GNU Scientific Library

Release 2.7

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Jan 13, 2022

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CHAPTER

ONE

INTRODUCTION

The GNU Scientific Library (GSL) is a collection of routines for numerical computing. The routines have been written from scratch in C, and present a modern Applications Programming Interface (API) for C programmers, allowing wrappers to be written for very high level languages. The source code is distributed under the GNU General Public License.

1.1 Routines available in GSL

The library covers a wide range of topics in numerical computing. Routines are available for the following areas,

Complex Numbers	Roots of Polynomials	Special Functions
Vectors and Matrices	Permutations	Combinations
Sorting	BLAS Support	Linear Algebra
CBLAS Library	Fast Fourier Transforms	Eigensystems
Random Numbers	Quadrature	Random Distributions
Quasi-Random Sequences	Histograms	Statistics
Monte Carlo Integration	N-Tuples	Differential Equations
Simulated Annealing	Numerical Differentiation	Interpolation
Series Acceleration	Chebyshev Approximations	Root-Finding
Discrete Hankel Transforms	Least-Squares Fitting	Minimization
IEEE Floating-Point	Physical Constants	Basis Splines
Wavelets	Sparse BLAS Support	Sparse Linear Algebra

The use of these routines is described in this manual. Each chapter provides detailed definitions of the functions, followed by example programs and references to the articles on which the algorithms are based.

Where possible the routines have been based on reliable public-domain packages such as FFTPACK and QUADPACK, which the developers of GSL have reimplemented in C with modern coding conventions.

1.2 GSL is Free Software

The subroutines in the GNU Scientific Library are “free software”; this means that everyone is free to use them, and to redistribute them in other free programs. The library is not in the public domain; it is copyrighted and there are conditions on its distribution. These conditions are designed to permit everything that a good cooperating citizen would want to do. What is not allowed is to try to prevent others from further sharing any version of the software that they might get from you.

Specifically, we want to make sure that you have the right to share copies of programs that you are given which use the GNU Scientific Library, that you receive their source code or else can get it if you want it, that you can change these programs or use pieces of them in new free programs, and that you know you can do these things.

To make sure that everyone has such rights, we have to forbid you to deprive anyone else of these rights. For example, if you distribute copies of any code which uses the GNU Scientific Library, you must give the recipients all the rights that you have received. You must make sure that they, too, receive or can get the source code, both to the library and the code which uses it. And you must tell them their rights. This means that the library should not be redistributed in proprietary programs.

Also, for our own protection, we must make certain that everyone finds out that there is no warranty for the GNU Scientific Library. If these programs are modified by someone else and passed on, we want their recipients to know that what they have is not what we distributed, so that any problems introduced by others will not reflect on our reputation.

The precise conditions for the distribution of software related to the GNU Scientific Library are found in the GNU General Public License. Further information about this license is available from the GNU Project webpage Frequently Asked Questions about the GNU GPL.

The Free Software Foundation also operates a license consulting service for commercial users (contact details available from http://www.fsf.org.

1.3 Obtaining GSL

The source code for the library can be obtained in different ways, by copying it from a friend, purchasing it on CDROM or downloading it from the internet. A list of public ftp servers which carry the source code can be found on the GNU website, http://www.gnu.org/software/gsl/.

The preferred platform for the library is a GNU system, which allows it to take advantage of additional features in the GNU C compiler and GNU C library. However, the library is fully portable and should compile on most systems with a C compiler.

Announcements of new releases, updates and other relevant events are made on the info-gsl@gnu.org mailing list. To subscribe to this low-volume list, send an email of the following form:

```
To: info-gsl-request@gnu.org
Subject: subscribe
```

You will receive a response asking you to reply in order to confirm your subscription.

1.4 No Warranty

The software described in this manual has no warranty, it is provided “as is”. It is your responsibility to validate the behavior of the routines and their accuracy using the source code provided, or to purchase support and warranties from commercial redistributors. Consult the GNU General Public License for further details.

1.5 Reporting Bugs

A list of known bugs can be found in the `BUGS` file included in the GSL distribution or online in the GSL bug tracker.[1] Details of compilation problems can be found in the `INSTALL` file.

If you find a bug which is not listed in these files, please report it to bug-gsl@gnu.org.

All bug reports should include:

- The version number of GSL
- The hardware and operating system
- The compiler used, including version number and compilation options
- A description of the bug behavior
- A short program which exercises the bug

It is useful if you can check whether the same problem occurs when the library is compiled without optimization. Thank you.

Any errors or omissions in this manual can also be reported to the same address.

1.6 Further Information

Additional information, including online copies of this manual, links to related projects, and mailing list archives are available from the website mentioned above.

Any questions about the use and installation of the library can be asked on the mailing list help-gsl@gnu.org. To subscribe to this list, send an email of the following form:

```
To: help-gsl-request@gnu.org
Subject: subscribe
```

This mailing list can be used to ask questions not covered by this manual, and to contact the developers of the library.

If you would like to refer to the GNU Scientific Library in a journal article, the recommended way is to cite this reference manual, e.g.:

```
M. Galassi et al, GNU Scientific Library Reference Manual (3rd Ed.), ISBN 0954612078.
```

If you want to give a url, use "http://www.gnu.org/software/gsl/".

1.7 Conventions used in this manual

This manual contains many examples which can be typed at the keyboard. A command entered at the terminal is shown like this:

```
$ command
```

The first character on the line is the terminal prompt, and should not be typed. The dollar sign $ is used as the standard prompt in this manual, although some systems may use a different character.

[1] http://savannah.gnu.org/bugs/?group=gsl

The examples assume the use of the GNU operating system. There may be minor differences in the output on other systems. The commands for setting environment variables use the Bourne shell syntax of the standard GNU shell (`bash`).

CHAPTER

TWO

USING THE LIBRARY

This chapter describes how to compile programs that use GSL, and introduces its conventions.

2.1 An Example Program

The following short program demonstrates the use of the library by computing the value of the Bessel function $J_0(x)$ for $x = 5$:

```
#include <stdio.h>
#include <gsl/gsl_sf_bessel.h>

int
main (void)
{
  double x = 5.0;
  double y = gsl_sf_bessel_J0 (x);
  printf ("J0(%g) = %.18e\n", x, y);
  return 0;
}
```

The output is shown below, and should be correct to double-precision accuracy[1],

```
J0(5) = -1.775967713143382642e-01
```

The steps needed to compile this program are described in the following sections.

2.2 Compiling and Linking

The library header files are installed in their own `gsl` directory. You should write any preprocessor include statements with a `gsl/` directory prefix thus:

```
#include <gsl/gsl_math.h>
```

If the directory is not installed on the standard search path of your compiler you will also need to provide its location to the preprocessor as a command line flag. The default location of the `gsl` directory is `/usr/local/include/gsl`. A typical compilation command for a source file `example.c` with the GNU C compiler `gcc` is:

[1] The last few digits may vary slightly depending on the compiler and platform used—this is normal

```
$ gcc -Wall -I/usr/local/include -c example.c
```

This results in an object file `example.o`. The default include path for `gcc` searches `/usr/local/include` automatically so the `-I` option can actually be omitted when GSL is installed in its default location.

2.2.1 Linking programs with the library

The library is installed as a single file, `libgsl.a`. A shared version of the library `libgsl.so` is also installed on systems that support shared libraries. The default location of these files is `/usr/local/lib`. If this directory is not on the standard search path of your linker you will also need to provide its location as a command line flag.

To link against the library you need to specify both the main library and a supporting CBLAS library, which provides standard basic linear algebra subroutines. A suitable CBLAS implementation is provided in the library `libgslcblas.a` if your system does not provide one. The following example shows how to link an application with the library:

```
$ gcc -L/usr/local/lib example.o -lgsl -lgslcblas -lm
```

The default library path for `gcc` searches `/usr/local/lib` automatically so the `-L` option can be omitted when GSL is installed in its default location.

The option `-lm` links with the system math library. On some systems it is not needed.[2]

For a tutorial introduction to the GNU C Compiler and related programs, see "An Introduction to GCC" (ISBN 0954161793).[3]

2.2.2 Linking with an alternative BLAS library

The following command line shows how you would link the same application with an alternative CBLAS library `libcblas.a`:

```
$ gcc example.o -lgsl -lcblas -lm
```

For the best performance an optimized platform-specific CBLAS library should be used for `-lcblas`. The library must conform to the CBLAS standard. The ATLAS package provides a portable high-performance BLAS library with a CBLAS interface. It is free software and should be installed for any work requiring fast vector and matrix operations. The following command line will link with the ATLAS library and its CBLAS interface:

```
$ gcc example.o -lgsl -lcblas -latlas -lm
```

If the ATLAS library is installed in a non-standard directory use the `-L` option to add it to the search path, as described above.

For more information about BLAS functions see *BLAS Support*.

[2] It is not needed on MacOS X
[3] http://www.network-theory.co.uk/gcc/intro/

2.3 Shared Libraries

To run a program linked with the shared version of the library the operating system must be able to locate the corresponding `.so` file at runtime. If the library cannot be found, the following error will occur:

```
$ ./a.out
./a.out: error while loading shared libraries:
libgsl.so.0: cannot open shared object file: No such file or directory
```

To avoid this error, either modify the system dynamic linker configuration[4] or define the shell variable `LD_LIBRARY_PATH` to include the directory where the library is installed.

For example, in the Bourne shell (`/bin/sh` or `/bin/bash`), the library search path can be set with the following commands:

```
$ LD_LIBRARY_PATH=/usr/local/lib
$ export LD_LIBRARY_PATH
$ ./example
```

In the C-shell (`/bin/csh` or `/bin/tcsh`) the equivalent command is:

```
% setenv LD_LIBRARY_PATH /usr/local/lib
```

The standard prompt for the C-shell in the example above is the percent character %, and should not be typed as part of the command.

To save retyping these commands each session they can be placed in an individual or system-wide login file.

To compile a statically linked version of the program, use the `-static` flag in `gcc`:

```
$ gcc -static example.o -lgsl -lgslcblas -lm
```

2.4 ANSI C Compliance

The library is written in ANSI C and is intended to conform to the ANSI C standard (C89). It should be portable to any system with a working ANSI C compiler.

The library does not rely on any non-ANSI extensions in the interface it exports to the user. Programs you write using GSL can be ANSI compliant. Extensions which can be used in a way compatible with pure ANSI C are supported, however, via conditional compilation. This allows the library to take advantage of compiler extensions on those platforms which support them.

When an ANSI C feature is known to be broken on a particular system the library will exclude any related functions at compile-time. This should make it impossible to link a program that would use these functions and give incorrect results.

To avoid namespace conflicts all exported function names and variables have the prefix `gsl_`, while exported macros have the prefix `GSL_`.

[4] `/etc/ld.so.conf` on GNU/Linux systems

2.5 Inline functions

The `inline` keyword is not part of the original ANSI C standard (C89) so the library does not export any inline function definitions by default. Inline functions were introduced officially in the newer C99 standard but most C89 compilers have also included `inline` as an extension for a long time.

To allow the use of inline functions, the library provides optional inline versions of performance-critical routines by conditional compilation in the exported header files. The inline versions of these functions can be included by defining the macro `HAVE_INLINE` when compiling an application:

```
$ gcc -Wall -c -DHAVE_INLINE example.c
```

If you use `autoconf` this macro can be defined automatically. If you do not define the macro `HAVE_INLINE` then the slower non-inlined versions of the functions will be used instead.

By default, the actual form of the inline keyword is `extern inline`, which is a `gcc` extension that eliminates unnecessary function definitions. If the form `extern inline` causes problems with other compilers a stricter autoconf test can be used, see *Autoconf Macros*.

When compiling with `gcc` in C99 mode (`gcc -std=c99`) the header files automatically switch to C99-compatible inline function declarations instead of `extern inline`. With other C99 compilers, define the macro `GSL_C99_INLINE` to use these declarations.

2.6 Long double

In general, the algorithms in the library are written for double precision only. The `long double` type is not supported for actual computation.

One reason for this choice is that the precision of `long double` is platform dependent. The IEEE standard only specifies the minimum precision of extended precision numbers, while the precision of `double` is the same on all platforms.

However, it is sometimes necessary to interact with external data in long-double format, so the vector and matrix datatypes include long-double versions.

It should be noted that in some system libraries the `stdio.h` formatted input/output functions `printf` and `scanf` are not implemented correctly for `long double`. Undefined or incorrect results are avoided by testing these functions during the `configure` stage of library compilation and eliminating certain GSL functions which depend on them if necessary. The corresponding line in the `configure` output looks like this:

```
checking whether printf works with long double... no
```

Consequently when `long double` formatted input/output does not work on a given system it should be impossible to link a program which uses GSL functions dependent on this.

If it is necessary to work on a system which does not support formatted `long double` input/output then the options are to use binary formats or to convert `long double` results into `double` for reading and writing.

2.7 Portability functions

To help in writing portable applications GSL provides some implementations of functions that are found in other libraries, such as the BSD math library. You can write your application to use the native versions of these functions, and substitute the GSL versions via a preprocessor macro if they are unavailable on another platform.

For example, after determining whether the BSD function `hypot()` is available you can include the following macro definitions in a file `config.h` with your application:

```
/* Substitute gsl_hypot for missing system hypot */

#ifndef HAVE_HYPOT
#define hypot gsl_hypot
#endif
```

The application source files can then use the include command `#include <config.h>` to replace each occurrence of `hypot()` by *`gsl_hypot()`* when `hypot()` is not available. This substitution can be made automatically if you use `autoconf`, see *Autoconf Macros*.

In most circumstances the best strategy is to use the native versions of these functions when available, and fall back to GSL versions otherwise, since this allows your application to take advantage of any platform-specific optimizations in the system library. This is the strategy used within GSL itself.

2.8 Alternative optimized functions

The main implementation of some functions in the library will not be optimal on all architectures. For example, there are several ways to compute a Gaussian random variate and their relative speeds are platform-dependent. In cases like this the library provides alternative implementations of these functions with the same interface. If you write your application using calls to the standard implementation you can select an alternative version later via a preprocessor definition. It is also possible to introduce your own optimized functions this way while retaining portability. The following lines demonstrate the use of a platform-dependent choice of methods for sampling from the Gaussian distribution:

```
#ifdef SPARC
#define gsl_ran_gaussian gsl_ran_gaussian_ratio_method
#endif
#ifdef INTEL
#define gsl_ran_gaussian my_gaussian
#endif
```

These lines would be placed in the configuration header file `config.h` of the application, which should then be included by all the source files. Note that the alternative implementations will not produce bit-for-bit identical results, and in the case of random number distributions will produce an entirely different stream of random variates.

2.9 Support for different numeric types

Many functions in the library are defined for different numeric types. This feature is implemented by varying the name of the function with a type-related modifier—a primitive form of C++ templates. The modifier is inserted into the function name after the initial module prefix. The following table shows the function names defined for all the numeric types of an imaginary module `gsl_foo` with function `fn()`:

```
gsl_foo_fn               double
gsl_foo_long_double_fn   long double
gsl_foo_float_fn         float
gsl_foo_long_fn          long
gsl_foo_ulong_fn         unsigned long
gsl_foo_int_fn           int
gsl_foo_uint_fn          unsigned int
gsl_foo_short_fn         short
gsl_foo_ushort_fn        unsigned short
gsl_foo_char_fn          char
gsl_foo_uchar_fn         unsigned char
```

The normal numeric precision `double` is considered the default and does not require a suffix. For example, the function *`gsl_stats_mean()`* computes the mean of double precision numbers, while the function `gsl_stats_int_mean()` computes the mean of integers.

A corresponding scheme is used for library defined types, such as `gsl_vector` and `gsl_matrix`. In this case the modifier is appended to the type name. For example, if a module defines a new type-dependent struct or typedef `gsl_foo` it is modified for other types in the following way:

```
gsl_foo                  double
gsl_foo_long_double      long double
gsl_foo_float            float
gsl_foo_long             long
gsl_foo_ulong            unsigned long
gsl_foo_int              int
gsl_foo_uint             unsigned int
gsl_foo_short            short
gsl_foo_ushort           unsigned short
gsl_foo_char             char
gsl_foo_uchar            unsigned char
```

When a module contains type-dependent definitions the library provides individual header files for each type. The filenames are modified as shown in the below. For convenience the default header includes the definitions for all the types. To include only the double precision header file, or any other specific type, use its individual filename:

```
#include <gsl/gsl_foo.h>               All types
#include <gsl/gsl_foo_double.h>        double
#include <gsl/gsl_foo_long_double.h>   long double
#include <gsl/gsl_foo_float.h>         float
#include <gsl/gsl_foo_long.h>          long
#include <gsl/gsl_foo_ulong.h>         unsigned long
#include <gsl/gsl_foo_int.h>           int
#include <gsl/gsl_foo_uint.h>          unsigned int
#include <gsl/gsl_foo_short.h>         short
#include <gsl/gsl_foo_ushort.h>        unsigned short
```

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```
#include <gsl/gsl_foo_char.h>          char
#include <gsl/gsl_foo_uchar.h>         unsigned char
```

2.10 Compatibility with C++

The library header files automatically define functions to have `extern "C"` linkage when included in C++ programs. This allows the functions to be called directly from C++.

To use C++ exception handling within user-defined functions passed to the library as parameters, the library must be built with the additional `CFLAGS` compilation option `-fexceptions`.

2.11 Aliasing of arrays

The library assumes that arrays, vectors and matrices passed as modifiable arguments are not aliased and do not overlap with each other. This removes the need for the library to handle overlapping memory regions as a special case, and allows additional optimizations to be used. If overlapping memory regions are passed as modifiable arguments then the results of such functions will be undefined. If the arguments will not be modified (for example, if a function prototype declares them as `const` arguments) then overlapping or aliased memory regions can be safely used.

2.12 Thread-safety

The library can be used in multi-threaded programs. All the functions are thread-safe, in the sense that they do not use static variables. Memory is always associated with objects and not with functions. For functions which use *workspace* objects as temporary storage the workspaces should be allocated on a per-thread basis. For functions which use *table* objects as read-only memory the tables can be used by multiple threads simultaneously. Table arguments are always declared `const` in function prototypes, to indicate that they may be safely accessed by different threads.

There are a small number of static global variables which are used to control the overall behavior of the library (e.g. whether to use range-checking, the function to call on fatal error, etc). These variables are set directly by the user, so they should be initialized once at program startup and not modified by different threads.

2.13 Deprecated Functions

From time to time, it may be necessary for the definitions of some functions to be altered or removed from the library. In these circumstances the functions will first be declared *deprecated* and then removed from subsequent versions of the library. Functions that are deprecated can be disabled in the current release by setting the preprocessor definition `GSL_DISABLE_DEPRECATED`. This allows existing code to be tested for forwards compatibility.

2.14 Code Reuse

Where possible the routines in the library have been written to avoid dependencies between modules and files. This should make it possible to extract individual functions for use in your own applications, without needing to have the whole library installed. You may need to define certain macros such as `GSL_ERROR` and remove some `#include` statements in order to compile the files as standalone units. Reuse of the library code in this way is encouraged, subject to the terms of the GNU General Public License.

CHAPTER

THREE

ERROR HANDLING

This chapter describes the way that GSL functions report and handle errors. By examining the status information returned by every function you can determine whether it succeeded or failed, and if it failed you can find out what the precise cause of failure was. You can also define your own error handling functions to modify the default behavior of the library.

The functions described in this section are declared in the header file `gsl_errno.h`.

3.1 Error Reporting

The library follows the thread-safe error reporting conventions of the POSIX Threads library. Functions return a non-zero error code to indicate an error and `0` to indicate success:

```
int status = gsl_function (...)

if (status) { /* an error occurred */
  .....
  /* status value specifies the type of error */
}
```

The routines report an error whenever they cannot perform the task requested of them. For example, a root-finding function would return a non-zero error code if could not converge to the requested accuracy, or exceeded a limit on the number of iterations. Situations like this are a normal occurrence when using any mathematical library and you should check the return status of the functions that you call.

Whenever a routine reports an error the return value specifies the type of error. The return value is analogous to the value of the variable `errno` in the C library. The caller can examine the return code and decide what action to take, including ignoring the error if it is not considered serious.

In addition to reporting errors by return codes the library also has an error handler function `gsl_error()`. This function is called by other library functions when they report an error, just before they return to the caller. The default behavior of the error handler is to print a message and abort the program:

```
gsl: file.c:67: ERROR: invalid argument supplied by user
Default GSL error handler invoked.
Aborted
```

The purpose of the `gsl_error()` handler is to provide a function where a breakpoint can be set that will catch library errors when running under the debugger. It is not intended for use in production programs, which should handle any errors using the return codes.

3.2 Error Codes

The error code numbers returned by library functions are defined in the file `gsl_errno.h`. They all have the prefix `GSL_` and expand to non-zero constant integer values. Error codes above 1024 are reserved for applications, and are not used by the library. Many of the error codes use the same base name as the corresponding error code in the C library. Here are some of the most common error codes,

int **GSL_EDOM**

Domain error; used by mathematical functions when an argument value does not fall into the domain over which the function is defined (like `EDOM` in the C library)

int **GSL_ERANGE**

Range error; used by mathematical functions when the result value is not representable because of overflow or underflow (like `ERANGE` in the C library)

int **GSL_ENOMEM**

No memory available. The system cannot allocate more virtual memory because its capacity is full (like `ENOMEM` in the C library). This error is reported when a GSL routine encounters problems when trying to allocate memory with `malloc()`.

int **GSL_EINVAL**

Invalid argument. This is used to indicate various kinds of problems with passing the wrong argument to a library function (like `EINVAL` in the C library).

The error codes can be converted into an error message using the function *gsl_strerror()*.

const char ***gsl_strerror**(const int gsl_errno)

This function returns a pointer to a string describing the error code *gsl_errno*. For example:

```
printf ("error: %s\n", gsl_strerror (status));
```

would print an error message like `error:  output range error` for a status value of *GSL_ERANGE*.

3.3 Error Handlers

The default behavior of the GSL error handler is to print a short message and call `abort()`. When this default is in use programs will stop with a core-dump whenever a library routine reports an error. This is intended as a fail-safe default for programs which do not check the return status of library routines (we don't encourage you to write programs this way).

If you turn off the default error handler it is your responsibility to check the return values of routines and handle them yourself. You can also customize the error behavior by providing a new error handler. For example, an alternative error handler could log all errors to a file, ignore certain error conditions (such as underflows), or start the debugger and attach it to the current process when an error occurs.

All GSL error handlers have the type `gsl_error_handler_t`, which is defined in `gsl_errno.h`,

type **gsl_error_handler_t**

This is the type of GSL error handler functions. An error handler will be passed four arguments which specify the reason for the error (a string), the name of the source file in which it occurred (also a string), the line number in that file (an integer) and the error number (an integer). The source file and line number are set at compile time using the `__FILE__` and `__LINE__` directives in the preprocessor. An error handler function returns type `void`. Error handler functions should be defined like this:

```
void handler (const char * reason,
              const char * file,
              int line,
              int gsl_errno)
```

To request the use of your own error handler you need to call the function `gsl_set_error_handler()` which is also declared in `gsl_errno.h`,

gsl_error_handler_t ***gsl_set_error_handler**(*gsl_error_handler_t* *new_handler)

This function sets a new error handler, `new_handler`, for the GSL library routines. The previous handler is returned (so that you can restore it later). Note that the pointer to a user defined error handler function is stored in a static variable, so there can be only one error handler per program. This function should be not be used in multi-threaded programs except to set up a program-wide error handler from a master thread. The following example shows how to set and restore a new error handler:

```
/* save original handler, install new handler */
old_handler = gsl_set_error_handler (&my_handler);

/* code uses new handler */
.....

/* restore original handler */
gsl_set_error_handler (old_handler);
```

To use the default behavior (`abort()` on error) set the error handler to `NULL`:

```
old_handler = gsl_set_error_handler (NULL);
```

gsl_error_handler_t ***gsl_set_error_handler_off**()

This function turns off the error handler by defining an error handler which does nothing. This will cause the program to continue after any error, so the return values from any library routines must be checked. This is the recommended behavior for production programs. The previous handler is returned (so that you can restore it later).

The error behavior can be changed for specific applications by recompiling the library with a customized definition of the `GSL_ERROR` macro in the file `gsl_errno.h`.

3.4 Using GSL error reporting in your own functions

If you are writing numerical functions in a program which also uses GSL code you may find it convenient to adopt the same error reporting conventions as in the library.

To report an error you need to call the function `gsl_error()` with a string describing the error and then return an appropriate error code from `gsl_errno.h`, or a special value, such as `NaN`. For convenience the file `gsl_errno.h` defines two macros which carry out these steps:

GSL_ERROR(reason, gsl_errno)

This macro reports an error using the GSL conventions and returns a status value of `gsl_errno`. It expands to the following code fragment:

```
gsl_error (reason, __FILE__, __LINE__, gsl_errno);
return gsl_errno;
```

The macro definition in `gsl_errno.h` actually wraps the code in a `do { ... } while (0)` block to prevent possible parsing problems.

Here is an example of how the macro could be used to report that a routine did not achieve a requested tolerance. To report the error the routine needs to return the error code `GSL_ETOL`:

```
if (residual > tolerance)
  {
    GSL_ERROR("residual exceeds tolerance", GSL_ETOL);
  }
```

GSL_ERROR_VAL(reason, gsl_errno, value)

This macro is the same as `GSL_ERROR` but returns a user-defined value of `value` instead of an error code. It can be used for mathematical functions that return a floating point value.

The following example shows how to return a `NaN` at a mathematical singularity using the `GSL_ERROR_VAL` macro:

```
if (x == 0)
  {
    GSL_ERROR_VAL("argument lies on singularity", GSL_ERANGE, GSL_NAN);
  }
```

3.5 Examples

Here is an example of some code which checks the return value of a function where an error might be reported:

```
#include <stdio.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_fft_complex.h>

...
  int status;
  size_t n = 37;

  gsl_set_error_handler_off();

  status = gsl_fft_complex_radix2_forward (data, stride, n);

  if (status) {
    if (status == GSL_EINVAL) {
       fprintf (stderr, "invalid argument, n=%d\n", n);
    } else {
       fprintf (stderr, "failed, gsl_errno=%d\n", status);
    }
    exit (-1);
  }
...
```

The function *gsl_fft_complex_radix2_forward()* only accepts integer lengths which are a power of two. If the variable `n` is not a power of two then the call to the library function will return `GSL_EINVAL`, indicating that the length argument is invalid. The function call to *gsl_set_error_handler_off()* stops the default error handler from aborting the program. The `else` clause catches any other possible errors.

CHAPTER

FOUR

MATHEMATICAL FUNCTIONS

This chapter describes basic mathematical functions. Some of these functions are present in system libraries, but the alternative versions given here can be used as a substitute when the system functions are not available.

The functions and macros described in this chapter are defined in the header file `gsl_math.h`.

4.1 Mathematical Constants

The library ensures that the standard BSD mathematical constants are defined. For reference, here is a list of the constants:

`M_E`	The base of exponentials, e
`M_LOG2E`	The base-2 logarithm of e, $\log_2(e)$
`M_LOG10E`	The base-10 logarithm of e, $\log_{10}(e)$
`M_SQRT2`	The square root of two, $\sqrt{2}$
`M_SQRT1_2`	The square root of one-half, $\sqrt{1/2}$
`M_SQRT3`	The square root of three, $\sqrt{3}$
`M_PI`	The constant pi, π
`M_PI_2`	Pi divided by two, $\pi/2$
`M_PI_4`	Pi divided by four, $\pi/4$
`M_SQRTPI`	The square root of pi, $\sqrt{\pi}$
`M_2_SQRTPI`	Two divided by the square root of pi, $2/\sqrt{\pi}$
`M_1_PI`	The reciprocal of pi, $1/\pi$
`M_2_PI`	Twice the reciprocal of pi, $2/\pi$
`M_LN10`	The natural logarithm of ten, $\ln(10)$
`M_LN2`	The natural logarithm of two, $\ln(2)$
`M_LNPI`	The natural logarithm of pi, $\ln(\pi)$
`M_EULER`	Euler's constant, γ

4.2 Infinities and Not-a-number

`GSL_POSINF`

This macro contains the IEEE representation of positive infinity, $+\infty$. It is computed from the expression `+1.0/0.0`.

`GSL_NEGINF`

This macro contains the IEEE representation of negative infinity, $-\infty$. It is computed from the expression `-1.0/0.0`.

`GSL_NAN`

This macro contains the IEEE representation of the Not-a-Number symbol, `NaN`. It is computed from the ratio `0.0/0.0`.

int **gsl_isnan**(const double x)

This function returns 1 if *x* is not-a-number.

int **gsl_isinf**(const double x)

This function returns $+1$ if *x* is positive infinity, -1 if *x* is negative infinity and 0 otherwise.[1]

int **gsl_finite**(const double x)

This function returns 1 if *x* is a real number, and 0 if it is infinite or not-a-number.

4.3 Elementary Functions

The following routines provide portable implementations of functions found in the BSD math library. When native versions are not available the functions described here can be used instead. The substitution can be made automatically if you use `autoconf` to compile your application (see *Portability functions*).

double **gsl_log1p**(const double x)

This function computes the value of $\log(1+x)$ in a way that is accurate for small *x*. It provides an alternative to the BSD math function `log1p(x)`.

double **gsl_expm1**(const double x)

This function computes the value of $\exp(x)-1$ in a way that is accurate for small *x*. It provides an alternative to the BSD math function `expm1(x)`.

double **gsl_hypot**(const double x, const double y)

This function computes the value of $\sqrt{x^2+y^2}$ in a way that avoids overflow. It provides an alternative to the BSD math function `hypot(x,y)`.

double **gsl_hypot3**(const double x, const double y, const double z)

This function computes the value of $\sqrt{x^2+y^2+z^2}$ in a way that avoids overflow.

double **gsl_acosh**(const double x)

This function computes the value of $\operatorname{arccosh}(x)$. It provides an alternative to the standard math function `acosh(x)`.

double **gsl_asinh**(const double x)

This function computes the value of $\operatorname{arcsinh}(x)$. It provides an alternative to the standard math function `asinh(x)`.

[1] Note that the C99 standard only requires the system `isinf()` function to return a non-zero value, without the sign of the infinity. The implementation in some earlier versions of GSL used the system `isinf()` function and may have this behavior on some platforms. Therefore, it is advisable to test the sign of `x` separately, if needed, rather than relying the sign of the return value from `gsl_isinf()`.

double **gsl_atanh**(const double x)
: This function computes the value of $\operatorname{arctanh}(x)$. It provides an alternative to the standard math function `atanh(x)`.

double **gsl_ldexp**(double x, int e)
: This function computes the value of $x * 2^e$. It provides an alternative to the standard math function `ldexp(x,e)`.

double **gsl_frexp**(double x, int *e)
: This function splits the number `x` into its normalized fraction f and exponent e, such that $x = f * 2^e$ and $0.5 <= f < 1$. The function returns f and stores the exponent in e. If x is zero, both f and e are set to zero. This function provides an alternative to the standard math function `frexp(x, e)`.

4.4 Small integer powers

A common complaint about the standard C library is its lack of a function for calculating (small) integer powers. GSL provides some simple functions to fill this gap. For reasons of efficiency, these functions do not check for overflow or underflow conditions.

double **gsl_pow_int**(double x, int n)

double **gsl_pow_uint**(double x, unsigned int n)
: These routines computes the power x^n for integer `n`. The power is computed efficiently—for example, x^8 is computed as $((x^2)^2)^2$, requiring only 3 multiplications. A version of this function which also computes the numerical error in the result is available as *gsl_sf_pow_int_e()*.

double **gsl_pow_2**(const double x)

double **gsl_pow_3**(const double x)

double **gsl_pow_4**(const double x)

double **gsl_pow_5**(const double x)

double **gsl_pow_6**(const double x)

double **gsl_pow_7**(const double x)

double **gsl_pow_8**(const double x)

double **gsl_pow_9**(const double x)
: These functions can be used to compute small integer powers x^2, x^3, etc. efficiently. The functions will be inlined when `HAVE_INLINE` is defined, so that use of these functions should be as efficient as explicitly writing the corresponding product expression:

```
#include <gsl/gsl_math.h>
double y = gsl_pow_4 (3.141)  /* compute 3.141**4 */
```

4.5 Testing the Sign of Numbers

`GSL_SIGN(x)`

This macro returns the sign of `x`. It is defined as `((x) >= 0 ? 1 :  -1)`. Note that with this definition the sign of zero is positive (regardless of its IEEE sign bit).

4.6 Testing for Odd and Even Numbers

`GSL_IS_ODD(n)`

This macro evaluates to 1 if `n` is odd and 0 if `n` is even. The argument `n` must be of integer type.

`GSL_IS_EVEN(n)`

This macro is the opposite of *GSL_IS_ODD*. It evaluates to 1 if `n` is even and 0 if `n` is odd. The argument `n` must be of integer type.

4.7 Maximum and Minimum functions

Note that the following macros perform multiple evaluations of their arguments, so they should not be used with arguments that have side effects (such as a call to a random number generator).

GSL_MAX(a, b)

This macro returns the maximum of `a` and `b`. It is defined as `((a) > (b) ? (a):(b))`.

GSL_MIN(a, b)

This macro returns the minimum of `a` and `b`. It is defined as `((a) < (b) ? (a):(b))`.

extern inline double **GSL_MAX_DBL**(double a, double b)

This function returns the maximum of the double precision numbers *a* and *b* using an inline function. The use of a function allows for type checking of the arguments as an extra safety feature. On platforms where inline functions are not available the macro *GSL_MAX* will be automatically substituted.

extern inline double **GSL_MIN_DBL**(double a, double b)

This function returns the minimum of the double precision numbers *a* and *b* using an inline function. The use of a function allows for type checking of the arguments as an extra safety feature. On platforms where inline functions are not available the macro *GSL_MIN* will be automatically substituted.

extern inline int **GSL_MAX_INT**(int a, int b)

extern inline int **GSL_MIN_INT**(int a, int b)

These functions return the maximum or minimum of the integers *a* and *b* using an inline function. On platforms where inline functions are not available the macros *GSL_MAX* or *GSL_MIN* will be automatically substituted.

extern inline long double **GSL_MAX_LDBL**(long double a, long double b)

extern inline long double **GSL_MIN_LDBL**(long double a, long double b)

These functions return the maximum or minimum of the long doubles *a* and *b* using an inline function. On platforms where inline functions are not available the macros *GSL_MAX* or *GSL_MIN* will be automatically substituted.

4.8 Approximate Comparison of Floating Point Numbers

It is sometimes useful to be able to compare two floating point numbers approximately, to allow for rounding and truncation errors. The following function implements the approximate floating-point comparison algorithm proposed by D.E. Knuth in Section 4.2.2 of "Seminumerical Algorithms" (3rd edition).

int **gsl_fcmp**(double x, double y, double epsilon)

This function determines whether *x* and *y* are approximately equal to a relative accuracy *epsilon*.

The relative accuracy is measured using an interval of size 2δ, where $\delta = 2^k \epsilon$ and k is the maximum base-2 exponent of x and y as computed by the function `frexp()`.

If x and y lie within this interval, they are considered approximately equal and the function returns 0. Otherwise if $x < y$, the function returns -1, or if $x > y$, the function returns $+1$.

Note that x and y are compared to relative accuracy, so this function is not suitable for testing whether a value is approximately zero.

The implementation is based on the package `fcmp` by T.C. Belding.

CHAPTER

FIVE

COMPLEX NUMBERS

The functions described in this chapter provide support for complex numbers. The algorithms take care to avoid unnecessary intermediate underflows and overflows, allowing the functions to be evaluated over as much of the complex plane as possible.

For multiple-valued functions the branch cuts have been chosen to follow the conventions of Abramowitz and Stegun. The functions return principal values which are the same as those in GNU Calc, which in turn are the same as those in "Common Lisp, The Language (Second Edition)"[1] and the HP-28/48 series of calculators.

The complex types are defined in the header file `gsl_complex.h`, while the corresponding complex functions and arithmetic operations are defined in `gsl_complex_math.h`.

5.1 Representation of complex numbers

Complex numbers are represented using the type `gsl_complex`. The default interface defines `gsl_complex` as:

```
typedef struct
{
  double dat[2];
} gsl_complex;
```

The real and imaginary part are stored in contiguous elements of a two element array. This eliminates any padding between the real and imaginary parts, `dat[0]` and `dat[1]`, allowing the struct to be mapped correctly onto packed complex arrays.

If a C compiler is available which supports the C11 standard, and the `<complex.h>` header file is included *prior* to `gsl_complex.h`, then `gsl_complex` will be defined to be the native C complex type:

```
typedef double complex gsl_complex
```

This allows users to use `gsl_complex` in ordinary operations such as:

```
gsl_complex x = 2 + 5 * I;
gsl_complex y = x + (3 - 4*I);
```

Important: Native C support for complex numbers was introduced in the C99 standard, and additional functionality was added in C11. When `<complex.h>` is included in a user's program prior to `gsl_complex.h`, GSL uses the new C11 functionality to define the *`GSL_REAL`* and *`GSL_IMAG`* macros. It does not appear possible to properly define these macros using the C99 standard, and so using a C99 compiler will not define `gsl_complex` to the native complex type.

[1] Note that the first edition uses different definitions.

Some compilers, such as the gcc 4.8 series implement only a portion of the C11 standard and so they may fail to correctly compile GSL code when a user tries to turn on native complex functionality. A workaround for this issue is to either remove `<complex.h>` from the include list, or add `-DGSL_COMPLEX_LEGACY` to the compiler flags, which will use the older struct-based definition of `gsl_complex`.

5.2 Complex number macros

The following C macros offer convenient ways to manipulate complex numbers.

GSL_REAL(z)

GSL_IMAG(z)

These macros return a memory location (lvalue) corresponding to the real and imaginary parts respectively of the complex number `z`. This allows users to perform operations like:

```
gsl_complex x, y;

GSL_REAL(x) = 4;
GSL_IMAG(x) = 2;

GSL_REAL(y) = GSL_REAL(x);
GSL_IMAG(y) = GSL_REAL(x);
```

In other words, these macros can both read and write to the real and imaginary parts of a complex variable.

GSL_SET_COMPLEX(zp, x, y)

This macro uses the Cartesian components (`x`, `y`) to set the real and imaginary parts of the complex number pointed to by `zp`. For example:

```
GSL_SET_COMPLEX(&z, 3, 4)
```

sets z to be $3 + 4i$.

5.3 Assigning complex numbers

gsl_complex **gsl_complex_rect**(double x, double y)

This function uses the rectangular Cartesian components (x, y) to return the complex number $z = x + iy$. An inline version of this function is used when `HAVE_INLINE` is defined.

gsl_complex **gsl_complex_polar**(double r, double theta)

This function returns the complex number $z = r \exp(i\theta) = r(\cos(\theta) + i \sin(\theta))$ from the polar representation (*r*, *theta*).

5.4 Properties of complex numbers

double **gsl_complex_arg**(gsl_complex z)
This function returns the argument of the complex number z, $\arg(z)$, where $-\pi < \arg(z) <= \pi$.

double **gsl_complex_abs**(gsl_complex z)
This function returns the magnitude of the complex number z, $|z|$.

double **gsl_complex_abs2**(gsl_complex z)
This function returns the squared magnitude of the complex number z, $|z|^2$.

double **gsl_complex_logabs**(gsl_complex z)
This function returns the natural logarithm of the magnitude of the complex number z, $\log|z|$. It allows an accurate evaluation of $\log|z|$ when $|z|$ is close to one. The direct evaluation of `log(gsl_complex_abs(z))` would lead to a loss of precision in this case.

5.5 Complex arithmetic operators

gsl_complex **gsl_complex_add**(gsl_complex a, gsl_complex b)
This function returns the sum of the complex numbers a and b, $z = a + b$.

gsl_complex **gsl_complex_sub**(gsl_complex a, gsl_complex b)
This function returns the difference of the complex numbers a and b, $z = a - b$.

gsl_complex **gsl_complex_mul**(gsl_complex a, gsl_complex b)
This function returns the product of the complex numbers a and b, $z = ab$.

gsl_complex **gsl_complex_div**(gsl_complex a, gsl_complex b)
This function returns the quotient of the complex numbers a and b, $z = a/b$.

gsl_complex **gsl_complex_add_real**(gsl_complex a, double x)
This function returns the sum of the complex number a and the real number x, $z = a + x$.

gsl_complex **gsl_complex_sub_real**(gsl_complex a, double x)
This function returns the difference of the complex number a and the real number x, $z = a - x$.

gsl_complex **gsl_complex_mul_real**(gsl_complex a, double x)
This function returns the product of the complex number a and the real number x, $z = ax$.

gsl_complex **gsl_complex_div_real**(gsl_complex a, double x)
This function returns the quotient of the complex number a and the real number x, $z = a/x$.

gsl_complex **gsl_complex_add_imag**(gsl_complex a, double y)
This function returns the sum of the complex number a and the imaginary number iy, $z = a + iy$.

gsl_complex **gsl_complex_sub_imag**(gsl_complex a, double y)
This function returns the difference of the complex number a and the imaginary number iy, $z = a - iy$.

gsl_complex **gsl_complex_mul_imag**(gsl_complex a, double y)
This function returns the product of the complex number a and the imaginary number iy, $z = a * (iy)$.

gsl_complex **gsl_complex_div_imag**(gsl_complex a, double y)
This function returns the quotient of the complex number a and the imaginary number iy, $z = a/(iy)$.

gsl_complex **gsl_complex_conjugate**(gsl_complex z)
This function returns the complex conjugate of the complex number z, $z^* = x - iy$.

gsl_complex **gsl_complex_inverse**(gsl_complex z)
This function returns the inverse, or reciprocal, of the complex number z, $1/z = (x - iy)/(x^2 + y^2)$.

gsl_complex **gsl_complex_negative**(gsl_complex z)
: This function returns the negative of the complex number *z*, $-z = (-x) + i(-y)$.

5.6 Elementary Complex Functions

gsl_complex **gsl_complex_sqrt**(gsl_complex z)
: This function returns the square root of the complex number *z*, $\sqrt{z}$. The branch cut is the negative real axis. The result always lies in the right half of the complex plane.

gsl_complex **gsl_complex_sqrt_real**(double x)
: This function returns the complex square root of the real number *x*, where *x* may be negative.

gsl_complex **gsl_complex_pow**(gsl_complex z, gsl_complex a)
: The function returns the complex number *z* raised to the complex power *a*, z^a. This is computed as $\exp(\log(z) * a)$ using complex logarithms and complex exponentials.

gsl_complex **gsl_complex_pow_real**(gsl_complex z, double x)
: This function returns the complex number *z* raised to the real power *x*, z^x.

gsl_complex **gsl_complex_exp**(gsl_complex z)
: This function returns the complex exponential of the complex number *z*, $\exp(z)$.

gsl_complex **gsl_complex_log**(gsl_complex z)
: This function returns the complex natural logarithm (base e) of the complex number *z*, $\log(z)$. The branch cut is the negative real axis.

gsl_complex **gsl_complex_log10**(gsl_complex z)
: This function returns the complex base-10 logarithm of the complex number *z*, $\log_{10}(z)$.

gsl_complex **gsl_complex_log_b**(gsl_complex z, gsl_complex b)
: This function returns the complex base-*b* logarithm of the complex number *z*, $\log_b(z)$. This quantity is computed as the ratio $\log(z)/\log(b)$.

5.7 Complex Trigonometric Functions

gsl_complex **gsl_complex_sin**(gsl_complex z)
: This function returns the complex sine of the complex number *z*, $\sin(z) = (\exp(iz) - \exp(-iz))/(2i)$.

gsl_complex **gsl_complex_cos**(gsl_complex z)
: This function returns the complex cosine of the complex number *z*, $\cos(z) = (\exp(iz) + \exp(-iz))/2$.

gsl_complex **gsl_complex_tan**(gsl_complex z)
: This function returns the complex tangent of the complex number *z*, $\tan(z) = \sin(z)/\cos(z)$.

gsl_complex **gsl_complex_sec**(gsl_complex z)
: This function returns the complex secant of the complex number *z*, $\sec(z) = 1/\cos(z)$.

gsl_complex **gsl_complex_csc**(gsl_complex z)
: This function returns the complex cosecant of the complex number *z*, $\csc(z) = 1/\sin(z)$.

gsl_complex **gsl_complex_cot**(gsl_complex z)
: This function returns the complex cotangent of the complex number *z*, $\cot(z) = 1/\tan(z)$.

5.8 Inverse Complex Trigonometric Functions

gsl_complex **gsl_complex_arcsin**(gsl_complex z)
: This function returns the complex arcsine of the complex number *z*, $\arcsin(z)$. The branch cuts are on the real axis, less than -1 and greater than 1.

gsl_complex **gsl_complex_arcsin_real**(double z)
: This function returns the complex arcsine of the real number *z*, $\arcsin(z)$. For z between -1 and 1, the function returns a real value in the range $[-\pi/2, \pi/2]$. For z less than -1 the result has a real part of $-\pi/2$ and a positive imaginary part. For z greater than 1 the result has a real part of $\pi/2$ and a negative imaginary part.

gsl_complex **gsl_complex_arccos**(gsl_complex z)
: This function returns the complex arccosine of the complex number *z*, $\arccos(z)$. The branch cuts are on the real axis, less than -1 and greater than 1.

gsl_complex **gsl_complex_arccos_real**(double z)
: This function returns the complex arccosine of the real number *z*, $\arccos(z)$. For z between -1 and 1, the function returns a real value in the range $[0, \pi]$. For z less than -1 the result has a real part of π and a negative imaginary part. For z greater than 1 the result is purely imaginary and positive.

gsl_complex **gsl_complex_arctan**(gsl_complex z)
: This function returns the complex arctangent of the complex number *z*, $\arctan(z)$. The branch cuts are on the imaginary axis, below $-i$ and above i.

gsl_complex **gsl_complex_arcsec**(gsl_complex z)
: This function returns the complex arcsecant of the complex number *z*, $\mathrm{arcsec}(z) = \arccos(1/z)$.

gsl_complex **gsl_complex_arcsec_real**(double z)
: This function returns the complex arcsecant of the real number *z*, $\mathrm{arcsec}(z) = \arccos(1/z)$.

gsl_complex **gsl_complex_arccsc**(gsl_complex z)
: This function returns the complex arccosecant of the complex number *z*, $\mathrm{arccsc}(z) = \arcsin(1/z)$.

gsl_complex **gsl_complex_arccsc_real**(double z)
: This function returns the complex arccosecant of the real number *z*, $\mathrm{arccsc}(z) = \arcsin(1/z)$.

gsl_complex **gsl_complex_arccot**(gsl_complex z)
: This function returns the complex arccotangent of the complex number *z*, $\mathrm{arccot}(z) = \arctan(1/z)$.

5.9 Complex Hyperbolic Functions

gsl_complex **gsl_complex_sinh**(gsl_complex z)
: This function returns the complex hyperbolic sine of the complex number *z*, $\sinh(z) = (\exp(z) - \exp(-z))/2$.

gsl_complex **gsl_complex_cosh**(gsl_complex z)
: This function returns the complex hyperbolic cosine of the complex number *z*, $\cosh(z) = (\exp(z) + \exp(-z))/2$.

gsl_complex **gsl_complex_tanh**(gsl_complex z)
: This function returns the complex hyperbolic tangent of the complex number *z*, $\tanh(z) = \sinh(z)/\cosh(z)$.

gsl_complex **gsl_complex_sech**(gsl_complex z)
: This function returns the complex hyperbolic secant of the complex number *z*, $\mathrm{sech}(z) = 1/\cosh(z)$.

gsl_complex **gsl_complex_csch**(gsl_complex z)
: This function returns the complex hyperbolic cosecant of the complex number *z*, $\mathrm{csch}(z) = 1/\sinh(z)$.

gsl_complex **gsl_complex_coth**(gsl_complex z)
: This function returns the complex hyperbolic cotangent of the complex number *z*, $\coth(z) = 1/\tanh(z)$.

5.10 Inverse Complex Hyperbolic Functions

gsl_complex **gsl_complex_arcsinh**(gsl_complex z)
: This function returns the complex hyperbolic arcsine of the complex number z, $\text{arcsinh}(z)$. The branch cuts are on the imaginary axis, below $-i$ and above i.

gsl_complex **gsl_complex_arccosh**(gsl_complex z)
: This function returns the complex hyperbolic arccosine of the complex number z, $\text{arccosh}(z)$. The branch cut is on the real axis, less than 1. Note that in this case we use the negative square root in formula 4.6.21 of Abramowitz & Stegun giving $\text{arccosh}(z) = \log(z - \sqrt{z^2 - 1})$.

gsl_complex **gsl_complex_arccosh_real**(double z)
: This function returns the complex hyperbolic arccosine of the real number z, $\text{arccosh}(z)$.

gsl_complex **gsl_complex_arctanh**(gsl_complex z)
: This function returns the complex hyperbolic arctangent of the complex number z, $\text{arctanh}(z)$. The branch cuts are on the real axis, less than -1 and greater than 1.

gsl_complex **gsl_complex_arctanh_real**(double z)
: This function returns the complex hyperbolic arctangent of the real number z, $\text{arctanh}(z)$.

gsl_complex **gsl_complex_arcsech**(gsl_complex z)
: This function returns the complex hyperbolic arcsecant of the complex number z, $\text{arcsech}(z) = \text{arccosh}(1/z)$.

gsl_complex **gsl_complex_arccsch**(gsl_complex z)
: This function returns the complex hyperbolic arccosecant of the complex number z, $\text{arccsch}(z) = \text{arcsinh}(1/z)$.

gsl_complex **gsl_complex_arccoth**(gsl_complex z)
: This function returns the complex hyperbolic arccotangent of the complex number z, $\text{arccoth}(z) = \text{arctanh}(1/z)$.

5.11 References and Further Reading

The implementations of the elementary and trigonometric functions are based on the following papers,

- T. E. Hull, Thomas F. Fairgrieve, Ping Tak Peter Tang, "Implementing Complex Elementary Functions Using Exception Handling", ACM Transactions on Mathematical Software, Volume 20 (1994), pp 215–244, Corrigenda, p553
- T. E. Hull, Thomas F. Fairgrieve, Ping Tak Peter Tang, "Implementing the complex arcsin and arccosine functions using exception handling", ACM Transactions on Mathematical Software, Volume 23 (1997) pp 299–335

The general formulas and details of branch cuts can be found in the following books,

- Abramowitz and Stegun, Handbook of Mathematical Functions, "Circular Functions in Terms of Real and Imaginary Parts", Formulas 4.3.55–58, "Inverse Circular Functions in Terms of Real and Imaginary Parts", Formulas 4.4.37–39, "Hyperbolic Functions in Terms of Real and Imaginary Parts", Formulas 4.5.49–52, "Inverse Hyperbolic Functions—relation to Inverse Circular Functions", Formulas 4.6.14–19.
- Dave Gillespie, Calc Manual, Free Software Foundation, ISBN 1-882114-18-3

CHAPTER

SIX

POLYNOMIALS

This chapter describes functions for evaluating and solving polynomials. There are routines for finding real and complex roots of quadratic and cubic equations using analytic methods. An iterative polynomial solver is also available for finding the roots of general polynomials with real coefficients (of any order). The functions are declared in the header file `gsl_poly.h`.

6.1 Polynomial Evaluation

The functions described here evaluate the polynomial

$$P(x) = c[0] + c[1]x + c[2]x^2 + \cdots + c[len-1]x^{len-1}$$

using Horner's method for stability. Inline versions of these functions are used when `HAVE_INLINE` is defined.

double **`gsl_poly_eval`**(const double c[], const int len, const double x)
: This function evaluates a polynomial with real coefficients for the real variable *`x`*.

gsl_complex **`gsl_poly_complex_eval`**(const double c[], const int len, const gsl_complex z)
: This function evaluates a polynomial with real coefficients for the complex variable *`z`*.

gsl_complex **`gsl_complex_poly_complex_eval`**(const gsl_complex c[], const int len, const gsl_complex z)
: This function evaluates a polynomial with complex coefficients for the complex variable *`z`*.

int **`gsl_poly_eval_derivs`**(const double c[], const size_t lenc, const double x, double res[], const size_t lenres)
: This function evaluates a polynomial and its derivatives storing the results in the array *`res`* of size *`lenres`*. The output array contains the values of $d^kP(x)/dx^k$ for the specified value of *`x`* starting with $k = 0$.

6.2 Divided Difference Representation of Polynomials

The functions described here manipulate polynomials stored in Newton's divided-difference representation. The use of divided-differences is described in Abramowitz & Stegun sections 25.1.4 and 25.2.26, and Burden and Faires, chapter 3, and discussed briefly below.

Given a function $f(x)$, an nth degree interpolating polynomial $P_n(x)$ can be constructed which agrees with f at $n+1$ distinct points $x_0, x_1, ..., x_n$. This polynomial can be written in a form known as Newton's divided-difference representation

$$P_n(x) = f(x_0) + \sum_{k=1}^{n}[x_0, x_1, ..., x_k](x-x_0)(x-x_1)\cdots(x-x_{k-1})$$

where the divided differences $[x_0, x_1, ..., x_k]$ are defined in section 25.1.4 of Abramowitz and Stegun. Additionally, it is possible to construct an interpolating polynomial of degree $2n + 1$ which also matches the first derivatives of f at the points $x_0, x_1, ..., x_n$. This is called the Hermite interpolating polynomial and is defined as

$$H_{2n+1}(x) = f(z_0) + \sum_{k=1}^{2n+1} [z_0, z_1, ..., z_k](x - z_0)(x - z_1) \cdots (x - z_{k-1})$$

where the elements of $z = \{x_0, x_0, x_1, x_1, ..., x_n, x_n\}$ are defined by $z_{2k} = z_{2k+1} = x_k$. The divided-differences $[z_0, z_1, ..., z_k]$ are discussed in Burden and Faires, section 3.4.

int **gsl_poly_dd_init**(double dd[], const double xa[], const double ya[], size_t size)

This function computes a divided-difference representation of the interpolating polynomial for the points (x, y) stored in the arrays *xa* and *ya* of length *size*. On output the divided-differences of (*xa*, *ya*) are stored in the array *dd*, also of length *size*. Using the notation above, $dd[k] = [x_0, x_1, ..., x_k]$.

double **gsl_poly_dd_eval**(const double dd[], const double xa[], const size_t size, const double x)

This function evaluates the polynomial stored in divided-difference form in the arrays *dd* and *xa* of length *size* at the point *x*. An inline version of this function is used when `HAVE_INLINE` is defined.

int **gsl_poly_dd_taylor**(double c[], double xp, const double dd[], const double xa[], size_t size, double w[])

This function converts the divided-difference representation of a polynomial to a Taylor expansion. The divided-difference representation is supplied in the arrays *dd* and *xa* of length *size*. On output the Taylor coefficients of the polynomial expanded about the point *xp* are stored in the array *c* also of length *size*. A workspace of length *size* must be provided in the array *w*.

int **gsl_poly_dd_hermite_init**(double dd[], double za[], const double xa[], const double ya[], const double dya[], const size_t size)

This function computes a divided-difference representation of the interpolating Hermite polynomial for the points (x, y) stored in the arrays *xa* and *ya* of length *size*. Hermite interpolation constructs polynomials which also match first derivatives dy/dx which are provided in the array *dya* also of length *size*. The first derivatives can be incorported into the usual divided-difference algorithm by forming a new dataset $z = \{x_0, x_0, x_1, x_1, ...\}$, which is stored in the array *za* of length 2**size* on output. On output the divided-differences of the Hermite representation are stored in the array *dd*, also of length 2**size*. Using the notation above, $dd[k] = [z_0, z_1, ..., z_k]$. The resulting Hermite polynomial can be evaluated by calling `gsl_poly_dd_eval()` and using *za* for the input argument *xa*.

6.3 Quadratic Equations

int **gsl_poly_solve_quadratic**(double a, double b, double c, double *x0, double *x1)

This function finds the real roots of the quadratic equation,

$$ax^2 + bx + c = 0$$

The number of real roots (either zero, one or two) is returned, and their locations are stored in *x0* and *x1*. If no real roots are found then *x0* and *x1* are not modified. If one real root is found (i.e. if $a = 0$) then it is stored in *x0*. When two real roots are found they are stored in *x0* and *x1* in ascending order. The case of coincident roots is not considered special. For example $(x - 1)^2 = 0$ will have two roots, which happen to have exactly equal values.

The number of roots found depends on the sign of the discriminant $b^2 - 4ac$. This will be subject to rounding and cancellation errors when computed in double precision, and will also be subject to errors if the coefficients of the polynomial are inexact. These errors may cause a discrete change in the number of roots. However, for polynomials with small integer coefficients the discriminant can always be computed exactly.

int **gsl_poly_complex_solve_quadratic**(double a, double b, double c, gsl_complex *z0, gsl_complex *z1)

This function finds the complex roots of the quadratic equation,

$$az^2 + bz + c = 0$$

The number of complex roots is returned (either one or two) and the locations of the roots are stored in `z0` and `z1`. The roots are returned in ascending order, sorted first by their real components and then by their imaginary components. If only one real root is found (i.e. if $a = 0$) then it is stored in `z0`.

6.4 Cubic Equations

int **gsl_poly_solve_cubic**(double a, double b, double c, double *x0, double *x1, double *x2)

This function finds the real roots of the cubic equation,

$$x^3 + ax^2 + bx + c = 0$$

with a leading coefficient of unity. The number of real roots (either one or three) is returned, and their locations are stored in `x0`, `x1` and `x2`. If one real root is found then only `x0` is modified. When three real roots are found they are stored in `x0`, `x1` and `x2` in ascending order. The case of coincident roots is not considered special. For example, the equation $(x - 1)^3 = 0$ will have three roots with exactly equal values. As in the quadratic case, finite precision may cause equal or closely-spaced real roots to move off the real axis into the complex plane, leading to a discrete change in the number of real roots.

int **gsl_poly_complex_solve_cubic**(double a, double b, double c, gsl_complex *z0, gsl_complex *z1, gsl_complex *z2)

This function finds the complex roots of the cubic equation,

$$z^3 + az^2 + bz + c = 0$$

The number of complex roots is returned (always three) and the locations of the roots are stored in `z0`, `z1` and `z2`. The roots are returned in ascending order, sorted first by their real components and then by their imaginary components.

6.5 General Polynomial Equations

The roots of polynomial equations cannot be found analytically beyond the special cases of the quadratic, cubic and quartic equation. The algorithm described in this section uses an iterative method to find the approximate locations of roots of higher order polynomials.

type **gsl_poly_complex_workspace**

This workspace contains parameters used for finding roots of general polynomials

gsl_poly_complex_workspace ***gsl_poly_complex_workspace_alloc**(size_t n)

This function allocates space for a `gsl_poly_complex_workspace` struct and a workspace suitable for solving a polynomial with `n` coefficients using the routine `gsl_poly_complex_solve()`.

The function returns a pointer to the newly allocated `gsl_poly_complex_workspace` if no errors were detected, and a null pointer in the case of error.

void **gsl_poly_complex_workspace_free**(*gsl_poly_complex_workspace* *w)

This function frees all the memory associated with the workspace `w`.

int **gsl_poly_complex_solve**(const double *a, size_t n, *gsl_poly_complex_workspace* *w, gsl_complex_packed_ptr z)

This function computes the roots of the general polynomial

$$P(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1} x^{n-1}$$

using balanced-QR reduction of the companion matrix. The parameter `n` specifies the length of the coefficient array. The coefficient of the highest order term must be non-zero. The function requires a workspace `w` of the appropriate size. The $n-1$ roots are returned in the packed complex array `z` of length $2(n-1)$, alternating real and imaginary parts.

The function returns `GSL_SUCCESS` if all the roots are found. If the QR reduction does not converge, the error handler is invoked with an error code of `GSL_EFAILED`. Note that due to finite precision, roots of higher multiplicity are returned as a cluster of simple roots with reduced accuracy. The solution of polynomials with higher-order roots requires specialized algorithms that take the multiplicity structure into account (see e.g. Z. Zeng, Algorithm 835, ACM Transactions on Mathematical Software, Volume 30, Issue 2 (2004), pp 218–236).

6.6 Examples

To demonstrate the use of the general polynomial solver we will take the polynomial $P(x) = x^5 - 1$ which has these roots:

$$1, e^{2\pi i/5}, e^{4\pi i/5}, e^{6\pi i/5}, e^{8\pi i/5}$$

The following program will find these roots.

```c
#include <stdio.h>
#include <gsl/gsl_poly.h>

int
main (void)
{
  int i;
  /* coefficients of P(x) =  -1 + x^5  */
  double a[6] = { -1, 0, 0, 0, 0, 1 };
  double z[10];

  gsl_poly_complex_workspace * w
      = gsl_poly_complex_workspace_alloc (6);

  gsl_poly_complex_solve (a, 6, w, z);

  gsl_poly_complex_workspace_free (w);

  for (i = 0; i < 5; i++)
    {
      printf ("z%d = %+.18f %+.18f\n",
              i, z[2*i], z[2*i+1]);
    }

  return 0;
}
```

The output of the program is

```
z0 = -0.809016994374947673 +0.587785252292473359
z1 = -0.809016994374947673 -0.587785252292473359
z2 = +0.309016994374947507 +0.951056516295152976
z3 = +0.309016994374947507 -0.951056516295152976
z4 = +0.999999999999999889 +0.000000000000000000
```

which agrees with the analytic result, $z_n = \exp(2\pi n i/5)$.

6.7 References and Further Reading

The balanced-QR method and its error analysis are described in the following papers,

- R.S. Martin, G. Peters and J.H. Wilkinson, "The QR Algorithm for Real Hessenberg Matrices", Numerische Mathematik, 14 (1970), 219–231.
- B.N. Parlett and C. Reinsch, "Balancing a Matrix for Calculation of Eigenvalues and Eigenvectors", Numerische Mathematik, 13 (1969), 293–304.
- A. Edelman and H. Murakami, "Polynomial roots from companion matrix eigenvalues", Mathematics of Computation, Vol.: 64, No.: 210 (1995), 763–776.

The formulas for divided differences are given in the following texts,

- Abramowitz and Stegun, Handbook of Mathematical Functions, Sections 25.1.4 and 25.2.26.
- R. L. Burden and J. D. Faires, Numerical Analysis, 9th edition, ISBN 0-538-73351-9, 2011.

CHAPTER

SEVEN

SPECIAL FUNCTIONS

This chapter describes the GSL special function library. The library includes routines for calculating the values of Airy functions, Bessel functions, Clausen functions, Coulomb wave functions, Coupling coefficients, the Dawson function, Debye functions, Dilogarithms, Elliptic integrals, Jacobi elliptic functions, Error functions, Exponential integrals, Fermi-Dirac functions, Gamma functions, Gegenbauer functions, Hermite polynomials and functions, Hypergeometric functions, Laguerre functions, Legendre functions and Spherical Harmonics, the Psi (Digamma) Function, Synchrotron functions, Transport functions, Trigonometric functions and Zeta functions. Each routine also computes an estimate of the numerical error in the calculated value of the function.

The functions in this chapter are declared in individual header files, such as `gsl_sf_airy.h`, `gsl_sf_bessel.h`, etc. The complete set of header files can be included using the file `gsl_sf.h`.

7.1 Usage

The special functions are available in two calling conventions, a *natural form* which returns the numerical value of the function and an *error-handling form* which returns an error code. The two types of function provide alternative ways of accessing the same underlying code.

The *natural form* returns only the value of the function and can be used directly in mathematical expressions. For example, the following function call will compute the value of the Bessel function $J_0(x)$:

```
double y = gsl_sf_bessel_J0 (x);
```

There is no way to access an error code or to estimate the error using this method. To allow access to this information the alternative error-handling form stores the value and error in a modifiable argument:

```
gsl_sf_result result;
int status = gsl_sf_bessel_J0_e (x, &result);
```

The error-handling functions have the suffix `_e`. The returned status value indicates error conditions such as overflow, underflow or loss of precision. If there are no errors the error-handling functions return `GSL_SUCCESS`.

7.2 The gsl_sf_result struct

The error handling form of the special functions always calculate an error estimate along with the value of the result. Therefore, structures are provided for amalgamating a value and error estimate. These structures are declared in the header file `gsl_sf_result.h`.

The following struct contains value and error fields.

type **gsl_sf_result**

```
typedef struct
{
  double val;
  double err;
} gsl_sf_result;
```

The field `val` contains the value and the field `err` contains an estimate of the absolute error in the value.

In some cases, an overflow or underflow can be detected and handled by a function. In this case, it may be possible to return a scaling exponent as well as an error/value pair in order to save the result from exceeding the dynamic range of the built-in types. The following struct contains value and error fields as well as an exponent field such that the actual result is obtained as `result * 10^(e10)`.

type **gsl_sf_result_e10**

```
typedef struct
{
  double val;
  double err;
  int    e10;
} gsl_sf_result_e10;
```

7.3 Modes

The goal of the library is to achieve double precision accuracy wherever possible. However the cost of evaluating some special functions to double precision can be significant, particularly where very high order terms are required. In these cases a `mode` argument, of type *gsl_mode_t* allows the accuracy of the function to be reduced in order to improve performance. The following precision levels are available for the mode argument,

type **gsl_mode_t**

GSL_PREC_DOUBLE
Double-precision, a relative accuracy of approximately $2 * 10^{-16}$.

GSL_PREC_SINGLE
Single-precision, a relative accuracy of approximately 10^{-7}.

GSL_PREC_APPROX
Approximate values, a relative accuracy of approximately $5 * 10^{-4}$.

The approximate mode provides the fastest evaluation at the lowest accuracy.

7.4 Airy Functions and Derivatives

The Airy functions $Ai(x)$ and $Bi(x)$ are defined by the integral representations,

$$Ai(x) = \frac{1}{\pi} \int_0^\infty \cos(t^3/3 + xt)\,dt$$
$$Bi(x) = \frac{1}{\pi} \int_0^\infty (e^{-t^3/3+xt} + \sin(t^3/3 + xt))\,dt$$

For further information see Abramowitz & Stegun, Section 10.4. The Airy functions are defined in the header file `gsl_sf_airy.h`.

7.4.1 Airy Functions

double **gsl_sf_airy_Ai**(double x, *gsl_mode_t* mode)

int **gsl_sf_airy_Ai_e**(double x, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the Airy function $Ai(x)$ with an accuracy specified by `mode`.

double **gsl_sf_airy_Bi**(double x, *gsl_mode_t* mode)

int **gsl_sf_airy_Bi_e**(double x, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the Airy function $Bi(x)$ with an accuracy specified by `mode`.

double **gsl_sf_airy_Ai_scaled**(double x, *gsl_mode_t* mode)

int **gsl_sf_airy_Ai_scaled_e**(double x, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute a scaled version of the Airy function $S_A(x)Ai(x)$. For $x > 0$ the scaling factor $S_A(x)$ is $\exp(+(2/3)x^{3/2})$, and is 1 for $x < 0$.

double **gsl_sf_airy_Bi_scaled**(double x, *gsl_mode_t* mode)

int **gsl_sf_airy_Bi_scaled_e**(double x, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute a scaled version of the Airy function $S_B(x)Bi(x)$. For $x > 0$ the scaling factor $S_B(x)$ is $exp(-(2/3)x^{3/2})$, and is 1 for $x < 0$.

7.4.2 Derivatives of Airy Functions

double **gsl_sf_airy_Ai_deriv**(double x, *gsl_mode_t* mode)

int **gsl_sf_airy_Ai_deriv_e**(double x, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the Airy function derivative $Ai'(x)$ with an accuracy specified by `mode`.

double **gsl_sf_airy_Bi_deriv**(double x, *gsl_mode_t* mode)

int **gsl_sf_airy_Bi_deriv_e**(double x, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the Airy function derivative $Bi'(x)$ with an accuracy specified by `mode`.

double **gsl_sf_airy_Ai_deriv_scaled**(double x, *gsl_mode_t* mode)

int **gsl_sf_airy_Ai_deriv_scaled_e**(double x, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the scaled Airy function derivative $S_A(x)Ai'(x)$. For $x > 0$ the scaling factor $S_A(x)$ is $\exp(+(2/3)x^{3/2})$, and is 1 for $x < 0$.

double **gsl_sf_airy_Bi_deriv_scaled**(double x, *gsl_mode_t* mode)

int **gsl_sf_airy_Bi_deriv_scaled_e**(double x, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the scaled Airy function derivative $S_B(x)Bi'(x)$. For $x > 0$ the scaling factor $S_B(x)$ is $exp(-(2/3)x^{3/2})$, and is 1 for $x < 0$.

7.4.3 Zeros of Airy Functions

double **gsl_sf_airy_zero_Ai**(unsigned int s)

int **gsl_sf_airy_zero_Ai_e**(unsigned int s, *gsl_sf_result* *result)

These routines compute the location of the `s`-th zero of the Airy function $Ai(x)$.

double **gsl_sf_airy_zero_Bi**(unsigned int s)

int **gsl_sf_airy_zero_Bi_e**(unsigned int s, *gsl_sf_result* *result)

These routines compute the location of the `s`-th zero of the Airy function $Bi(x)$.

7.4.4 Zeros of Derivatives of Airy Functions

double **gsl_sf_airy_zero_Ai_deriv**(unsigned int s)

int **gsl_sf_airy_zero_Ai_deriv_e**(unsigned int s, *gsl_sf_result* *result)

These routines compute the location of the `s`-th zero of the Airy function derivative $Ai'(x)$.

double **gsl_sf_airy_zero_Bi_deriv**(unsigned int s)

int **gsl_sf_airy_zero_Bi_deriv_e**(unsigned int s, *gsl_sf_result* *result)

These routines compute the location of the `s`-th zero of the Airy function derivative $Bi'(x)$.

7.5 Bessel Functions

The routines described in this section compute the Cylindrical Bessel functions $J_n(x)$, $Y_n(x)$, Modified cylindrical Bessel functions $I_n(x)$, $K_n(x)$, Spherical Bessel functions $j_l(x)$, $y_l(x)$, and Modified Spherical Bessel functions $i_l(x)$, $k_l(x)$. For more information see Abramowitz & Stegun, Chapters 9 and 10. The Bessel functions are defined in the header file `gsl_sf_bessel.h`.

7.5.1 Regular Cylindrical Bessel Functions

double **gsl_sf_bessel_J0**(double x)

int **gsl_sf_bessel_J0_e**(double x, *gsl_sf_result* *result)

These routines compute the regular cylindrical Bessel function of zeroth order, $J_0(x)$.

double **gsl_sf_bessel_J1**(double x)

int **gsl_sf_bessel_J1_e**(double x, *gsl_sf_result* *result)

These routines compute the regular cylindrical Bessel function of first order, $J_1(x)$.

double **gsl_sf_bessel_Jn**(int n, double x)

int **gsl_sf_bessel_Jn_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the regular cylindrical Bessel function of order `n`, $J_n(x)$.

int **gsl_sf_bessel_Jn_array**(int nmin, int nmax, double x, double result_array[])

This routine computes the values of the regular cylindrical Bessel functions $J_n(x)$ for n from `nmin` to `nmax` inclusive, storing the results in the array `result_array`. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

7.5.2 Irregular Cylindrical Bessel Functions

double **gsl_sf_bessel_Y0**(double x)

int **gsl_sf_bessel_Y0_e**(double x, *gsl_sf_result* *result)

These routines compute the irregular cylindrical Bessel function of zeroth order, $Y_0(x)$, for $x > 0$.

double **gsl_sf_bessel_Y1**(double x)

int **gsl_sf_bessel_Y1_e**(double x, *gsl_sf_result* *result)

These routines compute the irregular cylindrical Bessel function of first order, $Y_1(x)$, for $x > 0$.

double **gsl_sf_bessel_Yn**(int n, double x)

int **gsl_sf_bessel_Yn_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the irregular cylindrical Bessel function of order `n`, $Y_n(x)$, for $x > 0$.

int **gsl_sf_bessel_Yn_array**(int nmin, int nmax, double x, double result_array[])

This routine computes the values of the irregular cylindrical Bessel functions $Y_n(x)$ for n from `nmin` to `nmax` inclusive, storing the results in the array `result_array`. The domain of the function is $x > 0$. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

7.5.3 Regular Modified Cylindrical Bessel Functions

double **gsl_sf_bessel_I0**(double x)

int **gsl_sf_bessel_I0_e**(double x, *gsl_sf_result* *result)

These routines compute the regular modified cylindrical Bessel function of zeroth order, $I_0(x)$.

double **gsl_sf_bessel_I1**(double x)

int **gsl_sf_bessel_I1_e**(double x, *gsl_sf_result* *result)

These routines compute the regular modified cylindrical Bessel function of first order, $I_1(x)$.

double **gsl_sf_bessel_In**(int n, double x)

int **gsl_sf_bessel_In_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the regular modified cylindrical Bessel function of order `n`, $I_n(x)$.

int **gsl_sf_bessel_In_array**(int nmin, int nmax, double x, double result_array[])

This routine computes the values of the regular modified cylindrical Bessel functions $I_n(x)$ for n from `nmin` to `nmax` inclusive, storing the results in the array `result_array`. The start of the range `nmin` must be positive or zero. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

double **gsl_sf_bessel_I0_scaled**(double x)

int **gsl_sf_bessel_I0_scaled_e**(double x, *gsl_sf_result* *result)

These routines compute the scaled regular modified cylindrical Bessel function of zeroth order $\exp(-|x|)I_0(x)$.

double **gsl_sf_bessel_I1_scaled**(double x)

int **gsl_sf_bessel_I1_scaled_e**(double x, *gsl_sf_result* *result)

These routines compute the scaled regular modified cylindrical Bessel function of first order $\exp(-|x|)I_1(x)$.

double **gsl_sf_bessel_In_scaled**(int n, double x)

int **gsl_sf_bessel_In_scaled_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the scaled regular modified cylindrical Bessel function of order `n`, $\exp(-|x|)I_n(x)$

int **gsl_sf_bessel_In_scaled_array**(int nmin, int nmax, double x, double result_array[])

This routine computes the values of the scaled regular cylindrical Bessel functions $\exp(-|x|)I_n(x)$ for n from `nmin` to `nmax` inclusive, storing the results in the array `result_array`. The start of the range `nmin` must be positive or zero. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

7.5.4 Irregular Modified Cylindrical Bessel Functions

double **gsl_sf_bessel_K0**(double x)

int **gsl_sf_bessel_K0_e**(double x, *gsl_sf_result* *result)

These routines compute the irregular modified cylindrical Bessel function of zeroth order, $K_0(x)$, for $x > 0$.

double **gsl_sf_bessel_K1**(double x)

int **gsl_sf_bessel_K1_e**(double x, *gsl_sf_result* *result)

These routines compute the irregular modified cylindrical Bessel function of first order, $K_1(x)$, for $x > 0$.

double **gsl_sf_bessel_Kn**(int n, double x)

int **gsl_sf_bessel_Kn_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the irregular modified cylindrical Bessel function of order `n`, $K_n(x)$, for $x > 0$.

int **gsl_sf_bessel_Kn_array**(int nmin, int nmax, double x, double result_array[])

This routine computes the values of the irregular modified cylindrical Bessel functions $K_n(x)$ for n from `nmin` to `nmax` inclusive, storing the results in the array `result_array`. The start of the range `nmin` must be positive or zero. The domain of the function is $x > 0$. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

double **gsl_sf_bessel_K0_scaled**(double x)

int **gsl_sf_bessel_K0_scaled_e**(double x, *gsl_sf_result* *result)

These routines compute the scaled irregular modified cylindrical Bessel function of zeroth order $\exp(x)K_0(x)$ for $x > 0$.

double **gsl_sf_bessel_K1_scaled**(double x)

int **gsl_sf_bessel_K1_scaled_e**(double x, *gsl_sf_result* *result)

These routines compute the scaled irregular modified cylindrical Bessel function of first order $\exp(x)K_1(x)$ for $x > 0$.

double **gsl_sf_bessel_Kn_scaled**(int n, double x)

int **gsl_sf_bessel_Kn_scaled_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the scaled irregular modified cylindrical Bessel function of order `n`, $\exp(x)K_n(x)$, for $x > 0$.

int **gsl_sf_bessel_Kn_scaled_array**(int nmin, int nmax, double x, double result_array[])

This routine computes the values of the scaled irregular cylindrical Bessel functions $\exp(x)K_n(x)$ for n from `nmin` to `nmax` inclusive, storing the results in the array `result_array`. The start of the range `nmin` must be positive or zero. The domain of the function is $x > 0$. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

7.5.5 Regular Spherical Bessel Functions

double **gsl_sf_bessel_j0**(double x)

int **gsl_sf_bessel_j0_e**(double x, *gsl_sf_result* *result)

These routines compute the regular spherical Bessel function of zeroth order, $j_0(x) = \sin(x)/x$.

double **gsl_sf_bessel_j1**(double x)

int **gsl_sf_bessel_j1_e**(double x, *gsl_sf_result* *result)

These routines compute the regular spherical Bessel function of first order, $j_1(x) = (\sin(x)/x - \cos(x))/x$.

double **gsl_sf_bessel_j2**(double x)

int **gsl_sf_bessel_j2_e**(double x, *gsl_sf_result* *result)

These routines compute the regular spherical Bessel function of second order, $j_2(x) = ((3/x^2 - 1)\sin(x) - 3\cos(x)/x)/x$.

double **gsl_sf_bessel_jl**(int l, double x)

int **gsl_sf_bessel_jl_e**(int l, double x, *gsl_sf_result* *result)

These routines compute the regular spherical Bessel function of order `l`, $j_l(x)$, for $l \geq 0$ and $x \geq 0$.

int **gsl_sf_bessel_jl_array**(int lmax, double x, double result_array[])

This routine computes the values of the regular spherical Bessel functions $j_l(x)$ for l from 0 to `lmax` inclusive for $lmax \geq 0$ and $x \geq 0$, storing the results in the array `result_array`. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

int **gsl_sf_bessel_jl_steed_array**(int lmax, double x, double *result_array)

This routine uses Steed's method to compute the values of the regular spherical Bessel functions $j_l(x)$ for l from 0 to `lmax` inclusive for $lmax \geq 0$ and $x \geq 0$, storing the results in the array `result_array`. The Steed/Barnett algorithm is described in Comp. Phys. Comm. 21, 297 (1981). Steed's method is more stable than the recurrence used in the other functions but is also slower.

7.5.6 Irregular Spherical Bessel Functions

double **gsl_sf_bessel_y0**(double x)

int **gsl_sf_bessel_y0_e**(double x, *gsl_sf_result* *result)

These routines compute the irregular spherical Bessel function of zeroth order, $y_0(x) = -\cos(x)/x$.

double **gsl_sf_bessel_y1**(double x)

int **gsl_sf_bessel_y1_e**(double x, *gsl_sf_result* *result)

These routines compute the irregular spherical Bessel function of first order, $y_1(x) = -(\cos(x)/x + \sin(x))/x$.

double **gsl_sf_bessel_y2**(double x)

int **gsl_sf_bessel_y2_e**(double x, *gsl_sf_result* *result)

These routines compute the irregular spherical Bessel function of second order, $y_2(x) = (-3/x^3 + 1/x)\cos(x) - (3/x^2)\sin(x)$.

double **gsl_sf_bessel_yl**(int l, double x)

int **gsl_sf_bessel_yl_e**(int l, double x, *gsl_sf_result* *result)

These routines compute the irregular spherical Bessel function of order `l`, $y_l(x)$, for $l \geq 0$.

int **gsl_sf_bessel_yl_array**(int lmax, double x, double result_array[])

This routine computes the values of the irregular spherical Bessel functions $y_l(x)$ for l from 0 to `lmax` inclusive for $lmax \geq 0$, storing the results in the array `result_array`. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

7.5.7 Regular Modified Spherical Bessel Functions

The regular modified spherical Bessel functions $i_l(x)$ are related to the modified Bessel functions of fractional order, $i_l(x) = \sqrt{\pi/(2x)} I_{l+1/2}(x)$

double **gsl_sf_bessel_i0_scaled**(double x)

int **gsl_sf_bessel_i0_scaled_e**(double x, *gsl_sf_result* *result)

These routines compute the scaled regular modified spherical Bessel function of zeroth order, $\exp(-|x|)i_0(x)$.

double **gsl_sf_bessel_i1_scaled**(double x)

int **gsl_sf_bessel_i1_scaled_e**(double x, *gsl_sf_result* *result)

These routines compute the scaled regular modified spherical Bessel function of first order, $\exp(-|x|)i_1(x)$.

double **gsl_sf_bessel_i2_scaled**(double x)

int **gsl_sf_bessel_i2_scaled_e**(double x, *gsl_sf_result* *result)

These routines compute the scaled regular modified spherical Bessel function of second order, $\exp(-|x|)i_2(x)$

double **gsl_sf_bessel_il_scaled**(int l, double x)

int **gsl_sf_bessel_il_scaled_e**(int l, double x, *gsl_sf_result* *result)

These routines compute the scaled regular modified spherical Bessel function of order `l`, $\exp(-|x|)i_l(x)$

int **gsl_sf_bessel_il_scaled_array**(int lmax, double x, double result_array[])
This routine computes the values of the scaled regular modified spherical Bessel functions $\exp(-|x|)i_l(x)$ for l from 0 to `lmax` inclusive for $lmax \geq 0$, storing the results in the array `result_array`. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

7.5.8 Irregular Modified Spherical Bessel Functions

The irregular modified spherical Bessel functions $k_l(x)$ are related to the irregular modified Bessel functions of fractional order, $k_l(x) = \sqrt{\pi/(2x)}K_{l+1/2}(x)$.

double **gsl_sf_bessel_k0_scaled**(double x)

int **gsl_sf_bessel_k0_scaled_e**(double x, *gsl_sf_result* *result)
These routines compute the scaled irregular modified spherical Bessel function of zeroth order, $\exp(x)k_0(x)$, for $x > 0$.

double **gsl_sf_bessel_k1_scaled**(double x)

int **gsl_sf_bessel_k1_scaled_e**(double x, *gsl_sf_result* *result)
These routines compute the scaled irregular modified spherical Bessel function of first order, $\exp(x)k_1(x)$, for $x > 0$.

double **gsl_sf_bessel_k2_scaled**(double x)

int **gsl_sf_bessel_k2_scaled_e**(double x, *gsl_sf_result* *result)
These routines compute the scaled irregular modified spherical Bessel function of second order, $\exp(x)k_2(x)$, for $x > 0$.

double **gsl_sf_bessel_kl_scaled**(int l, double x)

int **gsl_sf_bessel_kl_scaled_e**(int l, double x, *gsl_sf_result* *result)
These routines compute the scaled irregular modified spherical Bessel function of order `l`, $\exp(x)k_l(x)$, for $x > 0$.

int **gsl_sf_bessel_kl_scaled_array**(int lmax, double x, double result_array[])
This routine computes the values of the scaled irregular modified spherical Bessel functions $\exp(x)k_l(x)$ for l from 0 to `lmax` inclusive for $lmax \geq 0$ and $x > 0$, storing the results in the array `result_array`. The values are computed using recurrence relations for efficiency, and therefore may differ slightly from the exact values.

7.5.9 Regular Bessel Function—Fractional Order

double **gsl_sf_bessel_Jnu**(double nu, double x)

int **gsl_sf_bessel_Jnu_e**(double nu, double x, *gsl_sf_result* *result)
These routines compute the regular cylindrical Bessel function of fractional order ν, $J_\nu(x)$.

int **gsl_sf_bessel_sequence_Jnu_e**(double nu, *gsl_mode_t* mode, size_t size, double v[])
This function computes the regular cylindrical Bessel function of fractional order ν, $J_\nu(x)$, evaluated at a series of x values. The array `v` of length `size` contains the x values. They are assumed to be strictly ordered and positive. The array is over-written with the values of $J_\nu(x_i)$.

7.5.10 Irregular Bessel Functions—Fractional Order

double **gsl_sf_bessel_Ynu**(double nu, double x)

int **gsl_sf_bessel_Ynu_e**(double nu, double x, *gsl_sf_result* *result)

These routines compute the irregular cylindrical Bessel function of fractional order ν, $Y_\nu(x)$.

7.5.11 Regular Modified Bessel Functions—Fractional Order

double **gsl_sf_bessel_Inu**(double nu, double x)

int **gsl_sf_bessel_Inu_e**(double nu, double x, *gsl_sf_result* *result)

These routines compute the regular modified Bessel function of fractional order ν, $I_\nu(x)$ for $x > 0$, $\nu > 0$.

double **gsl_sf_bessel_Inu_scaled**(double nu, double x)

int **gsl_sf_bessel_Inu_scaled_e**(double nu, double x, *gsl_sf_result* *result)

These routines compute the scaled regular modified Bessel function of fractional order ν, $\exp(-|x|)I_\nu(x)$ for $x > 0$, $\nu > 0$.

7.5.12 Irregular Modified Bessel Functions—Fractional Order

double **gsl_sf_bessel_Knu**(double nu, double x)

int **gsl_sf_bessel_Knu_e**(double nu, double x, *gsl_sf_result* *result)

These routines compute the irregular modified Bessel function of fractional order ν, $K_\nu(x)$ for $x > 0$, $\nu > 0$.

double **gsl_sf_bessel_lnKnu**(double nu, double x)

int **gsl_sf_bessel_lnKnu_e**(double nu, double x, *gsl_sf_result* *result)

These routines compute the logarithm of the irregular modified Bessel function of fractional order ν, $\ln(K_\nu(x))$ for $x > 0$, $\nu > 0$.

double **gsl_sf_bessel_Knu_scaled**(double nu, double x)

int **gsl_sf_bessel_Knu_scaled_e**(double nu, double x, *gsl_sf_result* *result)

These routines compute the scaled irregular modified Bessel function of fractional order ν, $\exp(+|x|)K_\nu(x)$ for $x > 0$, $\nu > 0$.

7.5.13 Zeros of Regular Bessel Functions

double **gsl_sf_bessel_zero_J0**(unsigned int s)

int **gsl_sf_bessel_zero_J0_e**(unsigned int s, *gsl_sf_result* *result)

These routines compute the location of the `s`-th positive zero of the Bessel function $J_0(x)$.

double **gsl_sf_bessel_zero_J1**(unsigned int s)

int **gsl_sf_bessel_zero_J1_e**(unsigned int s, *gsl_sf_result* *result)

These routines compute the location of the `s`-th positive zero of the Bessel function $J_1(x)$.

double **gsl_sf_bessel_zero_Jnu**(double nu, unsigned int s)

int **gsl_sf_bessel_zero_Jnu_e**(double nu, unsigned int s, *gsl_sf_result* *result)

These routines compute the location of the `s`-th positive zero of the Bessel function $J_\nu(x)$. The current implementation does not support negative values of `nu`.

7.6 Clausen Functions

The Clausen function is defined by the following integral,

$$Cl_2(x) = -\int_0^x dt \log(2\sin(t/2))$$

It is related to the *dilogarithm* by $Cl_2(\theta) = \Im Li_2(\exp(i\theta))$. The Clausen functions are declared in the header file `gsl_sf_clausen.h`.

double **gsl_sf_clausen**(double x)

int **gsl_sf_clausen_e**(double x, *gsl_sf_result* *result)

These routines compute the Clausen integral $Cl_2(x)$.

7.7 Coulomb Functions

The prototypes of the Coulomb functions are declared in the header file `gsl_sf_coulomb.h`. Both bound state and scattering solutions are available.

7.7.1 Normalized Hydrogenic Bound States

double **gsl_sf_hydrogenicR_1**(double Z, double r)

int **gsl_sf_hydrogenicR_1_e**(double Z, double r, *gsl_sf_result* *result)

These routines compute the lowest-order normalized hydrogenic bound state radial wavefunction $R_1 := 2Z\sqrt{Z}\exp(-Zr)$.

double **gsl_sf_hydrogenicR**(int n, int l, double Z, double r)

int **gsl_sf_hydrogenicR_e**(int n, int l, double Z, double r, *gsl_sf_result* *result)

These routines compute the `n`-th normalized hydrogenic bound state radial wavefunction,

$$R_n := \frac{2Z^{3/2}}{n^2}\left(\frac{2Zr}{n}\right)^l \sqrt{\frac{(n-l-1)!}{(n+l)!}}\exp(-Zr/n)L^{2l+1}_{n-l-1}(2Zr/n).$$

where $L^a_b(x)$ is the *generalized Laguerre polynomial*. The normalization is chosen such that the wavefunction ψ is given by $\psi(n,l,r) = R_n Y_{lm}$.

7.7.2 Coulomb Wave Functions

The Coulomb wave functions $F_L(\eta, x)$, $G_L(\eta, x)$ are described in Abramowitz & Stegun, Chapter 14. Because there can be a large dynamic range of values for these functions, overflows are handled gracefully. If an overflow occurs, `GSL_EOVRFLW` is signalled and exponent(s) are returned through the modifiable parameters `exp_F`, `exp_G`. The full solution can be reconstructed from the following relations,

$$F_L(\eta, x) = fc[k_L] * \exp(exp_F)$$
$$G_L(\eta, x) = gc[k_L] * \exp(exp_G)$$

$$F_L'(\eta, x) = fcp[k_L] * \exp(exp_F)$$
$$G_L'(\eta, x) = gcp[k_L] * \exp(exp_G)$$

int **gsl_sf_coulomb_wave_FG_e**(double eta, double x, double L_F, int k, *gsl_sf_result* *F, *gsl_sf_result* *Fp, *gsl_sf_result* *G, *gsl_sf_result* *Gp, double *exp_F, double *exp_G)

This function computes the Coulomb wave functions $F_L(\eta, x)$, $G_{L-k}(\eta, x)$ and their derivatives $F_L'(\eta, x)$, $G_{L-k}'(\eta, x)$ with respect to x. The parameters are restricted to $L, L-k > -1/2$, $x > 0$ and integer k. Note that L itself is not restricted to being an integer. The results are stored in the parameters F, G for the function values and `Fp`, `Gp` for the derivative values. If an overflow occurs, `GSL_EOVRFLW` is returned and scaling exponents are stored in the modifiable parameters `exp_F`, `exp_G`.

int **gsl_sf_coulomb_wave_F_array**(double L_min, int kmax, double eta, double x, double fc_array[], double *F_exponent)

This function computes the Coulomb wave function $F_L(\eta, x)$ for $L = Lmin \dots Lmin + kmax$, storing the results in `fc_array`. In the case of overflow the exponent is stored in `F_exponent`.

int **gsl_sf_coulomb_wave_FG_array**(double L_min, int kmax, double eta, double x, double fc_array[], double gc_array[], double *F_exponent, double *G_exponent)

This function computes the functions $F_L(\eta, x)$, $G_L(\eta, x)$ for $L = Lmin \dots Lmin + kmax$ storing the results in `fc_array` and `gc_array`. In the case of overflow the exponents are stored in `F_exponent` and `G_exponent`.

int **gsl_sf_coulomb_wave_FGp_array**(double L_min, int kmax, double eta, double x, double fc_array[], double fcp_array[], double gc_array[], double gcp_array[], double *F_exponent, double *G_exponent)

This function computes the functions $F_L(\eta, x)$, $G_L(\eta, x)$ and their derivatives $F_L'(\eta, x)$, $G_L'(\eta, x)$ for $L = Lmin \dots Lmin + kmax$ storing the results in `fc_array`, `gc_array`, `fcp_array` and `gcp_array`. In the case of overflow the exponents are stored in `F_exponent` and `G_exponent`.

int **gsl_sf_coulomb_wave_sphF_array**(double L_min, int kmax, double eta, double x, double fc_array[], double F_exponent[])

This function computes the Coulomb wave function divided by the argument $F_L(\eta, x)/x$ for $L = Lmin \dots Lmin + kmax$, storing the results in `fc_array`. In the case of overflow the exponent is stored in `F_exponent`. This function reduces to spherical Bessel functions in the limit $\eta \to 0$.

7.7.3 Coulomb Wave Function Normalization Constant

The Coulomb wave function normalization constant is defined in Abramowitz 14.1.7.

int **gsl_sf_coulomb_CL_e**(double L, double eta, *gsl_sf_result* *result)

This function computes the Coulomb wave function normalization constant $C_L(\eta)$ for $L > -1$.

int **gsl_sf_coulomb_CL_array**(double Lmin, int kmax, double eta, double cl[])

This function computes the Coulomb wave function normalization constant $C_L(\eta)$ for $L = Lmin \dots Lmin + kmax$, $Lmin > -1$.

7.8 Coupling Coefficients

The Wigner 3-j, 6-j and 9-j symbols give the coupling coefficients for combined angular momentum vectors. Since the arguments of the standard coupling coefficient functions are integer or half-integer, the arguments of the following functions are, by convention, integers equal to twice the actual spin value. For information on the 3-j coefficients see Abramowitz & Stegun, Section 27.9. The functions described in this section are declared in the header file `gsl_sf_coupling.h`.

7.8.1 3-j Symbols

double **gsl_sf_coupling_3j**(int two_ja, int two_jb, int two_jc, int two_ma, int two_mb, int two_mc)

int **gsl_sf_coupling_3j_e**(int two_ja, int two_jb, int two_jc, int two_ma, int two_mb, int two_mc, *gsl_sf_result* *result)

These routines compute the Wigner 3-j coefficient,

$$\begin{pmatrix} ja & jb & jc \\ ma & mb & mc \end{pmatrix}$$

where the arguments are given in half-integer units, ja = `two_ja`/2, ma = `two_ma`/2, etc.

7.8.2 6-j Symbols

double **gsl_sf_coupling_6j**(int two_ja, int two_jb, int two_jc, int two_jd, int two_je, int two_jf)

int **gsl_sf_coupling_6j_e**(int two_ja, int two_jb, int two_jc, int two_jd, int two_je, int two_jf, *gsl_sf_result* *result)

These routines compute the Wigner 6-j coefficient,

$$\begin{Bmatrix} ja & jb & jc \\ jd & je & jf \end{Bmatrix}$$

where the arguments are given in half-integer units, ja = `two_ja`/2, ma = `two_ma`/2, etc.

7.8.3 9-j Symbols

double **gsl_sf_coupling_9j**(int two_ja, int two_jb, int two_jc, int two_jd, int two_je, int two_jf, int two_jg, int two_jh, int two_ji)

int **gsl_sf_coupling_9j_e**(int two_ja, int two_jb, int two_jc, int two_jd, int two_je, int two_jf, int two_jg, int two_jh, int two_ji, *gsl_sf_result* *result)

These routines compute the Wigner 9-j coefficient,

$$\begin{Bmatrix} ja & jb & jc \\ jd & je & jf \\ jg & jh & ji \end{Bmatrix}$$

where the arguments are given in half-integer units, ja = `two_ja`/2, ma = `two_ma`/2, etc.

7.9 Dawson Function

The Dawson integral is defined by

$$\exp(-x^2) \int_0^x dt \exp(t^2)$$

A table of Dawson's integral can be found in Abramowitz & Stegun, Table 7.5. The Dawson functions are declared in the header file `gsl_sf_dawson.h`.

double **gsl_sf_dawson**(double x)

int **gsl_sf_dawson_e**(double x, *gsl_sf_result* *result)

These routines compute the value of Dawson's integral for `x`.

7.10 Debye Functions

The Debye functions $D_n(x)$ are defined by the following integral,

$$D_n(x) = \frac{n}{x^n} \int_0^x dt \frac{t^n}{e^t - 1}$$

For further information see Abramowitz & Stegun, Section 27.1. The Debye functions are declared in the header file `gsl_sf_debye.h`.

double **gsl_sf_debye_1**(double x)

int **gsl_sf_debye_1_e**(double x, *gsl_sf_result* *result)

These routines compute the first-order Debye function $D_1(x)$.

double **gsl_sf_debye_2**(double x)

int **gsl_sf_debye_2_e**(double x, *gsl_sf_result* *result)

These routines compute the second-order Debye function $D_2(x)$.

double **gsl_sf_debye_3**(double x)

int **gsl_sf_debye_3_e**(double x, *gsl_sf_result* *result)

These routines compute the third-order Debye function $D_3(x)$.

double **gsl_sf_debye_4**(double x)

int **gsl_sf_debye_4_e**(double x, *gsl_sf_result* *result)

These routines compute the fourth-order Debye function $D_4(x)$.

double **gsl_sf_debye_5**(double x)

int **gsl_sf_debye_5_e**(double x, *gsl_sf_result* *result)

These routines compute the fifth-order Debye function $D_5(x)$.

double **gsl_sf_debye_6**(double x)

int **gsl_sf_debye_6_e**(double x, *gsl_sf_result* *result)

These routines compute the sixth-order Debye function $D_6(x)$.

7.11 Dilogarithm

The dilogarithm is defined as

$$Li_2(z) = -\int_0^z ds \frac{\log{(1-s)}}{s}$$

The functions described in this section are declared in the header file `gsl_sf_dilog.h`.

7.11.1 Real Argument

double **`gsl_sf_dilog`**(double x)

int **`gsl_sf_dilog_e`**(double x, *gsl_sf_result* *result)

These routines compute the dilogarithm for a real argument. In Lewin's notation this is $Li_2(x)$, the real part of the dilogarithm of a real x. It is defined by the integral representation

$$Li_2(x) = -\Re \int_0^x ds \log(1-s)/s$$

Note that $\Im(Li_2(x)) = 0$ for $x \le 1$, and $-\pi \log(x)$ for $x > 1$.

Note that Abramowitz & Stegun refer to the Spence integral $S(x) = Li_2(1-x)$ as the dilogarithm rather than $Li_2(x)$.

7.11.2 Complex Argument

int **`gsl_sf_complex_dilog_e`**(double r, double theta, *gsl_sf_result* *result_re, *gsl_sf_result* *result_im)

This function computes the full complex-valued dilogarithm for the complex argument $z = r\exp(i\theta)$. The real and imaginary parts of the result are returned in `result_re`, `result_im`.

7.12 Elementary Operations

The following functions allow for the propagation of errors when combining quantities by multiplication. The functions are declared in the header file `gsl_sf_elementary.h`.

double **`gsl_sf_multiply`**(double x, double y)

int **`gsl_sf_multiply_e`**(double x, double y, *gsl_sf_result* *result)

This function multiplies `x` and `y` storing the product and its associated error in `result`.

int **`gsl_sf_multiply_err_e`**(double x, double dx, double y, double dy, *gsl_sf_result* *result)

This function multiplies `x` and `y` with associated absolute errors `dx` and `dy`. The product $xy \pm xy\sqrt{(dx/x)^2 + (dy/y)^2}$ is stored in `result`.

7.13 Elliptic Integrals

The functions described in this section are declared in the header file `gsl_sf_ellint.h`. Further information about the elliptic integrals can be found in Abramowitz & Stegun, Chapter 17.

7.13.1 Definition of Legendre Forms

The Legendre forms of elliptic integrals $F(\phi, k)$, $E(\phi, k)$ and $\Pi(\phi, k, n)$ are defined by,

$$\begin{aligned}
F(\phi, k) &= \int_0^\phi dt \frac{1}{\sqrt{(1 - k^2 \sin^2(t))}} \\
E(\phi, k) &= \int_0^\phi dt \sqrt{(1 - k^2 \sin^2(t))} \\
\Pi(\phi, k, n) &= \int_0^\phi dt \frac{1}{(1 + n \sin^2(t))\sqrt{1 - k^2 \sin^2(t)}}
\end{aligned}$$

The complete Legendre forms are denoted by $K(k) = F(\pi/2, k)$ and $E(k) = E(\pi/2, k)$.

The notation used here is based on Carlson, "Numerische Mathematik" 33 (1979) 1 and differs slightly from that used by Abramowitz & Stegun, where the functions are given in terms of the parameter $m = k^2$ and n is replaced by $-n$.

7.13.2 Definition of Carlson Forms

The Carlson symmetric forms of elliptical integrals $RC(x, y)$, $RD(x, y, z)$, $RF(x, y, z)$ and $RJ(x, y, z, p)$ are defined by,

$$\begin{aligned}
RC(x, y) &= 1/2 \int_0^\infty dt (t + x)^{-1/2} (t + y)^{-1} \\
RD(x, y, z) &= 3/2 \int_0^\infty dt (t + x)^{-1/2} (t + y)^{-1/2} (t + z)^{-3/2} \\
RF(x, y, z) &= 1/2 \int_0^\infty dt (t + x)^{-1/2} (t + y)^{-1/2} (t + z)^{-1/2} \\
RJ(x, y, z, p) &= 3/2 \int_0^\infty dt (t + x)^{-1/2} (t + y)^{-1/2} (t + z)^{-1/2} (t + p)^{-1}
\end{aligned}$$

7.13.3 Legendre Form of Complete Elliptic Integrals

double **gsl_sf_ellint_Kcomp**(double k, *gsl_mode_t* mode)

int **gsl_sf_ellint_Kcomp_e**(double k, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the complete elliptic integral $K(k)$ to the accuracy specified by the mode variable `mode`. Note that Abramowitz & Stegun define this function in terms of the parameter $m = k^2$.

double **gsl_sf_ellint_Ecomp**(double k, *gsl_mode_t* mode)

int **gsl_sf_ellint_Ecomp_e**(double k, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the complete elliptic integral $E(k)$ to the accuracy specified by the mode variable `mode`. Note that Abramowitz & Stegun define this function in terms of the parameter $m = k^2$.

double **gsl_sf_ellint_Pcomp**(double k, double n, *gsl_mode_t* mode)

int **gsl_sf_ellint_Pcomp_e**(double k, double n, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the complete elliptic integral $\Pi(k, n)$ to the accuracy specified by the mode variable `mode`. Note that Abramowitz & Stegun define this function in terms of the parameters $m = k^2$ and $\sin^2(\alpha) = k^2$, with the change of sign $n \to -n$.

7.13.4 Legendre Form of Incomplete Elliptic Integrals

double **gsl_sf_ellint_F**(double phi, double k, *gsl_mode_t* mode)

int **gsl_sf_ellint_F_e**(double phi, double k, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the incomplete elliptic integral $F(\phi, k)$ to the accuracy specified by the mode variable `mode`. Note that Abramowitz & Stegun define this function in terms of the parameter $m = k^2$.

double **gsl_sf_ellint_E**(double phi, double k, *gsl_mode_t* mode)

int **gsl_sf_ellint_E_e**(double phi, double k, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the incomplete elliptic integral $E(\phi, k)$ to the accuracy specified by the mode variable `mode`. Note that Abramowitz & Stegun define this function in terms of the parameter $m = k^2$.

double **gsl_sf_ellint_P**(double phi, double k, double n, *gsl_mode_t* mode)

int **gsl_sf_ellint_P_e**(double phi, double k, double n, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the incomplete elliptic integral $\Pi(\phi, k, n)$ to the accuracy specified by the mode variable `mode`. Note that Abramowitz & Stegun define this function in terms of the parameters $m = k^2$ and $\sin^2(\alpha) = k^2$, with the change of sign $n \to -n$.

double **gsl_sf_ellint_D**(double phi, double k, *gsl_mode_t* mode)

int **gsl_sf_ellint_D_e**(double phi, double k, *gsl_mode_t* mode, *gsl_sf_result* *result)

These functions compute the incomplete elliptic integral $D(\phi, k)$ which is defined through the Carlson form $RD(x, y, z)$ by the following relation,

$$D(\phi, k) = \frac{1}{3}(\sin\phi)^3 RD(1 - \sin^2(\phi), 1 - k^2\sin^2(\phi), 1)$$

7.13.5 Carlson Forms

double **gsl_sf_ellint_RC**(double x, double y, *gsl_mode_t* mode)

int **gsl_sf_ellint_RC_e**(double x, double y, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the incomplete elliptic integral $RC(x, y)$ to the accuracy specified by the mode variable `mode`.

double **gsl_sf_ellint_RD**(double x, double y, double z, *gsl_mode_t* mode)

int **gsl_sf_ellint_RD_e**(double x, double y, double z, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the incomplete elliptic integral $RD(x, y, z)$ to the accuracy specified by the mode variable `mode`.

double **gsl_sf_ellint_RF**(double x, double y, double z, *gsl_mode_t* mode) int **gsl_sf_ellint_RF_e**(double x, double y, double z, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the incomplete elliptic integral $RF(x, y, z)$ to the accuracy specified by the mode variable `mode`.

double **gsl_sf_ellint_RJ**(double x, double y, double z, double p, *gsl_mode_t* mode)

int **gsl_sf_ellint_RJ_e**(double x, double y, double z, double p, *gsl_mode_t* mode, *gsl_sf_result* *result)

These routines compute the incomplete elliptic integral $RJ(x, y, z, p)$ to the accuracy specified by the mode variable `mode`.

7.14 Elliptic Functions (Jacobi)

The Jacobian Elliptic functions are defined in Abramowitz & Stegun, Chapter 16. The functions are declared in the header file `gsl_sf_elljac.h`.

int **gsl_sf_elljac_e**(double u, double m, double *sn, double *cn, double *dn)

This function computes the Jacobian elliptic functions $sn(u|m)$, $cn(u|m)$, $dn(u|m)$ by descending Landen transformations.

7.15 Error Functions

The error function is described in Abramowitz & Stegun, Chapter 7. The functions in this section are declared in the header file `gsl_sf_erf.h`.

7.15.1 Error Function

double **gsl_sf_erf**(double x)

int **gsl_sf_erf_e**(double x, *gsl_sf_result* *result)

These routines compute the error function $\mathrm{erf}(x)$, where $\mathrm{erf}(x) = (2/\sqrt{\pi}) \int_0^x dt \exp(-t^2)$.

7.15.2 Complementary Error Function

double **gsl_sf_erfc**(double x)

int **gsl_sf_erfc_e**(double x, *gsl_sf_result* *result)

These routines compute the complementary error function $\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) = (2/\sqrt{\pi}) \int_x^\infty \exp(-t^2)$

7.15.3 Log Complementary Error Function

double **gsl_sf_log_erfc**(double x)

int **gsl_sf_log_erfc_e**(double x, *gsl_sf_result* *result)

These routines compute the logarithm of the complementary error function $\log(\mathrm{erfc}(x))$.

7.15.4 Probability functions

The probability functions for the Normal or Gaussian distribution are described in Abramowitz & Stegun, Section 26.2.

double **gsl_sf_erf_Z**(double x)

int **gsl_sf_erf_Z_e**(double x, *gsl_sf_result* *result)

These routines compute the Gaussian probability density function $Z(x) = (1/\sqrt{2\pi})\exp(-x^2/2)$

double **gsl_sf_erf_Q**(double x)

int **gsl_sf_erf_Q_e**(double x, *gsl_sf_result* *result)

These routines compute the upper tail of the Gaussian probability function $Q(x) = (1/\sqrt{2\pi})\int_x^\infty dt \exp(-t^2/2)$

The *hazard function* for the normal distribution, also known as the inverse Mills' ratio, is defined as,

$$h(x) = \frac{Z(x)}{Q(x)} = \sqrt{\frac{2}{\pi}}\frac{\exp(-x^2/2)}{\operatorname{erfc}(x/\sqrt{2})}$$

It decreases rapidly as x approaches $-\infty$ and asymptotes to $h(x) \sim x$ as x approaches $+\infty$.

double **gsl_sf_hazard**(double x)

int **gsl_sf_hazard_e**(double x, *gsl_sf_result* *result)

These routines compute the hazard function for the normal distribution.

7.16 Exponential Functions

The functions described in this section are declared in the header file `gsl_sf_exp.h`.

7.16.1 Exponential Function

double **gsl_sf_exp**(double x)

int **gsl_sf_exp_e**(double x, *gsl_sf_result* *result)

These routines provide an exponential function $\exp(x)$ using GSL semantics and error checking.

int **gsl_sf_exp_e10_e**(double x, *gsl_sf_result_e10* *result)

This function computes the exponential $\exp(x)$ using the `gsl_sf_result_e10` type to return a result with extended range. This function may be useful if the value of $\exp(x)$ would overflow the numeric range of `double`.

double **gsl_sf_exp_mult**(double x, double y)

int **gsl_sf_exp_mult_e**(double x, double y, *gsl_sf_result* *result)

These routines exponentiate `x` and multiply by the factor `y` to return the product $y\exp(x)$.

int **gsl_sf_exp_mult_e10_e**(const double x, const double y, *gsl_sf_result_e10* *result)

This function computes the product $y\exp(x)$ using the `gsl_sf_result_e10` type to return a result with extended numeric range.

7.16.2 Relative Exponential Functions

double **gsl_sf_expm1**(double x)

int **gsl_sf_expm1_e**(double x, *gsl_sf_result* *result)

These routines compute the quantity $\exp(x) - 1$ using an algorithm that is accurate for small x.

double **gsl_sf_exprel**(double x)

int **gsl_sf_exprel_e**(double x, *gsl_sf_result* *result)

These routines compute the quantity $(\exp(x) - 1)/x$ using an algorithm that is accurate for small `x`. For small `x` the algorithm is based on the expansion $(\exp(x) - 1)/x = 1 + x/2 + x^2/(2 * 3) + x^3/(2 * 3 * 4) + \dots$.

double **gsl_sf_exprel_2**(double x)

int **gsl_sf_exprel_2_e**(double x, *gsl_sf_result* *result)

These routines compute the quantity $2(\exp(x) - 1 - x)/x^2$ using an algorithm that is accurate for small `x`. For small `x` the algorithm is based on the expansion $2(\exp(x) - 1 - x)/x^2 = 1 + x/3 + x^2/(3*4) + x^3/(3*4*5) + \dots$.

double **gsl_sf_exprel_n**(int n, double x)

int **gsl_sf_exprel_n_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the N-relative exponential, which is the `n`-th generalization of the functions `gsl_sf_exprel()` and `gsl_sf_exprel_2()`. The N-relative exponential is given by,

$$\begin{aligned}\mathrm{exprel}_N(x) &= N!/x^N \left(\exp(x) - \sum_{k=0}^{N-1} x^k/k!\right)\\ &= 1 + x/(N+1) + x^2/((N+1)(N+2)) + \dots\\ &= {}_1F_1(1, 1+N, x)\end{aligned}$$

7.16.3 Exponentiation With Error Estimate

int **gsl_sf_exp_err_e**(double x, double dx, *gsl_sf_result* *result)

This function exponentiates `x` with an associated absolute error `dx`.

int **gsl_sf_exp_err_e10_e**(double x, double dx, *gsl_sf_result_e10* *result)

This function exponentiates a quantity `x` with an associated absolute error `dx` using the `gsl_sf_result_e10` type to return a result with extended range.

int **gsl_sf_exp_mult_err_e**(double x, double dx, double y, double dy, *gsl_sf_result* *result)

This routine computes the product $y \exp(x)$ for the quantities `x`, `y` with associated absolute errors `dx`, `dy`.

int **gsl_sf_exp_mult_err_e10_e**(double x, double dx, double y, double dy, *gsl_sf_result_e10* *result)

This routine computes the product $y \exp(x)$ for the quantities `x`, `y` with associated absolute errors `dx`, `dy` using the `gsl_sf_result_e10` type to return a result with extended range.

7.17 Exponential Integrals

Information on the exponential integrals can be found in Abramowitz & Stegun, Chapter 5. These functions are declared in the header file `gsl_sf_expint.h`.

7.17.1 Exponential Integral

double **gsl_sf_expint_E1**(double x)

int **gsl_sf_expint_E1_e**(double x, *gsl_sf_result* *result)

These routines compute the exponential integral $E_1(x)$,

$$E_1(x) := \Re \int_1^\infty dt \exp(-xt)/t.$$

double **gsl_sf_expint_E2**(double x)

int **gsl_sf_expint_E2_e**(double x, *gsl_sf_result* *result)

These routines compute the second-order exponential integral $E_2(x)$,

$$E_2(x) := \Re \int_1^\infty dt \exp(-xt)/t^2$$

double **gsl_sf_expint_En**(int n, double x)

int **gsl_sf_expint_En_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the exponential integral $E_n(x)$ of order n,

$$E_n(x) := \Re \int_1^\infty dt \exp(-xt)/t^n.$$

7.17.2 Ei(x)

double **gsl_sf_expint_Ei**(double x)

int **gsl_sf_expint_Ei_e**(double x, *gsl_sf_result* *result)

These routines compute the exponential integral $Ei(x)$,

$$\mathrm{Ei}(x) = -PV\left(\int_{-x}^\infty dt \exp(-t)/t\right)$$

where PV denotes the principal value of the integral.

7.17.3 Hyperbolic Integrals

double **gsl_sf_Shi**(double x)

int **gsl_sf_Shi_e**(double x, *gsl_sf_result* *result)

These routines compute the integral

$$\mathrm{Shi}(x) = \int_0^x dt \sinh(t)/t$$

double **gsl_sf_Chi**(double x)

int **gsl_sf_Chi_e**(double x, *gsl_sf_result* *result)

These routines compute the integral

$$\mathrm{Chi}(x) := \Re\left[\gamma_E + \log(x) + \int_0^x dt(\cosh(t) - 1)/t\right]$$

where γ_E is the Euler constant (available as the macro `M_EULER`).

7.17.4 Ei_3(x)

double **gsl_sf_expint_3**(double x)

int **gsl_sf_expint_3_e**(double x, *gsl_sf_result* *result)

These routines compute the third-order exponential integral

$$\mathrm{Ei}_3(x) = \int_0^x dt \exp(-t^3)$$

for $x \geq 0$.

7.17.5 Trigonometric Integrals

double **gsl_sf_Si**(const double x)

int **gsl_sf_Si_e**(double x, *gsl_sf_result* *result)

These routines compute the Sine integral

$$\mathrm{Si}(x) = \int_0^x dt \sin(t)/t$$

double **gsl_sf_Ci**(const double x)

int **gsl_sf_Ci_e**(double x, *gsl_sf_result* *result)

These routines compute the Cosine integral

$$\mathrm{Ci}(x) = -\int_x^\infty dt \cos(t)/t$$

for $x > 0$

7.17.6 Arctangent Integral

double **gsl_sf_atanint**(double x)

int **gsl_sf_atanint_e**(double x, *gsl_sf_result* *result)

These routines compute the Arctangent integral, which is defined as

$$\mathrm{AtanInt}(x) = \int_0^x dt \arctan(t)/t$$

7.18 Fermi-Dirac Function

The functions described in this section are declared in the header file `gsl_sf_fermi_dirac.h`.

7.18.1 Complete Fermi-Dirac Integrals

The complete Fermi-Dirac integral $F_j(x)$ is given by,

$$F_j(x) := \frac{1}{\Gamma(j+1)} \int_0^\infty dt \frac{t^j}{(\exp(t-x)+1)}$$

Note that the Fermi-Dirac integral is sometimes defined without the normalisation factor in other texts.

double **gsl_sf_fermi_dirac_m1**(double x)

int **gsl_sf_fermi_dirac_m1_e**(double x, *gsl_sf_result* *result)

These routines compute the complete Fermi-Dirac integral with an index of -1. This integral is given by $F_{-1}(x) = e^x/(1+e^x)$.

double **gsl_sf_fermi_dirac_0**(double x)

int **gsl_sf_fermi_dirac_0_e**(double x, *gsl_sf_result* *result)

These routines compute the complete Fermi-Dirac integral with an index of 0. This integral is given by $F_0(x) = \ln(1+e^x)$.

double **gsl_sf_fermi_dirac_1**(double x)

int **gsl_sf_fermi_dirac_1_e**(double x, *gsl_sf_result* *result)

These routines compute the complete Fermi-Dirac integral with an index of 1, $F_1(x) = \int_0^\infty dt(t/(\exp(t-x)+1))$.

double **gsl_sf_fermi_dirac_2**(double x)

int **gsl_sf_fermi_dirac_2_e**(double x, *gsl_sf_result* *result)

These routines compute the complete Fermi-Dirac integral with an index of 2, $F_2(x) = (1/2)\int_0^\infty dt(t^2/(\exp(t-x)+1))$.

double **gsl_sf_fermi_dirac_int**(int j, double x)

int **gsl_sf_fermi_dirac_int_e**(int j, double x, *gsl_sf_result* *result)

These routines compute the complete Fermi-Dirac integral with an integer index of j, $F_j(x) = (1/\Gamma(j+1))\int_0^\infty dt(t^j/(\exp(t-x)+1))$.

double **gsl_sf_fermi_dirac_mhalf**(double x)

int **gsl_sf_fermi_dirac_mhalf_e**(double x, *gsl_sf_result* *result)

These routines compute the complete Fermi-Dirac integral $F_{-1/2}(x)$.

double **gsl_sf_fermi_dirac_half**(double x)

int **gsl_sf_fermi_dirac_half_e**(double x, *gsl_sf_result* *result)

These routines compute the complete Fermi-Dirac integral $F_{1/2}(x)$.

double **gsl_sf_fermi_dirac_3half**(double x) int **gsl_sf_fermi_dirac_3half_e**(double x, *gsl_sf_result* *result)

These routines compute the complete Fermi-Dirac integral $F_{3/2}(x)$.

7.18.2 Incomplete Fermi-Dirac Integrals

The incomplete Fermi-Dirac integral $F_j(x,b)$ is given by,

$$F_j(x,b) := \frac{1}{\Gamma(j+1)} \int_b^\infty dt \frac{t^j}{(\exp(t-x)+1)}$$

double **gsl_sf_fermi_dirac_inc_0**(double x, double b)

int **gsl_sf_fermi_dirac_inc_0_e**(double x, double b, *gsl_sf_result* *result)

These routines compute the incomplete Fermi-Dirac integral with an index of zero, $F_0(x,b) = \ln(1+e^{b-x}) - (b-x)$

7.19 Gamma and Beta Functions

The following routines compute the gamma and beta functions in their full and incomplete forms, as well as various kinds of factorials. The functions described in this section are declared in the header file `gsl_sf_gamma.h`.

7.19.1 Gamma Functions

The Gamma function is defined by the following integral,

$$\Gamma(x) = \int_0^\infty dt t^{x-1} \exp(-t)$$

It is related to the factorial function by $\Gamma(n) = (n-1)!$ for positive integer n. Further information on the Gamma function can be found in Abramowitz & Stegun, Chapter 6.

double **gsl_sf_gamma**(double x)

int **gsl_sf_gamma_e**(double x, *gsl_sf_result* *result)

These routines compute the Gamma function $\Gamma(x)$, subject to x not being a negative integer or zero. The function is computed using the real Lanczos method. The maximum value of x such that $\Gamma(x)$ is not considered an overflow is given by the macro `GSL_SF_GAMMA_XMAX` and is 171.0.

double **gsl_sf_lngamma**(double x)

int **gsl_sf_lngamma_e**(double x, *gsl_sf_result* *result)

These routines compute the logarithm of the Gamma function, $\log(\Gamma(x))$, subject to x not being a negative integer or zero. For $x < 0$ the real part of $\log(\Gamma(x))$ is returned, which is equivalent to $\log(|\Gamma(x)|)$. The function is computed using the real Lanczos method.

int **gsl_sf_lngamma_sgn_e**(double x, *gsl_sf_result* *result_lg, double *sgn)

This routine computes the sign of the gamma function and the logarithm of its magnitude, subject to x not being a negative integer or zero. The function is computed using the real Lanczos method. The value of the gamma function and its error can be reconstructed using the relation $\Gamma(x) = sgn * \exp(result\_lg)$, taking into account the two components of `result_lg`.

double **gsl_sf_gammastar**(double x)

int **gsl_sf_gammastar_e**(double x, *gsl_sf_result* *result)

These routines compute the regulated Gamma Function $\Gamma^*(x)$ for $x > 0$. The regulated gamma function is given by,

$$\Gamma^*(x) = \Gamma(x)/(\sqrt{2\pi}x^{(x-1/2)}\exp(-x)) \\ = \left(1 + \frac{1}{12x} + ...\right) \quad \text{for } x \to \infty$$

and is a useful suggestion of Temme.

double **gsl_sf_gammainv**(double x)

int **gsl_sf_gammainv_e**(double x, *gsl_sf_result* *result)

These routines compute the reciprocal of the gamma function, $1/\Gamma(x)$ using the real Lanczos method.

int **gsl_sf_lngamma_complex_e**(double zr, double zi, *gsl_sf_result* *lnr, *gsl_sf_result* *arg)

This routine computes $\log(\Gamma(z))$ for complex $z = z_r + iz_i$ and z not a negative integer or zero, using the complex Lanczos method. The returned parameters are $lnr = \log|\Gamma(z)|$ and $arg = \arg(\Gamma(z))$ in $(-\pi, \pi]$. Note that the phase part (`arg`) is not well-determined when $|z|$ is very large, due to inevitable roundoff in restricting to $(-\pi, \pi]$. This will result in a `GSL_ELOSS` error when it occurs. The absolute value part (`lnr`), however, never suffers from loss of precision.

7.19.2 Factorials

Although factorials can be computed from the Gamma function, using the relation $n! = \Gamma(n + 1)$ for non-negative integer n, it is usually more efficient to call the functions in this section, particularly for small values of n, whose factorial values are maintained in hardcoded tables.

double **gsl_sf_fact**(unsigned int n)

int **gsl_sf_fact_e**(unsigned int n, *gsl_sf_result* *result)

These routines compute the factorial $n!$. The factorial is related to the Gamma function by $n! = \Gamma(n + 1)$. The maximum value of n such that $n!$ is not considered an overflow is given by the macro `GSL_SF_FACT_NMAX` and is 170.

double **gsl_sf_doublefact**(unsigned int n)

int **gsl_sf_doublefact_e**(unsigned int n, *gsl_sf_result* *result)

These routines compute the double factorial $n!! = n(n - 2)(n - 4)\dots$. The maximum value of n such that $n!!$ is not considered an overflow is given by the macro `GSL_SF_DOUBLEFACT_NMAX` and is 297.

double **gsl_sf_lnfact**(unsigned int n)

int **gsl_sf_lnfact_e**(unsigned int n, *gsl_sf_result* *result)

These routines compute the logarithm of the factorial of `n`, $\log(n!)$. The algorithm is faster than computing $\ln(\Gamma(n + 1))$ via `gsl_sf_lngamma()` for $n < 170$, but defers for larger `n`.

double **gsl_sf_lndoublefact**(unsigned int n)

int **gsl_sf_lndoublefact_e**(unsigned int n, *gsl_sf_result* *result)

These routines compute the logarithm of the double factorial of `n`, $\log(n!!)$.

double **gsl_sf_choose**(unsigned int n, unsigned int m) int **gsl_sf_choose_e**(unsigned int n, unsigned int m, *gsl_sf_result* *result)

These routines compute the combinatorial factor `n choose m` $= n!/(m!(n-m)!)$

double **gsl_sf_lnchoose**(unsigned int n, unsigned int m)

int **gsl_sf_lnchoose_e**(unsigned int n, unsigned int m, *gsl_sf_result* *result)

These routines compute the logarithm of `n choose m`. This is equivalent to the sum $\log(n!) - \log(m!) - \log((n-m)!)$.

double **gsl_sf_taylorcoeff**(int n, double x)

int **gsl_sf_taylorcoeff_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the Taylor coefficient $x^n/n!$ for $x \geq 0$, $n \geq 0$

7.19.3 Pochhammer Symbol

double **gsl_sf_poch**(double a, double x)

int **gsl_sf_poch_e**(double a, double x, *gsl_sf_result* *result)

These routines compute the Pochhammer symbol $(a)_x = \Gamma(a+x)/\Gamma(a)$. The Pochhammer symbol is also known as the Apell symbol and sometimes written as (a,x). When a and $a+x$ are negative integers or zero, the limiting value of the ratio is returned.

double **gsl_sf_lnpoch**(double a, double x)

int **gsl_sf_lnpoch_e**(double a, double x, *gsl_sf_result* *result)

These routines compute the logarithm of the Pochhammer symbol, $\log((a)_x) = \log(\Gamma(a+x)/\Gamma(a))$.

int **gsl_sf_lnpoch_sgn_e**(double a, double x, *gsl_sf_result* *result, double *sgn)

These routines compute the sign of the Pochhammer symbol and the logarithm of its magnitude. The computed parameters are $result = \log(|(a)_x|)$ with a corresponding error term, and $sgn = \mathrm{sgn}((a)_x)$ where $(a)_x = \Gamma(a+x)/\Gamma(a)$.

double **gsl_sf_pochrel**(double a, double x)

int **gsl_sf_pochrel_e**(double a, double x, *gsl_sf_result* *result)

These routines compute the relative Pochhammer symbol $((a)_x - 1)/x$ where $(a)_x = \Gamma(a+x)/\Gamma(a)$.

7.19.4 Incomplete Gamma Functions

double **gsl_sf_gamma_inc**(double a, double x)

int **gsl_sf_gamma_inc_e**(double a, double x, *gsl_sf_result* *result)

These functions compute the unnormalized incomplete Gamma Function $\Gamma(a,x) = \int_x^\infty dt t^{(a-1)} \exp(-t)$ for a real and $x \geq 0$.

double **gsl_sf_gamma_inc_Q**(double a, double x)

int **gsl_sf_gamma_inc_Q_e**(double a, double x, *gsl_sf_result* *result)

These routines compute the normalized incomplete Gamma Function $Q(a,x) = 1/\Gamma(a) \int_x^\infty dt t^{(a-1)} \exp(-t)$ for $a > 0$, $x \geq 0$.

double **gsl_sf_gamma_inc_P**(double a, double x) int **gsl_sf_gamma_inc_P_e**(double a, double x, *gsl_sf_result* *result)

These routines compute the complementary normalized incomplete Gamma Function $P(a,x) = 1 - Q(a,x) = 1/\Gamma(a)\int_0^x dt t^{(a-1)}\exp(-t)$ for $a > 0$, $x \geq 0$.

Note that Abramowitz & Stegun call $P(a,x)$ the incomplete gamma function (section 6.5).

7.19.5 Beta Functions

double **gsl_sf_beta**(double a, double b)

int **gsl_sf_beta_e**(double a, double b, *gsl_sf_result* *result)

These routines compute the Beta Function, $B(a,b) = \Gamma(a)\Gamma(b)/\Gamma(a+b)$ subject to a and b not being negative integers.

double **gsl_sf_lnbeta**(double a, double b)

int **gsl_sf_lnbeta_e**(double a, double b, *gsl_sf_result* *result)

These routines compute the logarithm of the Beta Function, $\log(B(a,b))$ subject to a and b not being negative integers.

7.19.6 Incomplete Beta Function

double **gsl_sf_beta_inc**(double a, double b, double x)

int **gsl_sf_beta_inc_e**(double a, double b, double x, *gsl_sf_result* *result)

These routines compute the normalized incomplete Beta function $I_x(a,b) = B_x(a,b)/B(a,b)$ where

$$B_x(a,b) = \int_0^x t^{a-1}(1-t)^{b-1}dt$$

for $0 \leq x \leq 1$. For $a > 0$, $b > 0$ the value is computed using a continued fraction expansion. For all other values it is computed using the relation

$$I_x(a,b,x) = (1/a)x^a {}_2F_1(a, 1-b, a+1, x)/B(a,b)$$

7.20 Gegenbauer Functions

The Gegenbauer polynomials are defined in Abramowitz & Stegun, Chapter 22, where they are known as Ultraspherical polynomials. The functions described in this section are declared in the header file `gsl_sf_gegenbauer.h`.

double **gsl_sf_gegenpoly_1**(double lambda, double x)

double **gsl_sf_gegenpoly_2**(double lambda, double x)

double **gsl_sf_gegenpoly_3**(double lambda, double x)

int **gsl_sf_gegenpoly_1_e**(double lambda, double x, *gsl_sf_result* *result)

int **gsl_sf_gegenpoly_2_e**(double lambda, double x, *gsl_sf_result* *result) int **gsl_sf_gegenpoly_3_e**(double lambda, double x, *gsl_sf_result* *result)

These functions evaluate the Gegenbauer polynomials $C_n^{(\lambda)}(x)$ using explicit representations for $n = 1, 2, 3$.

double **gsl_sf_gegenpoly_n**(int n, double lambda, double x)

int **gsl_sf_gegenpoly_n_e**(int n, double lambda, double x, *gsl_sf_result* *result)

These functions evaluate the Gegenbauer polynomial $C_n^{(\lambda)}(x)$ for a specific value of `n`, `lambda`, `x` subject to $\lambda > -1/2$, $n \geq 0$.

int **gsl_sf_gegenpoly_array**(int nmax, double lambda, double x, double result_array[])

This function computes an array of Gegenbauer polynomials $C_n^{(\lambda)}(x)$ for $n = 0, 1, 2, \dots, nmax$, subject to $\lambda > -1/2$, $nmax \geq 0$.

7.21 Hermite Polynomials and Functions

Hermite polynomials and functions are discussed in Abramowitz & Stegun, Chapter 22 and Szego, Gabor (1939, 1958, 1967), Orthogonal Polynomials, American Mathematical Society. The Hermite polynomials and functions are defined in the header file `gsl_sf_hermite.h`.

7.21.1 Hermite Polynomials

The Hermite polynomials exist in two variants: the physicist version $H_n(x)$ and the probabilist version $He_n(x)$. They are defined by the derivatives

$$H_n(x) = (-1)^n e^{x^2} \left(\frac{d}{dx}\right)^n e^{-x^2}$$
$$He_n(x) = (-1)^n e^{x^2/2} \left(\frac{d}{dx}\right)^n e^{-x^2/2}$$

They are connected via

$$H_n(x) = 2^{n/2} He_n\left(\sqrt{2}x\right)$$
$$He_n(x) = 2^{-n/2} H_n\left(\frac{x}{\sqrt{2}}\right)$$

and satisfy the ordinary differential equations

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$$
$$He_n''(x) - xHe_n'(x) + nHe_n(x) = 0$$

double **gsl_sf_hermite**(const int n, const double x)

int **gsl_sf_hermite_e**(const int n, const double x, *gsl_sf_result* *result)

These routines evaluate the physicist Hermite polynomial $H_n(x)$ of order `n` at position `x`. If an overflow is detected, `GSL_EOVRFLW` is returned without calling the error handler.

int **gsl_sf_hermite_array**(const int nmax, const double x, double *result_array)

This routine evaluates all physicist Hermite polynomials H_n up to order `nmax` at position `x`. The results are stored in `result_array`.

double **gsl_sf_hermite_series**(const int n, const double x, const double *a) int **gsl_sf_hermite_series_e**(const int n, const double x, const double *a, *gsl_sf_result* *result)

These routines evaluate the series $\sum_{j=0}^{n} a_j H_j(x)$ with H_j being the j-th physicist Hermite polynomial using the Clenshaw algorithm.

double **gsl_sf_hermite_prob**(const int n, const double x)

int **gsl_sf_hermite_prob_e**(const int n, const double x, *gsl_sf_result* *result)

These routines evaluate the probabilist Hermite polynomial $He_n(x)$ of order `n` at position `x`. If an overflow is detected, `GSL_EOVRFLW` is returned without calling the error handler.

int **gsl_sf_hermite_prob_array**(const int nmax, const double x, double *result_array)

This routine evaluates all probabilist Hermite polynomials $He_n(x)$ up to order `nmax` at position `x`. The results are stored in `result_array`.

double **gsl_sf_hermite_prob_series**(const int n, const double x, const double *a)

int **gsl_sf_hermite_prob_series_e**(const int n, const double x, const double *a, *gsl_sf_result* *result)

These routines evaluate the series $\sum_{j=0}^{n} a_j He_j(x)$ with He_j being the j-th probabilist Hermite polynomial using the Clenshaw algorithm.

7.21.2 Derivatives of Hermite Polynomials

double **gsl_sf_hermite_deriv**(const int m, const int n, const double x)

int **gsl_sf_hermite_deriv_e**(const int m, const int n, const double x, *gsl_sf_result* *result)

These routines evaluate the `m`-th derivative of the physicist Hermite polynomial $H_n(x)$ of order `n` at position `x`.

int **gsl_sf_hermite_array_deriv**(const int m, const int nmax, const double x, double *result_array)

This routine evaluates the `m`-th derivative of all physicist Hermite polynomials $H_n(x)$ from orders $0, \ldots,$ nmax at position `x`. The result $d^m/dx^m H_n(x)$ is stored in `result_array[n]`. The output `result_array` must have length at least `nmax + 1`.

int **gsl_sf_hermite_deriv_array**(const int mmax, const int n, const double x, double *result_array)

This routine evaluates all derivative orders from $0, \ldots,$ mmax of the physicist Hermite polynomial of order `n`, H_n, at position `x`. The result $d^m/dx^m H_n(x)$ is stored in `result_array[m]`. The output `result_array` must have length at least `mmax + 1`.

double **gsl_sf_hermite_prob_deriv**(const int m, const int n, const double x)

int **gsl_sf_hermite_prob_deriv_e**(const int m, const int n, const double x, *gsl_sf_result* *result)

These routines evaluate the `m`-th derivative of the probabilist Hermite polynomial $He_n(x)$ of order `n` at position `x`.

int **gsl_sf_hermite_prob_array_deriv**(const int m, const int nmax, const double x, double *result_array)

This routine evaluates the `m`-th derivative of all probabilist Hermite polynomials $He_n(x)$ from orders $0, \ldots,$ nmax at position `x`. The result $d^m/dx^m He_n(x)$ is stored in `result_array[n]`. The output `result_array` must have length at least `nmax + 1`.

int **gsl_sf_hermite_prob_deriv_array**(const int mmax, const int n, const double x, double *result_array)

This routine evaluates all derivative orders from $0, \ldots,$ mmax of the probabilist Hermite polynomial of order `n`, He_n, at position `x`. The result $d^m/dx^m He_n(x)$ is stored in `result_array[m]`. The output `result_array` must have length at least `mmax + 1`.

7.21.3 Hermite Functions

The Hermite functions are defined by

$$\psi_n(x) = \left(2^n n! \sqrt{\pi}\right)^{-1/2} e^{-x^2/2} H_n\left(x\right)$$

and satisfy the Schrödinger equation for a quantum mechanical harmonic oscillator

$$\psi_n''(x) + (2n + 1 - x^2)\psi_n(x) = 0$$

They are orthonormal,

$$\int_{-\infty}^{\infty} \psi_m(x)\psi_n(x)dx = \delta_{mn}$$

and form an orthonormal basis of $L^2(\mathbb{R})$. The Hermite functions are also eigenfunctions of the continuous Fourier transform. GSL offers two methods for evaluating the Hermite functions. The first uses the standard three-term recurrence relation which has $O(n)$ complexity and is the most accurate. The second uses a Cauchy integral approach due to Bunck (2009) which has $O(\sqrt{n})$ complexity which represents a significant speed improvement for large n, although it is slightly less accurate.

double **gsl_sf_hermite_func**(const int n, const double x)

int **gsl_sf_hermite_func_e**(const int n, const double x, *gsl_sf_result* *result)

These routines evaluate the Hermite function $\psi_n(x)$ of order `n` at position `x` using a three term recurrence relation. The algorithm complexity is $O(n)$.

double **gsl_sf_hermite_func_fast**(const int n, const double x)

int **gsl_sf_hermite_func_fast_e**(const int n, const double x, *gsl_sf_result* *result)

These routines evaluate the Hermite function $\psi_n(x)$ of order `n` at position `x` using a the Cauchy integral algorithm due to Bunck, 2009. The algorithm complexity is $O(\sqrt{n})$.

int **gsl_sf_hermite_func_array**(const int nmax, const double x, double *result_array)

This routine evaluates all Hermite functions $\psi_n(x)$ for orders $n = 0, \dots,$ nmax at position `x`, using the recurrence relation algorithm. The results are stored in `result_array` which has length at least `nmax + 1`.

double **gsl_sf_hermite_func_series**(const int n, const double x, const double *a)

int **gsl_sf_hermite_func_series_e**(const int n, const double x, const double *a, *gsl_sf_result* *result)

These routines evaluate the series $\sum_{j=0}^{n} a_j \psi_j(x)$ with ψ_j being the j-th Hermite function using the Clenshaw algorithm.

7.21.4 Derivatives of Hermite Functions

double **gsl_sf_hermite_func_der**(const int m, const int n, const double x)

int **gsl_sf_hermite_func_der_e**(const int m, const int n, const double x, *gsl_sf_result* *result)

These routines evaluate the `m`-th derivative of the Hermite function $\psi_n(x)$ of order `n` at position `x`.

7.21.5 Zeros of Hermite Polynomials and Hermite Functions

These routines calculate the s-th zero of the Hermite polynomial/function of order n. Since the zeros are symmetrical around zero, only positive zeros are calculated, ordered from smallest to largest, starting from index 1. Only for odd polynomial orders a zeroth zero exists, its value always being zero.

double **gsl_sf_hermite_zero**(const int n, const int s)

int **gsl_sf_hermite_zero_e**(const int n, const int s, *gsl_sf_result* *result)

These routines evaluate the `s`-th zero of the physicist Hermite polynomial $H_n(x)$ of order `n`.

double **gsl_sf_hermite_prob_zero**(const int n, const int s)

int **gsl_sf_hermite_prob_zero_e**(const int n, const int s, *gsl_sf_result* *result)

These routines evaluate the `s`-th zero of the probabilist Hermite polynomial $He_n(x)$ of order `n`.

double **gsl_sf_hermite_func_zero**(const int n, const int s)

int **gsl_sf_hermite_func_zero_e**(const int n, const int s, *gsl_sf_result* *result)

These routines evaluate the `s`-th zero of the Hermite function $\psi_n(x)$ of order `n`.

7.22 Hypergeometric Functions

Hypergeometric functions are described in Abramowitz & Stegun, Chapters 13 and 15. These functions are declared in the header file `gsl_sf_hyperg.h`.

double **gsl_sf_hyperg_0F1**(double c, double x)

int **gsl_sf_hyperg_0F1_e**(double c, double x, *gsl_sf_result* *result)

These routines compute the hypergeometric function

$$ {}_0F_1(c,x) $$

double **gsl_sf_hyperg_1F1_int**(int m, int n, double x)

int **gsl_sf_hyperg_1F1_int_e**(int m, int n, double x, *gsl_sf_result* *result)

These routines compute the confluent hypergeometric function

$$ {}_1F_1(m,n,x) = M(m,n,x) $$

for integer parameters `m`, `n`.

double **gsl_sf_hyperg_1F1**(double a, double b, double x)

int **gsl_sf_hyperg_1F1_e**(double a, double b, double x, *gsl_sf_result* *result)

These routines compute the confluent hypergeometric function

$$ {}_1F_1(a,b,x) = M(a,b,x) $$

for general parameters `a`, `b`.

double **gsl_sf_hyperg_U_int**(int m, int n, double x)

int **gsl_sf_hyperg_U_int_e**(int m, int n, double x, *gsl_sf_result* *result)
These routines compute the confluent hypergeometric function $U(m, n, x)$ for integer parameters `m`, `n`.

int **gsl_sf_hyperg_U_int_e10_e**(int m, int n, double x, *gsl_sf_result_e10* *result)
This routine computes the confluent hypergeometric function $U(m, n, x)$ for integer parameters `m`, `n` using the `gsl_sf_result_e10` type to return a result with extended range.

double **gsl_sf_hyperg_U**(double a, double b, double x)

int **gsl_sf_hyperg_U_e**(double a, double b, double x, *gsl_sf_result* *result)
These routines compute the confluent hypergeometric function $U(a, b, x)$.

int **gsl_sf_hyperg_U_e10_e**(double a, double b, double x, *gsl_sf_result_e10* *result)
This routine computes the confluent hypergeometric function $U(a, b, x)$ using the `gsl_sf_result_e10` type to return a result with extended range.

double **gsl_sf_hyperg_2F1**(double a, double b, double c, double x)

int **gsl_sf_hyperg_2F1_e**(double a, double b, double c, double x, *gsl_sf_result* *result)
These routines compute the Gauss hypergeometric function

$$ {}_2F_1(a, b, c, x) = F(a, b, c, x) $$

for $|x| < 1$. If the arguments (a, b, c, x) are too close to a singularity then the function can return the error code `GSL_EMAXITER` when the series approximation converges too slowly. This occurs in the region of $x = 1$, $c - a - b = m$ for integer m.

double **gsl_sf_hyperg_2F1_conj**(double aR, double aI, double c, double x)

int **gsl_sf_hyperg_2F1_conj_e**(double aR, double aI, double c, double x, *gsl_sf_result* *result)
These routines compute the Gauss hypergeometric function

$$ {}_2F_1(a_R + ia_I, aR - iaI, c, x) $$

with complex parameters for $|x| < 1$.

double **gsl_sf_hyperg_2F1_renorm**(double a, double b, double c, double x)

int **gsl_sf_hyperg_2F1_renorm_e**(double a, double b, double c, double x, *gsl_sf_result* *result)
These routines compute the renormalized Gauss hypergeometric function

$$ {}_2F_1(a, b, c, x)/\Gamma(c) $$

for $|x| < 1$.

double **gsl_sf_hyperg_2F1_conj_renorm**(double aR, double aI, double c, double x)

int **gsl_sf_hyperg_2F1_conj_renorm_e**(double aR, double aI, double c, double x, *gsl_sf_result* *result)
These routines compute the renormalized Gauss hypergeometric function

$$ {}_2F_1(a_R + ia_I, a_R - ia_I, c, x)/\Gamma(c) $$

for $|x| < 1$.

double **gsl_sf_hyperg_2F0**(double a, double b, double x) int **gsl_sf_hyperg_2F0_e**(double a, double b, double x, *gsl_sf_result* *result)

These routines compute the hypergeometric function

$$ {}_2F_0(a,b,x) $$

The series representation is a divergent hypergeometric series. However, for $x < 0$ we have

$$ {}_2F_0(a,b,x) = (-1/x)^a U(a, 1+a-b, -1/x) $$

7.23 Laguerre Functions

The generalized Laguerre polynomials, sometimes referred to as associated Laguerre polynomials, are defined in terms of confluent hypergeometric functions as

$$ L^a_n(x) = \frac{(a+1)_n}{n!} {}_1F_1(-n, a+1, x) $$

where $(a)_n$ is the *Pochhammer symbol* (rising factorial). They are related to the plain Laguerre polynomials $L_n(x)$ by $L^0_n(x) = L_n(x)$ and $L^k_n(x) = (-1)^k (d^k/dx^k) L_{(n+k)}(x)$ For more information see Abramowitz & Stegun, Chapter 22.

The functions described in this section are declared in the header file `gsl_sf_laguerre.h`.

double **gsl_sf_laguerre_1**(double a, double x)

double **gsl_sf_laguerre_2**(double a, double x)

double **gsl_sf_laguerre_3**(double a, double x)

int **gsl_sf_laguerre_1_e**(double a, double x, *gsl_sf_result* *result)

int **gsl_sf_laguerre_2_e**(double a, double x, *gsl_sf_result* *result)

int **gsl_sf_laguerre_3_e**(double a, double x, *gsl_sf_result* *result)

These routines evaluate the generalized Laguerre polynomials $L^a_1(x)$, $L^a_2(x)$, $L^a_3(x)$ using explicit representations.

double **gsl_sf_laguerre_n**(const int n, const double a, const double x)

int **gsl_sf_laguerre_n_e**(int n, double a, double x, *gsl_sf_result* *result)

These routines evaluate the generalized Laguerre polynomials $L^a_n(x)$ for $a > -1$, $n \geq 0$.

7.24 Lambert W Functions

Lambert's W functions, $W(x)$, are defined to be solutions of the equation $W(x)\exp(W(x)) = x$. This function has multiple branches for $x < 0$; however, it has only two real-valued branches. We define $W_0(x)$ to be the principal branch, where $W > -1$ for $x < 0$, and $W_{-1}(x)$ to be the other real branch, where $W < -1$ for $x < 0$. The Lambert functions are declared in the header file `gsl_sf_lambert.h`.

double **gsl_sf_lambert_W0**(double x)

int **gsl_sf_lambert_W0_e**(double x, *gsl_sf_result* *result)

These compute the principal branch of the Lambert W function, $W_0(x)$.

double **gsl_sf_lambert_Wm1**(double x)

int **gsl_sf_lambert_Wm1_e**(double x, *gsl_sf_result* *result)

These compute the secondary real-valued branch of the Lambert W function, $W_{-1}(x)$.

7.25 Legendre Functions and Spherical Harmonics

The Legendre Functions and Legendre Polynomials are described in Abramowitz & Stegun, Chapter 8. These functions are declared in the header file `gsl_sf_legendre.h`.

7.25.1 Legendre Polynomials

double **gsl_sf_legendre_P1**(double x)

double **gsl_sf_legendre_P2**(double x)

double **gsl_sf_legendre_P3**(double x)

int **gsl_sf_legendre_P1_e**(double x, *gsl_sf_result* *result)

int **gsl_sf_legendre_P2_e**(double x, *gsl_sf_result* *result)

int **gsl_sf_legendre_P3_e**(double x, *gsl_sf_result* *result)

These functions evaluate the Legendre polynomials $P_l(x)$ using explicit representations for $l = 1, 2, 3$.

double **gsl_sf_legendre_Pl**(int l, double x)

int **gsl_sf_legendre_Pl_e**(int l, double x, *gsl_sf_result* *result)

These functions evaluate the Legendre polynomial $P_l(x)$ for a specific value of `l`, `x` subject to $l \geq 0$ and $|x| \leq 1$.

int **gsl_sf_legendre_Pl_array**(int lmax, double x, double result_array[])

int **gsl_sf_legendre_Pl_deriv_array**(int lmax, double x, double result_array[], double result_deriv_array[])

These functions compute arrays of Legendre polynomials $P_l(x)$ and derivatives $dP_l(x)/dx$ for $l = 0, \dots, lmax$ and $|x| \leq 1$.

double **gsl_sf_legendre_Q0**(double x)

int **gsl_sf_legendre_Q0_e**(double x, *gsl_sf_result* *result)

These routines compute the Legendre function $Q_0(x)$ for $x > -1$ and $x \neq 1$.

double **gsl_sf_legendre_Q1**(double x)

int **gsl_sf_legendre_Q1_e**(double x, *gsl_sf_result* *result)

These routines compute the Legendre function $Q_1(x)$ for $x > -1$ and $x \neq 1$.

double **gsl_sf_legendre_Ql**(int l, double x) int **gsl_sf_legendre_Ql_e**(int l, double x, *gsl_sf_result* *result)

These routines compute the Legendre function $Q_l(x)$ for $x > -1$, $x \neq 1$ and $l \geq 0$.

7.25.2 Associated Legendre Polynomials and Spherical Harmonics

The following functions compute the associated Legendre polynomials $P_l^m(x)$ which are solutions of the differential equation

$$(1-x^2)\frac{d^2}{dx^2}P_l^m(x) - 2x\frac{d}{dx}P_l^m(x) + \left(l(l+1) - \frac{m^2}{1-x^2}\right)P_l^m(x) = 0$$

where the degree l and order m satisfy $0 \leq l$ and $0 \leq m \leq l$. The functions $P_l^m(x)$ grow combinatorially with l and can overflow for l larger than about 150. Alternatively, one may calculate normalized associated Legendre polynomials. There are a number of different normalization conventions, and these functions can be stably computed up to degree and order 2700. The following normalizations are provided:

- Schmidt semi-normalization

  Schmidt semi-normalized associated Legendre polynomials are often used in the magnetics community and are defined as

  $$S_l^0(x) = P_l^0(x)$$
  $$S_l^m(x) = (-1)^m\sqrt{2\frac{(l-m)!}{(l+m)!}}P_l^m(x), m > 0$$

  The factor of $(-1)^m$ is called the Condon-Shortley phase factor and can be excluded if desired by setting the parameter `csphase = 1` in the functions below.

- Spherical Harmonic Normalization

  The associated Legendre polynomials suitable for calculating spherical harmonics are defined as

  $$Y_l^m(x) = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(x)$$

  where again the phase factor $(-1)^m$ can be included or excluded if desired.

- Full Normalization

  The fully normalized associated Legendre polynomials are defined as

  $$N_l^m(x) = (-1)^m\sqrt{(l+\frac{1}{2})\frac{(l-m)!}{(l+m)!}}P_l^m(x)$$

  and have the property

  $$\int_{-1}^{1} N_l^m(x)^2 dx = 1$$

The normalized associated Legendre routines below use a recurrence relation which is stable up to a degree and order of about 2700. Beyond this, the computed functions could suffer from underflow leading to incorrect results. Routines are provided to compute first and second derivatives $dP_l^m(x)/dx$ and $d^2P_l^m(x)/dx^2$ as well as their alternate versions $dP_l^m(\cos\theta)/d\theta$ and $d^2P_l^m(\cos\theta)/d\theta^2$. While there is a simple scaling relationship between the two forms, the derivatives involving θ are heavily used in spherical harmonic expansions and so these routines are also provided.

In the functions below, a parameter of type `gsl_sf_legendre_t` specifies the type of normalization to use. The possible values are type **gsl_sf_legendre_t**

Value	Description
GSL_SF_LEGENDRE_NONE	The unnormalized associated Legendre polynomials $P_l^m(x)$
GSL_SF_LEGENDRE_SCHMIDT	The Schmidt semi-normalized associated Legendre polynomials $S_l^m(x)$
GSL_SF_LEGENDRE_SPHARM	The spherical harmonic associated Legendre polynomials $Y_l^m(x)$
GSL_SF_LEGENDRE_FULL	The fully normalized associated Legendre polynomials $N_l^m(x)$

int **gsl_sf_legendre_array**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, double result_array[])

int **gsl_sf_legendre_array_e**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, const double csphase, double result_array[])

These functions calculate all normalized associated Legendre polynomials for $0 \leq l \leq lmax$ and $0 \leq m \leq l$ for $|x| \leq 1$. The `norm` parameter specifies which normalization is used. The normalized $P_l^m(x)$ values are stored in `result_array`, whose minimum size can be obtained from calling `gsl_sf_legendre_array_n()`. The array index of $P_l^m(x)$ is obtained from calling `gsl_sf_legendre_array_index(l, m)`. To include or exclude the Condon-Shortley phase factor of $(-1)^m$, set the parameter `csphase` to either -1 or 1 respectively in the `_e` function. This factor is excluded by default.

int **gsl_sf_legendre_deriv_array**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, double result_array[], double result_deriv_array[])

int **gsl_sf_legendre_deriv_array_e**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, const double csphase, double result_array[], double result_deriv_array[])

These functions calculate all normalized associated Legendre functions and their first derivatives up to degree `lmax` for $|x| < 1$. The parameter `norm` specifies the normalization used. The normalized $P_l^m(x)$ values and their derivatives $dP_l^m(x)/dx$ are stored in `result_array` and `result_deriv_array` respectively. To include or exclude the Condon-Shortley phase factor of $(-1)^m$, set the parameter `csphase` to either -1 or 1 respectively in the `_e` function. This factor is excluded by default.

int **gsl_sf_legendre_deriv_alt_array**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, double result_array[], double result_deriv_array[])

int **gsl_sf_legendre_deriv_alt_array_e**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, const double csphase, double result_array[], double result_deriv_array[])

These functions calculate all normalized associated Legendre functions and their (alternate) first derivatives up to degree `lmax` for $|x| < 1$. The normalized $P_l^m(x)$ values and their derivatives $dP_l^m(\cos\theta)/d\theta$ are stored in `result_array` and `result_deriv_array` respectively. To include or exclude the Condon-Shortley phase factor of $(-1)^m$, set the parameter `csphase` to either -1 or 1 respectively in the `_e` function. This factor is excluded by default.

int **gsl_sf_legendre_deriv2_array**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, double result_array[], double result_deriv_array[], double result_deriv2_array[])

int **gsl_sf_legendre_deriv2_array_e**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, const double csphase, double result_array[], double result_deriv_array[], double result_deriv2_array[])

These functions calculate all normalized associated Legendre functions and their first and second derivatives up to degree `lmax` for $|x| < 1$. The parameter `norm` specifies the normalization used. The normalized $P_l^m(x)$, their first derivatives $dP_l^m(x)/dx$, and their second derivatives $d^2P_l^m(x)/dx^2$ are stored in `result_array`, `result_deriv_array`, and `result_deriv2_array` respectively. To include or exclude the Condon-Shortley phase factor of $(-1)^m$, set the parameter `csphase` to either -1 or 1 respectively in the `_e` function. This factor is excluded by default.

int **gsl_sf_legendre_deriv2_alt_array**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, double result_array[], double result_deriv_array[], double result_deriv2_array[])

int **gsl_sf_legendre_deriv2_alt_array_e**(const *gsl_sf_legendre_t* norm, const size_t lmax, const double x, const double csphase, double result_array[], double result_deriv_array[], double result_deriv2_array[])

These functions calculate all normalized associated Legendre functions and their (alternate) first and second derivatives up to degree `lmax` for $|x| < 1$. The parameter `norm` specifies the normalization used. The normalized $P_l^m(x)$, their first derivatives $dP_l^m(\cos\theta)/d\theta$, and their second derivatives $d^2P_l^m(\cos\theta)/d\theta^2$ are stored in `result_array`, `result_deriv_array`, and `result_deriv2_array` respectively. To include or exclude the Condon-Shortley phase factor of $(-1)^m$, set the parameter `csphase` to either -1 or 1 respectively in the `_e` function. This factor is excluded by default.

size_t **gsl_sf_legendre_nlm**(const size_t lmax)

This function returns the total number of associated Legendre functions $P_l^m(x)$ for a given `lmax`. The number is `(lmax+1) * (lmax+2) / 2`.

size_t **gsl_sf_legendre_array_n**(const size_t lmax)

This function returns the minimum array size for maximum degree `lmax` needed for the array versions of the associated Legendre functions. Size is calculated as the total number of $P_l^m(x)$ functions (see `gsl_sf_legendre_nlm()`), plus extra space for precomputing multiplicative factors used in the recurrence relations.

size_t **gsl_sf_legendre_array_index**(const size_t l, const size_t m)

This function returns the index into `result_array`, `result_deriv_array`, or `result_deriv2_array` corresponding to $P_l^m(x)$, $P_l^{'m}(x)$, or $P_l^{''m}(x)$. The index is given by $l(l+1)/2 + m$.

An inline version of this function is used if `HAVE_INLINE` is defined.

double **gsl_sf_legendre_Plm**(int l, int m, double x)

int **gsl_sf_legendre_Plm_e**(int l, int m, double x, *gsl_sf_result* *result)

These routines compute the associated Legendre polynomial $P_l^m(x)$ for $m \geq 0$, $l \geq m$, and $|x| \leq 1$.

double **gsl_sf_legendre_sphPlm**(int l, int m, double x)

int **gsl_sf_legendre_sphPlm_e**(int l, int m, double x, *gsl_sf_result* *result)

These routines compute the normalized associated Legendre polynomial $\sqrt{(2l+1)/(4\pi)}\sqrt{(l-m)!/(l+m)!}P_l^m(x)$ suitable for use in spherical harmonics. The parameters must satisfy $m \geq 0$, $l \geq m$, and $|x| \leq 1$. These routines avoid the overflows that occur for the standard normalization of $P_l^m(x)$.

int **gsl_sf_legendre_Plm_array**(int lmax, int m, double x, double result_array[])

int **gsl_sf_legendre_Plm_deriv_array**(int lmax, int m, double x, double result_array[], double result_deriv_array[])

These functions are now deprecated and will be removed in a future release; see `gsl_sf_legendre_array()` and `gsl_sf_legendre_deriv_array()`.

int **gsl_sf_legendre_sphPlm_array**(int lmax, int m, double x, double result_array[])

int **gsl_sf_legendre_sphPlm_deriv_array**(int lmax, int m, double x, double result_array[], double result_deriv_array[])

These functions are now deprecated and will be removed in a future release; see *gsl_sf_legendre_array()* and *gsl_sf_legendre_deriv_array()*.

int **gsl_sf_legendre_array_size**(const int lmax, const int m)

This function is now deprecated and will be removed in a future release.

7.25.3 Conical Functions

The Conical Functions $P^{\mu}_{-(1/2)+i\lambda}(x)$ and $Q^{\mu}_{-(1/2)+i\lambda}$ are described in Abramowitz & Stegun, Section 8.12.

double **gsl_sf_conicalP_half**(double lambda, double x)

int **gsl_sf_conicalP_half_e**(double lambda, double x, *gsl_sf_result* *result)

These routines compute the irregular Spherical Conical Function $P^{1/2}_{-1/2+i\lambda}(x)$ for $x > -1$.

double **gsl_sf_conicalP_mhalf**(double lambda, double x)

int **gsl_sf_conicalP_mhalf_e**(double lambda, double x, *gsl_sf_result* *result)

These routines compute the regular Spherical Conical Function $P^{-1/2}_{-1/2+i\lambda}(x)$ for $x > -1$.

double **gsl_sf_conicalP_0**(double lambda, double x)

int **gsl_sf_conicalP_0_e**(double lambda, double x, *gsl_sf_result* *result)

These routines compute the conical function $P^{0}_{-1/2+i\lambda}(x)$ for $x > -1$.

double **gsl_sf_conicalP_1**(double lambda, double x)

int **gsl_sf_conicalP_1_e**(double lambda, double x, *gsl_sf_result* *result)

These routines compute the conical function $P^{1}_{-1/2+i\lambda}(x)$ for $x > -1$.

double **gsl_sf_conicalP_sph_reg**(int l, double lambda, double x)

int **gsl_sf_conicalP_sph_reg_e**(int l, double lambda, double x, *gsl_sf_result* *result)

These routines compute the Regular Spherical Conical Function $P^{-1/2-l}_{-1/2+i\lambda}(x)$ for $x > -1$ and $l \geq -1$.

double **gsl_sf_conicalP_cyl_reg**(int m, double lambda, double x)

int **gsl_sf_conicalP_cyl_reg_e**(int m, double lambda, double x, *gsl_sf_result* *result)

These routines compute the Regular Cylindrical Conical Function $P^{-m}_{-1/2+i\lambda}(x)$ for $x > -1$ and $m \geq -1$.

7.25.4 Radial Functions for Hyperbolic Space

The following spherical functions are specializations of Legendre functions which give the regular eigenfunctions of the Laplacian on a 3-dimensional hyperbolic space H^3. Of particular interest is the flat limit, $\lambda \to \infty$, $\eta \to 0$, $\lambda\eta$ fixed.

double **gsl_sf_legendre_H3d_0**(double lambda, double eta) int **gsl_sf_legendre_H3d_0_e**(double lambda, double eta, *gsl_sf_result* *result)

These routines compute the zeroth radial eigenfunction of the Laplacian on the 3-dimensional hyperbolic space,

$$L^{H3d}_0(\lambda,\eta) := \frac{\sin(\lambda\eta)}{\lambda\sinh(\eta)}$$

for $\eta \geq 0$. In the flat limit this takes the form $L^{H3d}_0(\lambda,\eta) = j_0(\lambda\eta)$.

double **gsl_sf_legendre_H3d_1**(double lambda, double eta)

int **gsl_sf_legendre_H3d_1_e**(double lambda, double eta, *gsl_sf_result* *result)

These routines compute the first radial eigenfunction of the Laplacian on the 3-dimensional hyperbolic space,

$$L^{H3d}_1(\lambda,\eta) := \frac{1}{\sqrt{\lambda^2+1}}\left(\frac{\sin(\lambda\eta)}{\lambda\sinh(\eta)}\right)(\coth(\eta) - \lambda\cot(\lambda\eta))$$

for $\eta \geq 0$ In the flat limit this takes the form $L^{H3d}_1(\lambda,\eta) = j_1(\lambda\eta)$.

double **gsl_sf_legendre_H3d**(int l, double lambda, double eta)

int **gsl_sf_legendre_H3d_e**(int l, double lambda, double eta, *gsl_sf_result* *result)

These routines compute the `l`-th radial eigenfunction of the Laplacian on the 3-dimensional hyperbolic space $\eta \geq 0$ and $l \geq 0$. In the flat limit this takes the form $L^{H3d}_l(\lambda,\eta) = j_l(\lambda\eta)$.

int **gsl_sf_legendre_H3d_array**(int lmax, double lambda, double eta, double result_array[])

This function computes an array of radial eigenfunctions $L^{H3d}_l(\lambda,\eta)$ for $0 \leq l \leq lmax$.

7.26 Logarithm and Related Functions

Information on the properties of the Logarithm function can be found in Abramowitz & Stegun, Chapter 4. The functions described in this section are declared in the header file `gsl_sf_log.h`.

double **gsl_sf_log**(double x)

int **gsl_sf_log_e**(double x, *gsl_sf_result* *result)

These routines compute the logarithm of `x`, $\log(x)$, for $x > 0$.

double **gsl_sf_log_abs**(double x)

int **gsl_sf_log_abs_e**(double x, *gsl_sf_result* *result)

These routines compute the logarithm of the magnitude of `x`, $\log(|x|)$, for $x \neq 0$.

int **gsl_sf_complex_log_e**(double zr, double zi, *gsl_sf_result* *lnr, *gsl_sf_result* *theta)

This routine computes the complex logarithm of $z = z_r + iz_i$. The results are returned as `lnr`, `theta` such that $\exp(lnr + i\theta) = z_r + iz_i$, where θ lies in the range $[-\pi, \pi]$.

double **gsl_sf_log_1plusx**(double x)

int **gsl_sf_log_1plusx_e**(double x, *gsl_sf_result* *result)

These routines compute $\log(1 + x)$ for $x > -1$ using an algorithm that is accurate for small `x`.

double **gsl_sf_log_1plusx_mx**(double x)

int **gsl_sf_log_1plusx_mx_e**(double x, *gsl_sf_result* *result)

These routines compute $\log(1 + x) - x$ for $x > -1$ using an algorithm that is accurate for small `x`.

7.27 Mathieu Functions

The routines described in this section compute the angular and radial Mathieu functions, and their characteristic values. Mathieu functions are the solutions of the following two differential equations:

$$\frac{d^2y}{dv^2} + (a - 2q\cos 2v)y = 0$$
$$\frac{d^2f}{du^2} - (a - 2q\cosh 2u)f = 0$$

The angular Mathieu functions $ce_r(x,q)$, $se_r(x,q)$ are the even and odd periodic solutions of the first equation, which is known as Mathieu's equation. These exist only for the discrete sequence of characteristic values $a = a_r(q)$ (even-periodic) and $a = b_r(q)$ (odd-periodic).

The radial Mathieu functions $Mc_r^{(j)}(z,q)$ and $Ms_r^{(j)}(z,q)$ are the solutions of the second equation, which is referred to as Mathieu's modified equation. The radial Mathieu functions of the first, second, third and fourth kind are denoted by the parameter j, which takes the value 1, 2, 3 or 4.

For more information on the Mathieu functions, see Abramowitz and Stegun, Chapter 20. These functions are defined in the header file `gsl_sf_mathieu.h`.

7.27.1 Mathieu Function Workspace

The Mathieu functions can be computed for a single order or for multiple orders, using array-based routines. The array-based routines require a preallocated workspace.

type **gsl_sf_mathieu_workspace**

Workspace required for array-based routines

gsl_sf_mathieu_workspace ***gsl_sf_mathieu_alloc**(size_t n, double qmax)

This function returns a workspace for the array versions of the Mathieu routines. The arguments n and `qmax` specify the maximum order and q-value of Mathieu functions which can be computed with this workspace.

void **gsl_sf_mathieu_free**(*gsl_sf_mathieu_workspace* *work)

This function frees the workspace `work`.

7.27.2 Mathieu Function Characteristic Values

int **gsl_sf_mathieu_a**(int n, double q)

int **gsl_sf_mathieu_a_e**(int n, double q, *gsl_sf_result* *result)

int **gsl_sf_mathieu_b**(int n, double q)

int **gsl_sf_mathieu_b_e**(int n, double q, *gsl_sf_result* *result)

These routines compute the characteristic values $a_n(q)$, $b_n(q)$ of the Mathieu functions $ce_n(q,x)$ and $se_n(q,x)$, respectively.

int **gsl_sf_mathieu_a_array**(int order_min, int order_max, double q, *gsl_sf_mathieu_workspace* *work, double result_array[])

int **gsl_sf_mathieu_b_array**(int order_min, int order_max, double q, *gsl_sf_mathieu_workspace* *work, double result_array[])

These routines compute a series of Mathieu characteristic values $a_n(q)$, $b_n(q)$ for n from `order_min` to `order_max` inclusive, storing the results in the array `result_array`.

7.27.3 Angular Mathieu Functions

int **gsl_sf_mathieu_ce**(int n, double q, double x)

int **gsl_sf_mathieu_ce_e**(int n, double q, double x, *gsl_sf_result* *result)

int **gsl_sf_mathieu_se**(int n, double q, double x)

int **gsl_sf_mathieu_se_e**(int n, double q, double x, *gsl_sf_result* *result)

These routines compute the angular Mathieu functions $ce_n(q, x)$ and $se_n(q, x)$, respectively.

int **gsl_sf_mathieu_ce_array**(int nmin, int nmax, double q, double x, *gsl_sf_mathieu_workspace* *work, double result_array[])

int **gsl_sf_mathieu_se_array**(int nmin, int nmax, double q, double x, *gsl_sf_mathieu_workspace* *work, double result_array[])

These routines compute a series of the angular Mathieu functions $ce_n(q, x)$ and $se_n(q, x)$ of order n from `nmin` to `nmax` inclusive, storing the results in the array `result_array`.

7.27.4 Radial Mathieu Functions

int **gsl_sf_mathieu_Mc**(int j, int n, double q, double x)

int **gsl_sf_mathieu_Mc_e**(int j, int n, double q, double x, *gsl_sf_result* *result)

int **gsl_sf_mathieu_Ms**(int j, int n, double q, double x)

int **gsl_sf_mathieu_Ms_e**(int j, int n, double q, double x, *gsl_sf_result* *result)

These routines compute the radial `j`-th kind Mathieu functions $Mc_n^{(j)}(q, x)$ and $Ms_n^{(j)}(q, x)$ of order `n`.

The allowed values of `j` are 1 and 2. The functions for $j = 3, 4$ can be computed as $M_n^{(3)} = M_n^{(1)} + iM_n^{(2)}$ and $M_n^{(4)} = M_n^{(1)} - iM_n^{(2)}$, where $M_n^{(j)} = Mc_n^{(j)}$ or $Ms_n^{(j)}$.

int **gsl_sf_mathieu_Mc_array**(int j, int nmin, int nmax, double q, double x, *gsl_sf_mathieu_workspace* *work, double result_array[])

int **gsl_sf_mathieu_Ms_array**(int j, int nmin, int nmax, double q, double x, *gsl_sf_mathieu_workspace* *work, double result_array[])

These routines compute a series of the radial Mathieu functions of kind `j`, with order from `nmin` to `nmax` inclusive, storing the results in the array `result_array`.

7.28 Power Function

The following functions are equivalent to the function `gsl_pow_int()` with an error estimate. These functions are declared in the header file `gsl_sf_pow_int.h`.

double **gsl_sf_pow_int**(double x, int n) int **gsl_sf_pow_int_e**(double x, int n, *gsl_sf_result* *result)

These routines compute the power x^n for integer `n`. The power is computed using the minimum number of multiplications. For example, x^8 is computed as $((x^2)^2)^2$, requiring only 3 multiplications. For reasons of efficiency, these functions do not check for overflow or underflow conditions. The following is a simple example:

```
#include <gsl/gsl_sf_pow_int.h>
/* compute 3.0**12 */
double y = gsl_sf_pow_int(3.0, 12);
```

7.29 Psi (Digamma) Function

The polygamma functions of order n are defined by

$$\psi^{(n)}(x) = \left(\frac{d}{dx}\right)^n \psi(x) = \left(\frac{d}{dx}\right)^{n+1} \log(\Gamma(x))$$

where $\psi(x) = \Gamma'(x)/\Gamma(x)$ is known as the digamma function. These functions are declared in the header file `gsl_sf_psi.h`.

7.29.1 Digamma Function

double **gsl_sf_psi_int**(int n)

int **gsl_sf_psi_int_e**(int n, *gsl_sf_result* *result)

These routines compute the digamma function $\psi(n)$ for positive integer `n`. The digamma function is also called the Psi function.

double **gsl_sf_psi**(double x)

int **gsl_sf_psi_e**(double x, *gsl_sf_result* *result)

These routines compute the digamma function $\psi(x)$ for general `x`, $x \neq 0$.

double **gsl_sf_psi_1piy**(double y)

int **gsl_sf_psi_1piy_e**(double y, *gsl_sf_result* *result)

These routines compute the real part of the digamma function on the line $1 + iy$, $\Re[\psi(1 + iy)]$.

7.29.2 Trigamma Function

double **gsl_sf_psi_1_int**(int n)

int **gsl_sf_psi_1_int_e**(int n, *gsl_sf_result* *result)

These routines compute the Trigamma function $\psi'(n)$ for positive integer n.

double **gsl_sf_psi_1**(double x)

int **gsl_sf_psi_1_e**(double x, *gsl_sf_result* *result)

These routines compute the Trigamma function $\psi'(x)$ for general `x`.

7.29.3 Polygamma Function

double **gsl_sf_psi_n**(int n, double x)

int **gsl_sf_psi_n_e**(int n, double x, *gsl_sf_result* *result)

These routines compute the polygamma function $\psi^{(n)}(x)$ for $n \geq 0$, $x > 0$.

7.30 Synchrotron Functions

The functions described in this section are declared in the header file `gsl_sf_synchrotron.h`.

double **gsl_sf_synchrotron_1**(double x)

int **gsl_sf_synchrotron_1_e**(double x, *gsl_sf_result* *result)

These routines compute the first synchrotron function $x \int_x^\infty dt K_{5/3}(t)$ for $x \geq 0$.

double **gsl_sf_synchrotron_2**(double x)

int **gsl_sf_synchrotron_2_e**(double x, *gsl_sf_result* *result)

These routines compute the second synchrotron function $x K_{2/3}(x)$ for $x \geq 0$.

7.31 Transport Functions

The transport functions $J(n, x)$ are defined by the integral representations

$$J(n, x) = \int_0^x t^n e^t / (e^t - 1)^2 dt$$

They are declared in the header file `gsl_sf_transport.h`.

double **gsl_sf_transport_2**(double x)

int **gsl_sf_transport_2_e**(double x, *gsl_sf_result* *result)

These routines compute the transport function $J(2, x)$.

double **gsl_sf_transport_3**(double x)

int **gsl_sf_transport_3_e**(double x, *gsl_sf_result* *result)

These routines compute the transport function $J(3, x)$.

double **gsl_sf_transport_4**(double x)

int **gsl_sf_transport_4_e**(double x, *gsl_sf_result* *result)

These routines compute the transport function $J(4, x)$.

double **gsl_sf_transport_5**(double x)

int **gsl_sf_transport_5_e**(double x, *gsl_sf_result* *result)

These routines compute the transport function $J(5, x)$.

7.32 Trigonometric Functions

The library includes its own trigonometric functions in order to provide consistency across platforms and reliable error estimates. These functions are declared in the header file `gsl_sf_trig.h`.

7.32.1 Circular Trigonometric Functions

double **`gsl_sf_sin`**(double x)

int **`gsl_sf_sin_e`**(double x, *gsl_sf_result* *result)
 These routines compute the sine function $\sin(x)$.

double **`gsl_sf_cos`**(double x)

int **`gsl_sf_cos_e`**(double x, *gsl_sf_result* *result)
 These routines compute the cosine function $\cos(x)$.

double **`gsl_sf_hypot`**(double x, double y)

int **`gsl_sf_hypot_e`**(double x, double y, *gsl_sf_result* *result)
 These routines compute the hypotenuse function $\sqrt{x^2 + y^2}$ avoiding overflow and underflow.

double **`gsl_sf_sinc`**(double x)

int **`gsl_sf_sinc_e`**(double x, *gsl_sf_result* *result)
 These routines compute $\mathrm{sinc}(x) = \sin(\pi x)/(\pi x)$ for any value of `x`.

7.32.2 Trigonometric Functions for Complex Arguments

int **`gsl_sf_complex_sin_e`**(double zr, double zi, *gsl_sf_result* *szr, *gsl_sf_result* *szi)
 This function computes the complex sine, $\sin(z_r + iz_i)$ storing the real and imaginary parts in `szr`, `szi`.

int **`gsl_sf_complex_cos_e`**(double zr, double zi, *gsl_sf_result* *czr, *gsl_sf_result* *czi)
 This function computes the complex cosine, $\cos(z_r + iz_i)$ storing the real and imaginary parts in `czr`, `czi`.

int **`gsl_sf_complex_logsin_e`**(double zr, double zi, *gsl_sf_result* *lszr, *gsl_sf_result* *lszi)
 This function computes the logarithm of the complex sine, $\log(\sin(z_r + iz_i))$ storing the real and imaginary parts in `lszr`, `lszi`.

7.32.3 Hyperbolic Trigonometric Functions

double **`gsl_sf_lnsinh`**(double x)

int **`gsl_sf_lnsinh_e`**(double x, *gsl_sf_result* *result)
 These routines compute $\log(\sinh(x))$ for $x > 0$.

double **`gsl_sf_lncosh`**(double x)

int **`gsl_sf_lncosh_e`**(double x, *gsl_sf_result* *result)
 These routines compute $\log(\cosh(x))$ for any `x`.

7.32.4 Conversion Functions

int **gsl_sf_polar_to_rect**(double r, double theta, *gsl_sf_result* *x, *gsl_sf_result* *y)

This function converts the polar coordinates (`r`, `theta`) to rectilinear coordinates (`x`, `y`), $x = r\cos(\theta)$, $y = r\sin(\theta)$.

int **gsl_sf_rect_to_polar**(double x, double y, *gsl_sf_result* *r, *gsl_sf_result* *theta)

This function converts the rectilinear coordinates (`x`, `y`) to polar coordinates (`r`, `theta`), such that $x = r\cos(\theta)$, $y = r\sin(\theta)$. The argument `theta` lies in the range $[-\pi, \pi]$.

7.32.5 Restriction Functions

double **gsl_sf_angle_restrict_symm**(double theta)

int **gsl_sf_angle_restrict_symm_e**(double *theta)

These routines force the angle `theta` to lie in the range $(-\pi, \pi]$.

Note that the mathematical value of π is slightly greater than `M_PI`, so the machine numbers `M_PI` and `-M_PI` are included in the range.

double **gsl_sf_angle_restrict_pos**(double theta)

int **gsl_sf_angle_restrict_pos_e**(double *theta)

These routines force the angle `theta` to lie in the range $[0, 2\pi)$.

Note that the mathematical value of 2π is slightly greater than `2*M_PI`, so the machine number `2*M_PI` is included in the range.

7.32.6 Trigonometric Functions With Error Estimates

int **gsl_sf_sin_err_e**(double x, double dx, *gsl_sf_result* *result)

This routine computes the sine of an angle `x` with an associated absolute error `dx`, $\sin(x \pm dx)$. Note that this function is provided in the error-handling form only since its purpose is to compute the propagated error.

int **gsl_sf_cos_err_e**(double x, double dx, *gsl_sf_result* *result)

This routine computes the cosine of an angle `x` with an associated absolute error `dx`, $\cos(x \pm dx)$. Note that this function is provided in the error-handling form only since its purpose is to compute the propagated error.

7.33 Zeta Functions

The Riemann zeta function is defined in Abramowitz & Stegun, Section 23.2. The functions described in this section are declared in the header file `gsl_sf_zeta.h`.

7.33.1 Riemann Zeta Function

The Riemann zeta function is defined by the infinite sum

$$\zeta(s) = \sum_{k=1}^{\infty} k^{-s}$$

double **gsl_sf_zeta_int**(int n)

int **gsl_sf_zeta_int_e**(int n, *gsl_sf_result* *result)

These routines compute the Riemann zeta function $\zeta(n)$ for integer `n`, $n \neq 1$.

double **gsl_sf_zeta**(double s)

int **gsl_sf_zeta_e**(double s, *gsl_sf_result* *result)

These routines compute the Riemann zeta function $\zeta(s)$ for arbitrary `s`, $s \neq 1$.

7.33.2 Riemann Zeta Function Minus One

For large positive argument, the Riemann zeta function approaches one. In this region the fractional part is interesting, and therefore we need a function to evaluate it explicitly.

double **gsl_sf_zetam1_int**(int n)

int **gsl_sf_zetam1_int_e**(int n, *gsl_sf_result* *result)

These routines compute $\zeta(n) - 1$ for integer `n`, $n \neq 1$.

double **gsl_sf_zetam1**(double s)

int **gsl_sf_zetam1_e**(double s, *gsl_sf_result* *result)

These routines compute $\zeta(s) - 1$ for arbitrary `s`, $s \neq 1$.

7.33.3 Hurwitz Zeta Function

The Hurwitz zeta function is defined by

$$\zeta(s, q) = \sum_{0}^{\infty} (k + q)^{-s}$$

double **gsl_sf_hzeta**(double s, double q)

int **gsl_sf_hzeta_e**(double s, double q, *gsl_sf_result* *result)

These routines compute the Hurwitz zeta function $\zeta(s, q)$ for $s > 1$, $q > 0$.

7.33.4 Eta Function

The eta function is defined by

$$\eta(s) = (1 - 2^{1-s})\zeta(s)$$

double **gsl_sf_eta_int**(int n)

int **gsl_sf_eta_int_e**(int n, *gsl_sf_result* *result)

These routines compute the eta function $\eta(n)$ for integer `n`.

double **gsl_sf_eta**(double s)

int **gsl_sf_eta_e**(double s, *gsl_sf_result* *result)

These routines compute the eta function $\eta(s)$ for arbitrary `s`.

7.34 Examples

The following example demonstrates the use of the error handling form of the special functions, in this case to compute the Bessel function $J_0(5.0)$,

```
#include <stdio.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_sf_bessel.h>

int
main (void)
{
  double x = 5.0;
  gsl_sf_result result;

  double expected = -0.17759677131433830434739701;

  int status = gsl_sf_bessel_J0_e (x, &result);

  printf ("status  = %s\n", gsl_strerror(status));
  printf ("J0(5.0) = %.18f\n"
          "      +/- % .18f\n",
          result.val, result.err);
  printf ("exact   = %.18f\n", expected);
  return status;
}
```

Here are the results of running the program,

```
status  = success
J0(5.0) = -0.177596771314338264
      +/-  0.000000000000000193
exact   = -0.177596771314338292
```

The next program computes the same quantity using the natural form of the function. In this case the error term `result.err` and return status are not accessible.

```
#include <stdio.h>
#include <gsl/gsl_sf_bessel.h>

int
main (void)
{
  double x = 5.0;
  double expected = -0.17759677131433830434739701;

  double y = gsl_sf_bessel_J0 (x);

  printf ("J0(5.0) = %.18f\n", y);
  printf ("exact   = %.18f\n", expected);
  return 0;
}
```

The results of the function are the same,

```
J0(5.0) = -0.177596771314338264
exact   = -0.177596771314338292
```

7.35 References and Further Reading

The library follows the conventions of the following book where possible,

- Handbook of Mathematical Functions, edited by Abramowitz & Stegun, Dover, ISBN 0486612724.

The following papers contain information on the algorithms used to compute the special functions,

- Allan J. MacLeod, MISCFUN: A software package to compute uncommon special functions. ACM Trans. Math. Soft., vol.: 22, 1996, 288–301
- Bunck, B. F., A fast algorithm for evaluation of normalized Hermite functions, BIT Numer. Math, 49: 281-295, 2009.
- G.N. Watson, A Treatise on the Theory of Bessel Functions, 2nd Edition (Cambridge University Press, 1944).
- G. Nemeth, Mathematical Approximations of Special Functions, Nova Science Publishers, ISBN 1-56072-052-2
- B.C. Carlson, Special Functions of Applied Mathematics (1977)
- N. M. Temme, Special Functions: An Introduction to the Classical Functions of Mathematical Physics (1996), ISBN 978-0471113133.
- W.J. Thompson, Atlas for Computing Mathematical Functions, John Wiley & Sons, New York (1997).
- Y.Y. Luke, Algorithms for the Computation of Mathematical Functions, Academic Press, New York (1977).
- S. A. Holmes and W. E. Featherstone, A unified approach to the Clenshaw summation and the recursive computation of very high degree and order normalised associated Legendre functions, Journal of Geodesy, 76, pg. 279-299, 2002.

CHAPTER

EIGHT

VECTORS AND MATRICES

The functions described in this chapter provide a simple vector and matrix interface to ordinary C arrays. The memory management of these arrays is implemented using a single underlying type, known as a block. By writing your functions in terms of vectors and matrices you can pass a single structure containing both data and dimensions as an argument without needing additional function parameters. The structures are compatible with the vector and matrix formats used by BLAS routines.

8.1 Data types

All the functions are available for each of the standard data-types. The versions for `double` have the prefix `gsl_block`, `gsl_vector` and `gsl_matrix`. Similarly the versions for single-precision `float` arrays have the prefix `gsl_block_float`, `gsl_vector_float` and `gsl_matrix_float`. The full list of available types is given below,

Prefix	Type
gsl_block	double
gsl_block_float	float
gsl_block_long_double	long double
gsl_block_int	int
gsl_block_uint	unsigned int
gsl_block_long	long
gsl_block_ulong	unsigned long
gsl_block_short	short
gsl_block_ushort	unsigned short
gsl_block_char	char
gsl_block_uchar	unsigned char
gsl_block_complex	complex double
gsl_block_complex_float	complex float
gsl_block_complex_long_double	complex long double

Corresponding types exist for the `gsl_vector` and `gsl_matrix` functions.

8.2 Blocks

For consistency all memory is allocated through a `gsl_block` structure. The structure contains two components, the size of an area of memory and a pointer to the memory. The `gsl_block` structure looks like this,

type **`gsl_block`**

```
typedef struct
{
  size_t size;
  double * data;
} gsl_block;
```

Vectors and matrices are made by *slicing* an underlying block. A slice is a set of elements formed from an initial offset and a combination of indices and step-sizes. In the case of a matrix the step-size for the column index represents the row-length. The step-size for a vector is known as the *stride*.

The functions for allocating and deallocating blocks are defined in `gsl_block.h`.

8.2.1 Block allocation

The functions for allocating memory to a block follow the style of `malloc` and `free`. In addition they also perform their own error checking. If there is insufficient memory available to allocate a block then the functions call the GSL error handler (with an error number of *`GSL_ENOMEM`*) in addition to returning a null pointer. Thus if you use the library error handler to abort your program then it isn't necessary to check every `alloc`.

gsl_block ***`gsl_block_alloc`**(size_t n)

This function allocates memory for a block of *`n`* double-precision elements, returning a pointer to the block struct. The block is not initialized and so the values of its elements are undefined. Use the function *`gsl_block_calloc()`* if you want to ensure that all the elements are initialized to zero.

Zero-sized requests are valid and return a non-null result. A null pointer is returned if insufficient memory is available to create the block.

gsl_block ***`gsl_block_calloc`**(size_t n)

This function allocates memory for a block and initializes all the elements of the block to zero.

void **`gsl_block_free`**(*gsl_block* *b)

This function frees the memory used by a block *`b`* previously allocated with *`gsl_block_alloc()`* or *`gsl_block_calloc()`*.

8.2.2 Reading and writing blocks

The library provides functions for reading and writing blocks to a file as binary data or formatted text.

int **`gsl_block_fwrite`**(FILE *stream, const *gsl_block* *b)

This function writes the elements of the block *`b`* to the stream *`stream`* in binary format. The return value is 0 for success and `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

int **`gsl_block_fread`**(FILE *stream, *gsl_block* *b)

This function reads into the block *`b`* from the open stream *`stream`* in binary format. The block *`b`* must be preallocated with the correct length since the function uses the size of *`b`* to determine how many bytes to read. The return value is 0 for success and `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

int **gsl_block_fprintf**(FILE *stream, const *gsl_block* *b, const char *format)

This function writes the elements of the block *b* line-by-line to the stream *stream* using the format specifier *format*, which should be one of the %g, %e or %f formats for floating point numbers and %d for integers. The function returns 0 for success and GSL_EFAILED if there was a problem writing to the file.

int **gsl_block_fscanf**(FILE *stream, *gsl_block* *b)

This function reads formatted data from the stream *stream* into the block *b*. The block *b* must be preallocated with the correct length since the function uses the size of *b* to determine how many numbers to read. The function returns 0 for success and GSL_EFAILED if there was a problem reading from the file.

8.2.3 Example programs for blocks

The following program shows how to allocate a block,

```
#include <stdio.h>
#include <gsl/gsl_block.h>

int
main (void)
{
  gsl_block * b = gsl_block_alloc (100);

  printf ("length of block = %zu\n", b->size);
  printf ("block data address = %p\n", b->data);

  gsl_block_free (b);
  return 0;
}
```

Here is the output from the program,

```
length of block = 100
block data address = 0x804b0d8
```

8.3 Vectors

Vectors are defined by a *gsl_vector* structure which describes a slice of a block. Different vectors can be created which point to the same block. A vector slice is a set of equally-spaced elements of an area of memory.

The *gsl_vector* structure contains five components, the *size*, the *stride*, a pointer to the memory where the elements are stored, data, a pointer to the block owned by the vector, block, if any, and an ownership flag, owner. The structure is very simple and looks like this,

type **gsl_vector**

```
typedef struct
{
  size_t size;
  size_t stride;
  double * data;
  gsl_block * block;
```

(continues on next page)

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```
  int owner;
} gsl_vector;
```

The `size` is simply the number of vector elements. The range of valid indices runs from 0 to `size-1`. The `stride` is the step-size from one element to the next in physical memory, measured in units of the appropriate datatype. The pointer `data` gives the location of the first element of the vector in memory. The pointer `block` stores the location of the memory block in which the vector elements are located (if any). If the vector owns this block then the `owner` field is set to one and the block will be deallocated when the vector is freed. If the vector points to a block owned by another object then the `owner` field is zero and any underlying block will not be deallocated with the vector.

The functions for allocating and accessing vectors are defined in `gsl_vector.h`.

8.3.1 Vector allocation

The functions for allocating memory to a vector follow the style of `malloc` and `free`. In addition they also perform their own error checking. If there is insufficient memory available to allocate a vector then the functions call the GSL error handler (with an error number of *`GSL_ENOMEM`*) in addition to returning a null pointer. Thus if you use the library error handler to abort your program then it isn't necessary to check every `alloc`.

gsl_vector ***gsl_vector_alloc**(size_t n)

This function creates a vector of length n, returning a pointer to a newly initialized vector struct. A new block is allocated for the elements of the vector, and stored in the `block` component of the vector struct. The block is "owned" by the vector, and will be deallocated when the vector is deallocated. Zero-sized requests are valid and return a non-null result.

gsl_vector ***gsl_vector_calloc**(size_t n)

This function allocates memory for a vector of length *`n`* and initializes all the elements of the vector to zero.

void **gsl_vector_free**(*gsl_vector* *v)

This function frees a previously allocated vector *`v`*. If the vector was created using *`gsl_vector_alloc()`* then the block underlying the vector will also be deallocated. If the vector has been created from another object then the memory is still owned by that object and will not be deallocated.

8.3.2 Accessing vector elements

Unlike Fortran compilers, C compilers do not usually provide support for range checking of vectors and matrices.[1] The functions *`gsl_vector_get()`* and *`gsl_vector_set()`* can perform portable range checking for you and report an error if you attempt to access elements outside the allowed range.

The functions for accessing the elements of a vector or matrix are defined in `gsl_vector.h` and declared `extern inline` to eliminate function-call overhead. You must compile your program with the preprocessor macro `HAVE_INLINE` defined to use these functions.

GSL_RANGE_CHECK_OFF

If necessary you can turn off range checking completely without modifying any source files by recompiling your program with the preprocessor definition *`GSL_RANGE_CHECK_OFF`*. Provided your compiler supports inline functions the effect of turning off range checking is to replace calls to `gsl_vector_get(v,i)` by `v->data[i*v->stride]` and calls to `gsl_vector_set(v,i,x)` by `v->data[i*v->stride]=x`. Thus there should be no performance penalty for using the range checking functions when range checking is turned off.

GSL_C99_INLINE

If you use a C99 compiler which requires inline functions in header files to be declared `inline` instead of `extern`

[1] Range checking is available in the GNU C Compiler bounds-checking extension, but it is not part of the default installation of GCC. Memory accesses can also be checked with Valgrind or the `gcc -fmudflap` memory protection option.

`inline`, define the macro *`GSL_C99_INLINE`* (see *Inline functions*). With GCC this is selected automatically when compiling in C99 mode (`-std=c99`).

int **`gsl_check_range`**

If inline functions are not used, calls to the functions *`gsl_vector_get()`* and *`gsl_vector_set()`* will link to the compiled versions of these functions in the library itself. The range checking in these functions is controlled by the global integer variable `gsl_check_range`. It is enabled by default—to disable it, set `gsl_check_range` to zero. Due to function-call overhead, there is less benefit in disabling range checking here than for inline functions.

double **`gsl_vector_get`**(const *gsl_vector* *v, const size_t i)

This function returns the *`i`*-th element of a vector *`v`*. If *`i`* lies outside the allowed range of 0 to `size - 1` then the error handler is invoked and 0 is returned. An inline version of this function is used when `HAVE_INLINE` is defined.

void **`gsl_vector_set`**(*gsl_vector* *v, const size_t i, double x)

This function sets the value of the *`i`*-th element of a vector *`v`* to *`x`*. If *`i`* lies outside the allowed range of 0 to `size - 1` then the error handler is invoked. An inline version of this function is used when `HAVE_INLINE` is defined.

double ***`gsl_vector_ptr`**(*gsl_vector* *v, size_t i)

const double ***`gsl_vector_const_ptr`**(const *gsl_vector* *v, size_t i)

These functions return a pointer to the *`i`*-th element of a vector *`v`*. If *`i`* lies outside the allowed range of 0 to `size - 1` then the error handler is invoked and a null pointer is returned. Inline versions of these functions are used when `HAVE_INLINE` is defined.

8.3.3 Initializing vector elements

void **`gsl_vector_set_all`**(*gsl_vector* *v, double x)

This function sets all the elements of the vector *`v`* to the value *`x`*.

void **`gsl_vector_set_zero`**(*gsl_vector* *v)

This function sets all the elements of the vector *`v`* to zero.

int **`gsl_vector_set_basis`**(*gsl_vector* *v, size_t i)

This function makes a basis vector by setting all the elements of the vector *`v`* to zero except for the *`i`*-th element which is set to one.

8.3.4 Reading and writing vectors

The library provides functions for reading and writing vectors to a file as binary data or formatted text.

int **`gsl_vector_fwrite`**(FILE *stream, const *gsl_vector* *v)

This function writes the elements of the vector *`v`* to the stream *`stream`* in binary format. The return value is 0 for success and `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

int **`gsl_vector_fread`**(FILE *stream, *gsl_vector* *v)

This function reads into the vector *`v`* from the open stream *`stream`* in binary format. The vector *`v`* must be preallocated with the correct length since the function uses the size of *`v`* to determine how many bytes to read. The return value is 0 for success and `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

int **`gsl_vector_fprintf`**(FILE *stream, const *gsl_vector* *v, const char *format)

This function writes the elements of the vector *`v`* line-by-line to the stream *`stream`* using the format specifier *`format`*, which should be one of the `%g`, `%e` or `%f` formats for floating point numbers and `%d` for integers. The function returns 0 for success and `GSL_EFAILED` if there was a problem writing to the file.

int **gsl_vector_fscanf**(FILE *stream, *gsl_vector* *v)

This function reads formatted data from the stream *stream* into the vector *v*. The vector *v* must be preallocated with the correct length since the function uses the size of *v* to determine how many numbers to read. The function returns 0 for success and `GSL_EFAILED` if there was a problem reading from the file.

8.3.5 Vector views

In addition to creating vectors from slices of blocks it is also possible to slice vectors and create vector views. For example, a subvector of another vector can be described with a view, or two views can be made which provide access to the even and odd elements of a vector.

type **gsl_vector_view**

type **gsl_vector_const_view**

A vector view is a temporary object, stored on the stack, which can be used to operate on a subset of vector elements. Vector views can be defined for both constant and non-constant vectors, using separate types that preserve constness. A vector view has the type *gsl_vector_view* and a constant vector view has the type *gsl_vector_const_view*. In both cases the elements of the view can be accessed as a *gsl_vector* using the `vector` component of the view object. A pointer to a vector of type `gsl_vector *` or `const gsl_vector *` can be obtained by taking the address of this component with the `&` operator.

When using this pointer it is important to ensure that the view itself remains in scope—the simplest way to do so is by always writing the pointer as `&view.vector`, and never storing this value in another variable.

gsl_vector_view **gsl_vector_subvector**(*gsl_vector* *v, size_t offset, size_t n)

gsl_vector_const_view **gsl_vector_const_subvector**(const *gsl_vector* *v, size_t offset, size_t n)

These functions return a vector view of a subvector of another vector *v*. The start of the new vector is offset by *offset* elements from the start of the original vector. The new vector has *n* elements. Mathematically, the `i`-th element of the new vector `v'` is given by:

```
v'(i) = v->data[(offset + i)*v->stride]
```

where the index `i` runs from 0 to `n - 1`.

The `data` pointer of the returned vector struct is set to null if the combined parameters (*offset*, *n*) overrun the end of the original vector.

The new vector is only a view of the block underlying the original vector, *v*. The block containing the elements of *v* is not owned by the new vector. When the view goes out of scope the original vector *v* and its block will continue to exist. The original memory can only be deallocated by freeing the original vector. Of course, the original vector should not be deallocated while the view is still in use.

The function *gsl_vector_const_subvector()* is equivalent to *gsl_vector_subvector()* but can be used for vectors which are declared `const`.

gsl_vector_view **gsl_vector_subvector_with_stride**(*gsl_vector* *v, size_t offset, size_t stride, size_t n)

gsl_vector_const_view **gsl_vector_const_subvector_with_stride**(const *gsl_vector* *v, size_t offset, size_t stride, size_t n)

These functions return a vector view of a subvector of another vector *v* with an additional stride argument. The subvector is formed in the same way as for *gsl_vector_subvector()* but the new vector has *n* elements with a step-size of *stride* from one element to the next in the original vector. Mathematically, the `i`-th element of the new vector `v'` is given by:

```
v'(i) = v->data[(offset + i*stride)*v->stride]
```

where the index `i` runs from 0 to `n - 1`.

Note that subvector views give direct access to the underlying elements of the original vector. For example, the following code will zero the even elements of the vector *v* of length `n`, while leaving the odd elements untouched:

```
gsl_vector_view v_even = gsl_vector_subvector_with_stride (v, 0, 2, n/2);
gsl_vector_set_zero (&v_even.vector);
```

A vector view can be passed to any subroutine which takes a vector argument just as a directly allocated vector would be, using `&view.vector`. For example, the following code computes the norm of the odd elements of *v* using the BLAS routine `dnrm2`:

```
gsl_vector_view v_odd = gsl_vector_subvector_with_stride (v, 1, 2, n/2);
double r = gsl_blas_dnrm2 (&v_odd.vector);
```

The function *gsl_vector_const_subvector_with_stride()* is equivalent to *gsl_vector_subvector_with_stride()* but can be used for vectors which are declared `const`.

gsl_vector_view **gsl_vector_complex_real**(gsl_vector_complex *v)

gsl_vector_const_view **gsl_vector_complex_const_real**(const gsl_vector_complex *v)

These functions return a vector view of the real parts of the complex vector *v*.

The function *gsl_vector_complex_const_real()* is equivalent to *gsl_vector_complex_real()* but can be used for vectors which are declared `const`.

gsl_vector_view **gsl_vector_complex_imag**(gsl_vector_complex *v)

gsl_vector_const_view **gsl_vector_complex_const_imag**(const gsl_vector_complex *v)

These functions return a vector view of the imaginary parts of the complex vector *v*.

The function *gsl_vector_complex_const_imag()* is equivalent to *gsl_vector_complex_imag()* but can be used for vectors which are declared `const`.

gsl_vector_view **gsl_vector_view_array**(double *base, size_t n)

gsl_vector_const_view **gsl_vector_const_view_array**(const double *base, size_t n)

These functions return a vector view of an array. The start of the new vector is given by *base* and has *n* elements. Mathematically, the `i`-th element of the new vector `v'` is given by:

```
v'(i) = base[i]
```

where the index `i` runs from 0 to `n - 1`.

The array containing the elements of `v` is not owned by the new vector view. When the view goes out of scope the original array will continue to exist. The original memory can only be deallocated by freeing the original pointer *base*. Of course, the original array should not be deallocated while the view is still in use.

The function *gsl_vector_const_view_array()* is equivalent to *gsl_vector_view_array()* but can be used for arrays which are declared `const`.

gsl_vector_view **gsl_vector_view_array_with_stride**(double *base, size_t stride, size_t n) *gsl_vector_const_view* **gsl_vector_const_view_array_with_stride**(const double *base, size_t stride, size_t n)

These functions return a vector view of an array `base` with an additional stride argument. The subvector is formed in the same way as for `gsl_vector_view_array()` but the new vector has `n` elements with a step-size of `stride` from one element to the next in the original array. Mathematically, the `i`-th element of the new vector `v'` is given by:

```
v'(i) = base[i*stride]
```

where the index `i` runs from 0 to `n - 1`.

Note that the view gives direct access to the underlying elements of the original array. A vector view can be passed to any subroutine which takes a vector argument just as a directly allocated vector would be, using `&view.vector`.

The function `gsl_vector_const_view_array_with_stride()` is equivalent to `gsl_vector_view_array_with_stride()` but can be used for arrays which are declared `const`.

8.3.6 Copying vectors

Common operations on vectors such as addition and multiplication are available in the BLAS part of the library (see *BLAS Support*). However, it is useful to have a small number of utility functions which do not require the full BLAS code. The following functions fall into this category.

int **gsl_vector_memcpy**(*gsl_vector* *dest, const *gsl_vector* *src)

This function copies the elements of the vector `src` into the vector `dest`. The two vectors must have the same length.

int **gsl_vector_swap**(*gsl_vector* *v, *gsl_vector* *w)

This function exchanges the elements of the vectors `v` and `w` by copying. The two vectors must have the same length.

8.3.7 Exchanging elements

The following functions can be used to exchange, or permute, the elements of a vector.

int **gsl_vector_swap_elements**(*gsl_vector* *v, size_t i, size_t j)

This function exchanges the `i`-th and `j`-th elements of the vector `v` in-place.

int **gsl_vector_reverse**(*gsl_vector* *v)

This function reverses the order of the elements of the vector `v`.

8.3.8 Vector operations

int **gsl_vector_add**(*gsl_vector* *a, const *gsl_vector* *b)

This function adds the elements of vector `b` to the elements of vector `a`. The result $a_i \leftarrow a_i + b_i$ is stored in `a` and `b` remains unchanged. The two vectors must have the same length.

int **gsl_vector_sub**(*gsl_vector* *a, const *gsl_vector* *b)

This function subtracts the elements of vector `b` from the elements of vector `a`. The result $a_i \leftarrow a_i - b_i$ is stored in `a` and `b` remains unchanged. The two vectors must have the same length.

int **gsl_vector_mul**(*gsl_vector* *a, const *gsl_vector* *b)

This function multiplies the elements of vector `a` by the elements of vector `b`. The result $a_i \leftarrow a_i * b_i$ is stored in `a` and `b` remains unchanged. The two vectors must have the same length.

int **gsl_vector_div**(*gsl_vector* *a, const *gsl_vector* *b)
This function divides the elements of vector `a` by the elements of vector `b`. The result $a_i \leftarrow a_i/b_i$ is stored in `a` and `b` remains unchanged. The two vectors must have the same length.

int **gsl_vector_scale**(*gsl_vector* *a, const double x)
This function multiplies the elements of vector `a` by the constant factor `x`. The result $a_i \leftarrow xa_i$ is stored in `a`.

int **gsl_vector_add_constant**(*gsl_vector* *a, const double x)
This function adds the constant value `x` to the elements of the vector `a`. The result $a_i \leftarrow a_i + x$ is stored in `a`.

double **gsl_vector_sum**(const *gsl_vector* *a)
This function returns the sum of the elements of `a`, defined as $\sum_{i=1}^{n} a_i$

int **gsl_vector_axpby**(const double alpha, const *gsl_vector* *x, const double beta, *gsl_vector* *y)
This function performs the operation $y \leftarrow \alpha x + \beta y$. The vectors `x` and `y` must have the same length.

8.3.9 Finding maximum and minimum elements of vectors

The following operations are only defined for real vectors.

double **gsl_vector_max**(const *gsl_vector* *v)
This function returns the maximum value in the vector `v`.

double **gsl_vector_min**(const *gsl_vector* *v)
This function returns the minimum value in the vector `v`.

void **gsl_vector_minmax**(const *gsl_vector* *v, double *min_out, double *max_out)
This function returns the minimum and maximum values in the vector `v`, storing them in `min_out` and `max_out`.

size_t **gsl_vector_max_index**(const *gsl_vector* *v)
This function returns the index of the maximum value in the vector `v`. When there are several equal maximum elements then the lowest index is returned.

size_t **gsl_vector_min_index**(const *gsl_vector* *v)
This function returns the index of the minimum value in the vector `v`. When there are several equal minimum elements then the lowest index is returned.

void **gsl_vector_minmax_index**(const *gsl_vector* *v, size_t *imin, size_t *imax)
This function returns the indices of the minimum and maximum values in the vector `v`, storing them in `imin` and `imax`. When there are several equal minimum or maximum elements then the lowest indices are returned.

8.3.10 Vector properties

The following functions are defined for real and complex vectors. For complex vectors both the real and imaginary parts must satisfy the conditions.

int **gsl_vector_isnull**(const *gsl_vector* *v)

int **gsl_vector_ispos**(const *gsl_vector* *v)

int **gsl_vector_isneg**(const *gsl_vector* *v)

int **gsl_vector_isnonneg**(const *gsl_vector* *v)
These functions return 1 if all the elements of the vector `v` are zero, strictly positive, strictly negative, or non-negative respectively, and 0 otherwise.

int **gsl_vector_equal**(const *gsl_vector* *u, const *gsl_vector* *v)
This function returns 1 if the vectors `u` and `v` are equal (by comparison of element values) and 0 otherwise.

8.3.11 Example programs for vectors

This program shows how to allocate, initialize and read from a vector using the functions *gsl_vector_alloc()*, *gsl_vector_set()* and *gsl_vector_get()*.

```
#include <stdio.h>
#include <gsl/gsl_vector.h>

int
main (void)
{
  int i;
  gsl_vector * v = gsl_vector_alloc (3);

  for (i = 0; i < 3; i++)
    {
      gsl_vector_set (v, i, 1.23 + i);
    }

  for (i = 0; i < 100; i++) /* OUT OF RANGE ERROR */
    {
      printf ("v_%d = %g\n", i, gsl_vector_get (v, i));
    }

  gsl_vector_free (v);
  return 0;
}
```

Here is the output from the program. The final loop attempts to read outside the range of the vector `v`, and the error is trapped by the range-checking code in *gsl_vector_get()*.

```
$ ./a.out
v_0 = 1.23
v_1 = 2.23
v_2 = 3.23
gsl: vector_source.c:12: ERROR: index out of range
Default GSL error handler invoked.
Aborted (core dumped)
```

The next program shows how to write a vector to a file.

```
#include <stdio.h>
#include <gsl/gsl_vector.h>

int
main (void)
{
  int i;
  gsl_vector * v = gsl_vector_alloc (100);

  for (i = 0; i < 100; i++)
    {
      gsl_vector_set (v, i, 1.23 + i);
    }
```

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```
  {
     FILE * f = fopen ("test.dat", "w");
     gsl_vector_fprintf (f, v, "%.5g");
     fclose (f);
  }

  gsl_vector_free (v);
  return 0;
}
```

After running this program the file `test.dat` should contain the elements of `v`, written using the format specifier `%.5g`. The vector could then be read back in using the function `gsl_vector_fscanf (f, v)` as follows:

```
#include <stdio.h>
#include <gsl/gsl_vector.h>

int
main (void)
{
  int i;
  gsl_vector * v = gsl_vector_alloc (10);

  {
     FILE * f = fopen ("test.dat", "r");
     gsl_vector_fscanf (f, v);
     fclose (f);
  }

  for (i = 0; i < 10; i++)
    {
      printf ("%g\n", gsl_vector_get(v, i));
    }

  gsl_vector_free (v);
  return 0;
}
```

8.4 Matrices

Matrices are defined by a *gsl_matrix* structure which describes a generalized slice of a block. Like a vector it represents a set of elements in an area of memory, but uses two indices instead of one.

type **gsl_matrix**

The *gsl_matrix* structure contains six components, the two dimensions of the matrix, a physical dimension, a pointer to the memory where the elements of the matrix are stored, `data`, a pointer to the block owned by the matrix `block`, if any, and an ownership flag, `owner`. The physical dimension determines the memory layout and can differ from the matrix dimension to allow the use of submatrices. The *gsl_matrix* structure is very simple and looks like this:

```
typedef struct
{
  size_t size1;
  size_t size2;
  size_t tda;
  double * data;
  gsl_block * block;
  int owner;
} gsl_matrix;
```

Matrices are stored in row-major order, meaning that each row of elements forms a contiguous block in memory. This is the standard "C-language ordering" of two-dimensional arrays. Note that Fortran stores arrays in column-major order. The number of rows is `size1`. The range of valid row indices runs from 0 to `size1 - 1`. Similarly `size2` is the number of columns. The range of valid column indices runs from 0 to `size2 - 1`. The physical row dimension `tda`, or *trailing dimension*, specifies the size of a row of the matrix as laid out in memory.

For example, in the following matrix `size1` is 3, `size2` is 4, and `tda` is 8. The physical memory layout of the matrix begins in the top left hand-corner and proceeds from left to right along each row in turn.

```
00 01 02 03 XX XX XX XX
10 11 12 13 XX XX XX XX
20 21 22 23 XX XX XX XX
```

Each unused memory location is represented by "`XX`". The pointer `data` gives the location of the first element of the matrix in memory. The pointer `block` stores the location of the memory block in which the elements of the matrix are located (if any). If the matrix owns this block then the `owner` field is set to one and the block will be deallocated when the matrix is freed. If the matrix is only a slice of a block owned by another object then the `owner` field is zero and any underlying block will not be freed.

The functions for allocating and accessing matrices are defined in `gsl_matrix.h`.

8.4.1 Matrix allocation

The functions for allocating memory to a matrix follow the style of `malloc` and `free`. They also perform their own error checking. If there is insufficient memory available to allocate a matrix then the functions call the GSL error handler (with an error number of *`GSL_ENOMEM`*) in addition to returning a null pointer. Thus if you use the library error handler to abort your program then it isn't necessary to check every `alloc`.

gsl_matrix ***`gsl_matrix_alloc`**(size_t n1, size_t n2)

This function creates a matrix of size *`n1`* rows by *`n2`* columns, returning a pointer to a newly initialized matrix struct. A new block is allocated for the elements of the matrix, and stored in the `block` component of the matrix struct. The block is "owned" by the matrix, and will be deallocated when the matrix is deallocated. Requesting zero for *`n1`* or *`n2`* is valid and returns a non-null result.

gsl_matrix ***`gsl_matrix_calloc`**(size_t n1, size_t n2)

This function allocates memory for a matrix of size *`n1`* rows by *`n2`* columns and initializes all the elements of the matrix to zero.

void **`gsl_matrix_free`**(*gsl_matrix* *m)

This function frees a previously allocated matrix *`m`*. If the matrix was created using *`gsl_matrix_alloc()`* then the block underlying the matrix will also be deallocated. If the matrix has been created from another object then the memory is still owned by that object and will not be deallocated.

8.4.2 Accessing matrix elements

The functions for accessing the elements of a matrix use the same range checking system as vectors. You can turn off range checking by recompiling your program with the preprocessor definition *GSL_RANGE_CHECK_OFF*.

The elements of the matrix are stored in "C-order", where the second index moves continuously through memory. More precisely, the element accessed by the function `gsl_matrix_get(m,i,j)` and `gsl_matrix_set(m,i,j,x)` is:

```
m->data[i * m->tda + j]
```

where `tda` is the physical row-length of the matrix.

double **gsl_matrix_get**(const *gsl_matrix* *m, const size_t i, const size_t j)

This function returns the (i, j)-th element of a matrix *m*. If *i* or *j* lie outside the allowed range of 0 to `n1 - 1` and 0 to `n2 - 1` then the error handler is invoked and 0 is returned. An inline version of this function is used when `HAVE_INLINE` is defined.

void **gsl_matrix_set**(*gsl_matrix* *m, const size_t i, const size_t j, double x)

This function sets the value of the (i, j)-th element of a matrix *m* to *x*. If *i* or *j* lies outside the allowed range of 0 to `n1 - 1` and 0 to `n2 - 1` then the error handler is invoked. An inline version of this function is used when `HAVE_INLINE` is defined.

double ***gsl_matrix_ptr**(*gsl_matrix* *m, size_t i, size_t j)

const double ***gsl_matrix_const_ptr**(const *gsl_matrix* *m, size_t i, size_t j)

These functions return a pointer to the (i, j)-th element of a matrix *m*. If *i* or *j* lie outside the allowed range of 0 to `n1 - 1` and 0 to `n2 - 1` then the error handler is invoked and a null pointer is returned. Inline versions of these functions are used when `HAVE_INLINE` is defined.

8.4.3 Initializing matrix elements

void **gsl_matrix_set_all**(*gsl_matrix* *m, double x)

This function sets all the elements of the matrix *m* to the value *x*.

void **gsl_matrix_set_zero**(*gsl_matrix* *m)

This function sets all the elements of the matrix *m* to zero.

void **gsl_matrix_set_identity**(*gsl_matrix* *m)

This function sets the elements of the matrix *m* to the corresponding elements of the identity matrix, $m(i, j) = \delta(i, j)$, i.e. a unit diagonal with all off-diagonal elements zero. This applies to both square and rectangular matrices.

8.4.4 Reading and writing matrices

The library provides functions for reading and writing matrices to a file as binary data or formatted text.

int **gsl_matrix_fwrite**(FILE *stream, const *gsl_matrix* *m)

This function writes the elements of the matrix *m* to the stream *stream* in binary format. The return value is 0 for success and `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

int **gsl_matrix_fread**(FILE *stream, *gsl_matrix* *m)

This function reads into the matrix *m* from the open stream *stream* in binary format. The matrix *m* must be preallocated with the correct dimensions since the function uses the size of *m* to determine how many bytes to read. The return value is 0 for success and `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

int **gsl_matrix_fprintf**(FILE *stream, const *gsl_matrix* *m, const char *format)

This function writes the elements of the matrix *m* line-by-line to the stream *stream* using the format specifier *format*, which should be one of the %g, %e or %f formats for floating point numbers and %d for integers. The function returns 0 for success and GSL_EFAILED if there was a problem writing to the file.

int **gsl_matrix_fscanf**(FILE *stream, *gsl_matrix* *m)

This function reads formatted data from the stream *stream* into the matrix *m*. The matrix *m* must be preallocated with the correct dimensions since the function uses the size of *m* to determine how many numbers to read. The function returns 0 for success and GSL_EFAILED if there was a problem reading from the file.

8.4.5 Matrix views

type **gsl_matrix_view**

type **gsl_matrix_const_view**

A matrix view is a temporary object, stored on the stack, which can be used to operate on a subset of matrix elements. Matrix views can be defined for both constant and non-constant matrices using separate types that preserve constness. A matrix view has the type *gsl_matrix_view* and a constant matrix view has the type *gsl_matrix_const_view*. In both cases the elements of the view can by accessed using the matrix component of the view object. A pointer gsl_matrix * or const gsl_matrix * can be obtained by taking the address of the matrix component with the & operator. In addition to matrix views it is also possible to create vector views of a matrix, such as row or column views.

gsl_matrix_view **gsl_matrix_submatrix**(*gsl_matrix* *m, size_t k1, size_t k2, size_t n1, size_t n2)

gsl_matrix_const_view **gsl_matrix_const_submatrix**(const *gsl_matrix* *m, size_t k1, size_t k2, size_t n1, size_t n2)

These functions return a matrix view of a submatrix of the matrix *m*. The upper-left element of the submatrix is the element (*k1*, *k2*) of the original matrix. The submatrix has *n1* rows and *n2* columns. The physical number of columns in memory given by tda is unchanged. Mathematically, the (i, j)-th element of the new matrix is given by:

```
m'(i,j) = m->data[(k1*m->tda + k2) + i*m->tda + j]
```

where the index i runs from 0 to n1 - 1 and the index j runs from 0 to n2 - 1.

The data pointer of the returned matrix struct is set to null if the combined parameters (i, j, *n1*, *n2*, tda) overrun the ends of the original matrix.

The new matrix view is only a view of the block underlying the existing matrix, *m*. The block containing the elements of *m* is not owned by the new matrix view. When the view goes out of scope the original matrix *m* and its block will continue to exist. The original memory can only be deallocated by freeing the original matrix. Of course, the original matrix should not be deallocated while the view is still in use.

The function *gsl_matrix_const_submatrix()* is equivalent to *gsl_matrix_submatrix()* but can be used for matrices which are declared const.

gsl_matrix_view **gsl_matrix_view_array**(double *base, size_t n1, size_t n2)

gsl_matrix_const_view **gsl_matrix_const_view_array**(const double *base, size_t n1, size_t n2)

These functions return a matrix view of the array *base*. The matrix has *n1* rows and *n2* columns. The physical number of columns in memory is also given by *n2*. Mathematically, the (i, j)-th element of the new matrix is given by:

```
m'(i,j) = base[i*n2 + j]
```

where the index i runs from 0 to n1 - 1 and the index j runs from 0 to n2 - 1.

The new matrix is only a view of the array *base*. When the view goes out of scope the original array *base* will continue to exist. The original memory can only be deallocated by freeing the original array. Of course, the original array should not be deallocated while the view is still in use.

The function *gsl_matrix_const_view_array()* is equivalent to *gsl_matrix_view_array()* but can be used for matrices which are declared const.

gsl_matrix_view **gsl_matrix_view_array_with_tda**(double *base, size_t n1, size_t n2, size_t tda)

gsl_matrix_const_view **gsl_matrix_const_view_array_with_tda**(const double *base, size_t n1, size_t n2, size_t tda)

These functions return a matrix view of the array *base* with a physical number of columns *tda* which may differ from the corresponding dimension of the matrix. The matrix has *n1* rows and *n2* columns, and the physical number of columns in memory is given by *tda*. Mathematically, the (i, j)-th element of the new matrix is given by:

```
m'(i,j) = base[i*tda + j]
```

where the index i runs from 0 to n1 - 1 and the index j runs from 0 to n2 - 1.

The new matrix is only a view of the array *base*. When the view goes out of scope the original array *base* will continue to exist. The original memory can only be deallocated by freeing the original array. Of course, the original array should not be deallocated while the view is still in use.

The function *gsl_matrix_const_view_array_with_tda()* is equivalent to *gsl_matrix_view_array_with_tda()* but can be used for matrices which are declared const.

gsl_matrix_view **gsl_matrix_view_vector**(*gsl_vector* *v, size_t n1, size_t n2)

gsl_matrix_const_view **gsl_matrix_const_view_vector**(const *gsl_vector* *v, size_t n1, size_t n2)

These functions return a matrix view of the vector *v*. The matrix has *n1* rows and *n2* columns. The vector must have unit stride. The physical number of columns in memory is also given by *n2*. Mathematically, the (i, j)-th element of the new matrix is given by:

```
m'(i,j) = v->data[i*n2 + j]
```

where the index i runs from 0 to n1 - 1 and the index j runs from 0 to n2 - 1.

The new matrix is only a view of the vector *v*. When the view goes out of scope the original vector *v* will continue to exist. The original memory can only be deallocated by freeing the original vector. Of course, the original vector should not be deallocated while the view is still in use.

The function *gsl_matrix_const_view_vector()* is equivalent to *gsl_matrix_view_vector()* but can be used for matrices which are declared const.

gsl_matrix_view **gsl_matrix_view_vector_with_tda**(*gsl_vector* *v, size_t n1, size_t n2, size_t tda)

gsl_matrix_const_view **gsl_matrix_const_view_vector_with_tda**(const *gsl_vector* *v, size_t n1, size_t n2, size_t tda)

These functions return a matrix view of the vector *v* with a physical number of columns *tda* which may differ from the corresponding matrix dimension. The vector must have unit stride. The matrix has *n1* rows and *n2* columns, and the physical number of columns in memory is given by *tda*. Mathematically, the (i, j)-th element of the new matrix is given by:

```
m'(i,j) = v->data[i*tda + j]
```

where the index `i` runs from 0 to `n1 - 1` and the index `j` runs from 0 to `n2 - 1`.

The new matrix is only a view of the vector *v*. When the view goes out of scope the original vector *v* will continue to exist. The original memory can only be deallocated by freeing the original vector. Of course, the original vector should not be deallocated while the view is still in use.

The function *gsl_matrix_const_view_vector_with_tda()* is equivalent to *gsl_matrix_view_vector_with_tda()* but can be used for matrices which are declared `const`.

8.4.6 Creating row and column views

In general there are two ways to access an object, by reference or by copying. The functions described in this section create vector views which allow access to a row or column of a matrix by reference. Modifying elements of the view is equivalent to modifying the matrix, since both the vector view and the matrix point to the same memory block.

gsl_vector_view **gsl_matrix_row**(*gsl_matrix* *m, size_t i)

gsl_vector_const_view **gsl_matrix_const_row**(const *gsl_matrix* *m, size_t i)

These functions return a vector view of the *i*-th row of the matrix *m*. The `data` pointer of the new vector is set to null if *i* is out of range.

The function *gsl_matrix_const_row()* is equivalent to *gsl_matrix_row()* but can be used for matrices which are declared `const`.

gsl_vector_view **gsl_matrix_column**(*gsl_matrix* *m, size_t j)

gsl_vector_const_view **gsl_matrix_const_column**(const *gsl_matrix* *m, size_t j)

These functions return a vector view of the *j*-th column of the matrix *m*. The `data` pointer of the new vector is set to null if *j* is out of range.

The function *gsl_matrix_const_column()* is equivalent to *gsl_matrix_column()* but can be used for matrices which are declared `const`.

gsl_vector_view **gsl_matrix_subrow**(*gsl_matrix* *m, size_t i, size_t offset, size_t n)

gsl_vector_const_view **gsl_matrix_const_subrow**(const *gsl_matrix* *m, size_t i, size_t offset, size_t n)

These functions return a vector view of the *i*-th row of the matrix *m* beginning at *offset* elements past the first column and containing *n* elements. The `data` pointer of the new vector is set to null if *i*, *offset*, or *n* are out of range.

The function *gsl_matrix_const_subrow()* is equivalent to *gsl_matrix_subrow()* but can be used for matrices which are declared `const`.

gsl_vector_view **gsl_matrix_subcolumn**(*gsl_matrix* *m, size_t j, size_t offset, size_t n)

gsl_vector_const_view **gsl_matrix_const_subcolumn**(const *gsl_matrix* *m, size_t j, size_t offset, size_t n)

These functions return a vector view of the *j*-th column of the matrix *m* beginning at *offset* elements past the first row and containing *n* elements. The `data` pointer of the new vector is set to null if *j*, *offset*, or *n* are out of range.

The function *gsl_matrix_const_subcolumn()* is equivalent to *gsl_matrix_subcolumn()* but can be used for matrices which are declared `const`.

gsl_vector_view **gsl_matrix_diagonal**(*gsl_matrix* *m)

gsl_vector_const_view **gsl_matrix_const_diagonal**(const *gsl_matrix* *m)

These functions return a vector view of the diagonal of the matrix *m*. The matrix *m* is not required to be square. For a rectangular matrix the length of the diagonal is the same as the smaller dimension of the matrix.

The function `gsl_matrix_const_diagonal()` is equivalent to `gsl_matrix_diagonal()` but can be used for matrices which are declared `const`.

gsl_vector_view **`gsl_matrix_subdiagonal`**(*gsl_matrix* *m, size_t k)

gsl_vector_const_view **`gsl_matrix_const_subdiagonal`**(const *gsl_matrix* *m, size_t k)

These functions return a vector view of the `k`-th subdiagonal of the matrix `m`. The matrix `m` is not required to be square. The diagonal of the matrix corresponds to $k = 0$.

The function `gsl_matrix_const_subdiagonal()` is equivalent to `gsl_matrix_subdiagonal()` but can be used for matrices which are declared `const`.

gsl_vector_view **`gsl_matrix_superdiagonal`**(*gsl_matrix* *m, size_t k)

gsl_vector_const_view **`gsl_matrix_const_superdiagonal`**(const *gsl_matrix* *m, size_t k)

These functions return a vector view of the `k`-th superdiagonal of the matrix `m`. The matrix `m` is not required to be square. The diagonal of the matrix corresponds to $k = 0$.

The function `gsl_matrix_const_superdiagonal()` is equivalent to `gsl_matrix_superdiagonal()` but can be used for matrices which are declared `const`.

8.4.7 Copying matrices

int **`gsl_matrix_memcpy`**(*gsl_matrix* *dest, const *gsl_matrix* *src)

This function copies the elements of the matrix `src` into the matrix `dest`. The two matrices must have the same size.

int **`gsl_matrix_swap`**(*gsl_matrix* *m1, *gsl_matrix* *m2)

This function exchanges the elements of the matrices `m1` and `m2` by copying. The two matrices must have the same size.

8.4.8 Copying rows and columns

The functions described in this section copy a row or column of a matrix into a vector. This allows the elements of the vector and the matrix to be modified independently. Note that if the matrix and the vector point to overlapping regions of memory then the result will be undefined. The same effect can be achieved with more generality using `gsl_vector_memcpy()` with vector views of rows and columns.

int **`gsl_matrix_get_row`**(*gsl_vector* *v, const *gsl_matrix* *m, size_t i)

This function copies the elements of the `i`-th row of the matrix `m` into the vector `v`. The length of the vector must be the same as the length of the row.

int **`gsl_matrix_get_col`**(*gsl_vector* *v, const *gsl_matrix* *m, size_t j)

This function copies the elements of the `j`-th column of the matrix `m` into the vector `v`. The length of the vector must be the same as the length of the column.

int **`gsl_matrix_set_row`**(*gsl_matrix* *m, size_t i, const *gsl_vector* *v)

This function copies the elements of the vector `v` into the `i`-th row of the matrix `m`. The length of the vector must be the same as the length of the row.

int **`gsl_matrix_set_col`**(*gsl_matrix* *m, size_t j, const *gsl_vector* *v)

This function copies the elements of the vector `v` into the `j`-th column of the matrix `m`. The length of the vector must be the same as the length of the column.

8.4.9 Exchanging rows and columns

The following functions can be used to exchange the rows and columns of a matrix.

int **gsl_matrix_swap_rows**(*gsl_matrix* *m, size_t i, size_t j)
: This function exchanges the `i`-th and `j`-th rows of the matrix `m` in-place.

int **gsl_matrix_swap_columns**(*gsl_matrix* *m, size_t i, size_t j)
: This function exchanges the `i`-th and `j`-th columns of the matrix `m` in-place.

int **gsl_matrix_swap_rowcol**(*gsl_matrix* *m, size_t i, size_t j)
: This function exchanges the `i`-th row and `j`-th column of the matrix `m` in-place. The matrix must be square for this operation to be possible.

int **gsl_matrix_transpose_memcpy**(*gsl_matrix* *dest, const *gsl_matrix* *src)
: This function makes the matrix `dest` the transpose of the matrix `src` by copying the elements of `src` into `dest`. This function works for all matrices provided that the dimensions of the matrix `dest` match the transposed dimensions of the matrix `src`.

int **gsl_matrix_transpose**(*gsl_matrix* *m)
: This function replaces the matrix `m` by its transpose by copying the elements of the matrix in-place. The matrix must be square for this operation to be possible.

int **gsl_matrix_complex_conjtrans_memcpy**(*gsl_matrix* *dest, const *gsl_matrix* *src)
: This function makes the matrix `dest` the conjugate transpose of the matrix `src` by copying the complex conjugate elements of `src` into `dest`. This function works for all complex matrices provided that the dimensions of the matrix `dest` match the transposed dimensions of the matrix `src`.

8.4.10 Matrix operations

The following operations are defined for real and complex matrices.

int **gsl_matrix_add**(*gsl_matrix* *a, const *gsl_matrix* *b)
: This function adds the elements of matrix `b` to the elements of matrix `a`. The result $a(i,j) \leftarrow a(i,j) + b(i,j)$ is stored in `a` and `b` remains unchanged. The two matrices must have the same dimensions.

int **gsl_matrix_sub**(*gsl_matrix* *a, const *gsl_matrix* *b)
: This function subtracts the elements of matrix `b` from the elements of matrix `a`. The result $a(i,j) \leftarrow a(i,j) - b(i,j)$ is stored in `a` and `b` remains unchanged. The two matrices must have the same dimensions.

int **gsl_matrix_mul_elements**(*gsl_matrix* *a, const *gsl_matrix* *b)
: This function multiplies the elements of matrix `a` by the elements of matrix `b`. The result $a(i,j) \leftarrow a(i,j) * b(i,j)$ is stored in `a` and `b` remains unchanged. The two matrices must have the same dimensions.

int **gsl_matrix_div_elements**(*gsl_matrix* *a, const *gsl_matrix* *b)
: This function divides the elements of matrix `a` by the elements of matrix `b`. The result $a(i,j) \leftarrow a(i,j)/b(i,j)$ is stored in `a` and `b` remains unchanged. The two matrices must have the same dimensions.

int **gsl_matrix_scale**(*gsl_matrix* *a, const double x)
: This function multiplies the elements of matrix `a` by the constant factor `x`. The result $a(i,j) \leftarrow xa(i,j)$ is stored in `a`.

int **gsl_matrix_scale_columns**(*gsl_matrix* *A, const *gsl_vector* *x)
: This function scales the columns of the M-by-N matrix `A` by the elements of the vector `x`, of length N. The j-th column of `A` is multiplied by x_j. This is equivalent to forming

$$A \rightarrow AX$$

where $X = \text{diag}(x)$.

int **gsl_matrix_scale_rows**(*gsl_matrix* *A, const *gsl_vector* *x)

This function scales the rows of the M-by-N matrix `A` by the elements of the vector `x`, of length M. The i-th row of `A` is multiplied by x_i. This is equivalent to forming

$$A \to XA$$

where $X = \text{diag}(x)$.

int **gsl_matrix_add_constant**(*gsl_matrix* *a, const double x)

This function adds the constant value `x` to the elements of the matrix `a`. The result $a(i,j) \leftarrow a(i,j) + x$ is stored in `a`.

8.4.11 Finding maximum and minimum elements of matrices

The following operations are only defined for real matrices.

double **gsl_matrix_max**(const *gsl_matrix* *m)

This function returns the maximum value in the matrix `m`.

double **gsl_matrix_min**(const *gsl_matrix* *m)

This function returns the minimum value in the matrix `m`.

void **gsl_matrix_minmax**(const *gsl_matrix* *m, double *min_out, double *max_out)

This function returns the minimum and maximum values in the matrix `m`, storing them in `min_out` and `max_out`.

void **gsl_matrix_max_index**(const *gsl_matrix* *m, size_t *imax, size_t *jmax)

This function returns the indices of the maximum value in the matrix `m`, storing them in `imax` and `jmax`. When there are several equal maximum elements then the first element found is returned, searching in row-major order.

void **gsl_matrix_min_index**(const *gsl_matrix* *m, size_t *imin, size_t *jmin)

This function returns the indices of the minimum value in the matrix `m`, storing them in `imin` and `jmin`. When there are several equal minimum elements then the first element found is returned, searching in row-major order.

void **gsl_matrix_minmax_index**(const *gsl_matrix* *m, size_t *imin, size_t *jmin, size_t *imax, size_t *jmax)

This function returns the indices of the minimum and maximum values in the matrix `m`, storing them in (`imin`, `jmin`) and (`imax`, `jmax`). When there are several equal minimum or maximum elements then the first elements found are returned, searching in row-major order.

8.4.12 Matrix properties

The following functions are defined for real and complex matrices. For complex matrices both the real and imaginary parts must satisfy the conditions.

int **gsl_matrix_isnull**(const *gsl_matrix* *m)

int **gsl_matrix_ispos**(const *gsl_matrix* *m)

int **gsl_matrix_isneg**(const *gsl_matrix* *m)

int **gsl_matrix_isnonneg**(const *gsl_matrix* *m)

These functions return 1 if all the elements of the matrix `m` are zero, strictly positive, strictly negative, or non-negative respectively, and 0 otherwise. To test whether a matrix is positive-definite, use the *Cholesky decomposition*.

int **gsl_matrix_equal**(const *gsl_matrix* *a, const *gsl_matrix* *b)

This function returns 1 if the matrices `a` and `b` are equal (by comparison of element values) and 0 otherwise.

double **gsl_matrix_norm1**(const *gsl_matrix* *A)

This function returns the 1-norm of the m-by-n matrix `A`, defined as the maximum column sum,

$$||A||_1 = \max_{1 \le j \le n} \sum_{i=1}^{m} |A_{ij}|$$

8.4.13 Example programs for matrices

The program below shows how to allocate, initialize and read from a matrix using the functions `gsl_matrix_alloc()`, `gsl_matrix_set()` and `gsl_matrix_get()`.

```
#include <stdio.h>
#include <gsl/gsl_matrix.h>

int
main (void)
{
  int i, j;
  gsl_matrix * m = gsl_matrix_alloc (10, 3);

  for (i = 0; i < 10; i++)
    for (j = 0; j < 3; j++)
      gsl_matrix_set (m, i, j, 0.23 + 100*i + j);

  for (i = 0; i < 100; i++)  /* OUT OF RANGE ERROR */
    for (j = 0; j < 3; j++)
      printf ("m(%d,%d) = %g\n", i, j,
              gsl_matrix_get (m, i, j));

  gsl_matrix_free (m);

  return 0;
}
```

Here is the output from the program. The final loop attempts to read outside the range of the matrix `m`, and the error is trapped by the range-checking code in `gsl_matrix_get()`.

```
$ ./a.out
m(0,0) = 0.23
m(0,1) = 1.23
m(0,2) = 2.23
m(1,0) = 100.23
m(1,1) = 101.23
m(1,2) = 102.23
...
m(9,2) = 902.23
gsl: matrix_source.c:13: ERROR: first index out of range
Default GSL error handler invoked.
Aborted (core dumped)
```

The next program shows how to write a matrix to a file.

```
#include <stdio.h>
#include <gsl/gsl_matrix.h>

int
main (void)
{
  int i, j, k = 0;
  gsl_matrix * m = gsl_matrix_alloc (100, 100);
  gsl_matrix * a = gsl_matrix_alloc (100, 100);

  for (i = 0; i < 100; i++)
    for (j = 0; j < 100; j++)
      gsl_matrix_set (m, i, j, 0.23 + i + j);

  {
     FILE * f = fopen ("test.dat", "wb");
     gsl_matrix_fwrite (f, m);
     fclose (f);
  }

  {
     FILE * f = fopen ("test.dat", "rb");
     gsl_matrix_fread (f, a);
     fclose (f);
  }

  for (i = 0; i < 100; i++)
    for (j = 0; j < 100; j++)
      {
        double mij = gsl_matrix_get (m, i, j);
        double aij = gsl_matrix_get (a, i, j);
        if (mij != aij) k++;
      }

  gsl_matrix_free (m);
  gsl_matrix_free (a);

  printf ("differences = %d (should be zero)\n", k);
  return (k > 0);
}
```

After running this program the file `test.dat` should contain the elements of `m`, written in binary format. The matrix which is read back in using the function `gsl_matrix_fread()` should be exactly equal to the original matrix.

The following program demonstrates the use of vector views. The program computes the column norms of a matrix.

```
#include <math.h>
#include <stdio.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_blas.h>

int
main (void)
```

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```
{
  size_t i,j;

  gsl_matrix *m = gsl_matrix_alloc (10, 10);

  for (i = 0; i < 10; i++)
    for (j = 0; j < 10; j++)
      gsl_matrix_set (m, i, j, sin (i) + cos (j));

  for (j = 0; j < 10; j++)
    {
      gsl_vector_view column = gsl_matrix_column (m, j);
      double d;

      d = gsl_blas_dnrm2 (&column.vector);

      printf ("matrix column %zu, norm = %g\n", j, d);
    }

  gsl_matrix_free (m);

  return 0;
}
```

Here is the output of the program,

```
matrix column 0, norm = 4.31461
matrix column 1, norm = 3.1205
matrix column 2, norm = 2.19316
matrix column 3, norm = 3.26114
matrix column 4, norm = 2.53416
matrix column 5, norm = 2.57281
matrix column 6, norm = 4.20469
matrix column 7, norm = 3.65202
matrix column 8, norm = 2.08524
matrix column 9, norm = 3.07313
```

The results can be confirmed using GNU octave:

```
$ octave
GNU Octave, version 2.0.16.92
octave> m = sin(0:9)' * ones(1,10)
               + ones(10,1) * cos(0:9);
octave> sqrt(sum(m.^2))
ans =
  4.3146  3.1205  2.1932  3.2611  2.5342  2.5728
  4.2047  3.6520  2.0852  3.0731
```

8.4.14 References and Further Reading

The block, vector and matrix objects in GSL follow the `valarray` model of C++. A description of this model can be found in the following reference,

- B. Stroustrup, The C++ Programming Language (3rd Ed), Section 22.4 Vector Arithmetic. Addison-Wesley 1997, ISBN 0-201-88954-4.

CHAPTER

NINE

PERMUTATIONS

This chapter describes functions for creating and manipulating permutations. A permutation p is represented by an array of n integers in the range 0 to $n-1$, where each value p_i occurs once and only once. The application of a permutation p to a vector v yields a new vector v' where $v'_i = v_{p_i}$. For example, the array $(0,1,3,2)$ represents a permutation which exchanges the last two elements of a four element vector. The corresponding identity permutation is $(0,1,2,3)$.

Note that the permutations produced by the linear algebra routines correspond to the exchange of matrix columns, and so should be considered as applying to row-vectors in the form $v' = vP$ rather than column-vectors, when permuting the elements of a vector.

The functions described in this chapter are defined in the header file `gsl_permutation.h`.

9.1 The Permutation struct

type **gsl_permutation**

A permutation is defined by a structure containing two components, the size of the permutation and a pointer to the permutation array. The elements of the permutation array are all of type `size_t`. The *gsl_permutation* structure looks like this:

```
typedef struct
{
  size_t size;
  size_t * data;
} gsl_permutation;
```

9.2 Permutation allocation

gsl_permutation ***gsl_permutation_alloc**(size_t n)

This function allocates memory for a new permutation of size *n*. The permutation is not initialized and its elements are undefined. Use the function *gsl_permutation_calloc()* if you want to create a permutation which is initialized to the identity. A null pointer is returned if insufficient memory is available to create the permutation.

gsl_permutation ***gsl_permutation_calloc**(size_t n)

This function allocates memory for a new permutation of size *n* and initializes it to the identity. A null pointer is returned if insufficient memory is available to create the permutation.

void **gsl_permutation_init**(*gsl_permutation* *p)

This function initializes the permutation *p* to the identity, i.e. $(0,1,2,\ldots,n-1)$.

void **gsl_permutation_free**(*gsl_permutation* *p)
This function frees all the memory used by the permutation `p`.

int **gsl_permutation_memcpy**(*gsl_permutation* *dest, const *gsl_permutation* *src)
This function copies the elements of the permutation `src` into the permutation `dest`. The two permutations must have the same size.

9.3 Accessing permutation elements

The following functions can be used to access and manipulate permutations.

size_t **gsl_permutation_get**(const *gsl_permutation* *p, const size_t i)
This function returns the value of the `i`-th element of the permutation `p`. If `i` lies outside the allowed range of 0 to $n-1$ then the error handler is invoked and 0 is returned. An inline version of this function is used when `HAVE_INLINE` is defined.

int **gsl_permutation_swap**(*gsl_permutation* *p, const size_t i, const size_t j)
This function exchanges the `i`-th and `j`-th elements of the permutation `p`.

9.4 Permutation properties

size_t **gsl_permutation_size**(const *gsl_permutation* *p)
This function returns the size of the permutation `p`.

size_t ***gsl_permutation_data**(const *gsl_permutation* *p)
This function returns a pointer to the array of elements in the permutation `p`.

int **gsl_permutation_valid**(const *gsl_permutation* *p)
This function checks that the permutation `p` is valid. The `n` elements should contain each of the numbers 0 to `n - 1` once and only once.

9.5 Permutation functions

void **gsl_permutation_reverse**(*gsl_permutation* *p)
This function reverses the elements of the permutation `p`.

int **gsl_permutation_inverse**(*gsl_permutation* *inv, const *gsl_permutation* *p)
This function computes the inverse of the permutation `p`, storing the result in `inv`.

int **gsl_permutation_next**(*gsl_permutation* *p)
This function advances the permutation `p` to the next permutation in lexicographic order and returns `GSL_SUCCESS`. If no further permutations are available it returns `GSL_FAILURE` and leaves `p` unmodified. Starting with the identity permutation and repeatedly applying this function will iterate through all possible permutations of a given order.

int **gsl_permutation_prev**(*gsl_permutation* *p)
This function steps backwards from the permutation `p` to the previous permutation in lexicographic order, returning `GSL_SUCCESS`. If no previous permutation is available it returns `GSL_FAILURE` and leaves `p` unmodified.

9.6 Applying Permutations

The following functions are defined in the header files `gsl_permute.h` and `gsl_permute_vector.h`.

int **gsl_permute**(const size_t *p, double *data, size_t stride, size_t n)

This function applies the permutation `p` to the array `data` of size `n` with stride `stride`.

int **gsl_permute_inverse**(const size_t *p, double *data, size_t stride, size_t n)

This function applies the inverse of the permutation `p` to the array `data` of size `n` with stride `stride`.

int **gsl_permute_vector**(const *gsl_permutation* *p, *gsl_vector* *v)

This function applies the permutation `p` to the elements of the vector `v`, considered as a row-vector acted on by a permutation matrix from the right, $v' = vP$. The j-th column of the permutation matrix P is given by the p_j-th column of the identity matrix. The permutation `p` and the vector `v` must have the same length.

int **gsl_permute_vector_inverse**(const *gsl_permutation* *p, *gsl_vector* *v)

This function applies the inverse of the permutation `p` to the elements of the vector `v`, considered as a row-vector acted on by an inverse permutation matrix from the right, $v' = vP^T$. Note that for permutation matrices the inverse is the same as the transpose. The j-th column of the permutation matrix P is given by the p_j-th column of the identity matrix. The permutation `p` and the vector `v` must have the same length.

int **gsl_permute_matrix**(const *gsl_permutation* *p, *gsl_matrix* *A)

This function applies the permutation `p` to the matrix `A` from the right, $A' = AP$. The j-th column of the permutation matrix P is given by the p_j-th column of the identity matrix. This effectively permutes the columns of `A` according to the permutation `p`, and so the number of columns of `A` must equal the size of the permutation `p`.

int **gsl_permutation_mul**(*gsl_permutation* *p, const *gsl_permutation* *pa, const *gsl_permutation* *pb)

This function combines the two permutations `pa` and `pb` into a single permutation `p`, where $p = pa * pb$ The permutation `p` is equivalent to applying `pb` first and then `pa`.

9.7 Reading and writing permutations

The library provides functions for reading and writing permutations to a file as binary data or formatted text.

int **gsl_permutation_fwrite**(FILE *stream, const *gsl_permutation* *p)

This function writes the elements of the permutation `p` to the stream `stream` in binary format. The function returns `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

int **gsl_permutation_fread**(FILE *stream, *gsl_permutation* *p)

This function reads into the permutation `p` from the open stream `stream` in binary format. The permutation `p` must be preallocated with the correct length since the function uses the size of `p` to determine how many bytes to read. The function returns `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

int **gsl_permutation_fprintf**(FILE *stream, const *gsl_permutation* *p, const char *format)

This function writes the elements of the permutation `p` line-by-line to the stream `stream` using the format specifier `format`, which should be suitable for a type of `size_t`. In ISO C99 the type modifier `z` represents `size_t`, so `"%zu\n"` is a suitable format[1]. The function returns `GSL_EFAILED` if there was a problem writing to the file.

int **gsl_permutation_fscanf**(FILE *stream, *gsl_permutation* *p)

This function reads formatted data from the stream `stream` into the permutation `p`. The permutation `p` must be preallocated with the correct length since the function uses the size of `p` to determine how many numbers to read. The function returns `GSL_EFAILED` if there was a problem reading from the file.

[1] In versions of the GNU C library prior to the ISO C99 standard, the type modifier `Z` was used instead.

9.8 Permutations in cyclic form

A permutation can be represented in both *linear* and *cyclic* notations. The functions described in this section convert between the two forms. The linear notation is an index mapping, and has already been described above. The cyclic notation expresses a permutation as a series of circular rearrangements of groups of elements, or *cycles*.

For example, under the cycle (1 2 3), 1 is replaced by 2, 2 is replaced by 3 and 3 is replaced by 1 in a circular fashion. Cycles of different sets of elements can be combined independently, for example (1 2 3) (4 5) combines the cycle (1 2 3) with the cycle (4 5), which is an exchange of elements 4 and 5. A cycle of length one represents an element which is unchanged by the permutation and is referred to as a *singleton*.

It can be shown that every permutation can be decomposed into combinations of cycles. The decomposition is not unique, but can always be rearranged into a standard *canonical form* by a reordering of elements. The library uses the canonical form defined in Knuth's *Art of Computer Programming* (Vol 1, 3rd Ed, 1997) Section 1.3.3, p.178.

The procedure for obtaining the canonical form given by Knuth is,

1. Write all singleton cycles explicitly
2. Within each cycle, put the smallest number first
3. Order the cycles in decreasing order of the first number in the cycle.

For example, the linear representation (2 4 3 0 1) is represented as (1 4) (0 2 3) in canonical form. The permutation corresponds to an exchange of elements 1 and 4, and rotation of elements 0, 2 and 3.

The important property of the canonical form is that it can be reconstructed from the contents of each cycle without the brackets. In addition, by removing the brackets it can be considered as a linear representation of a different permutation. In the example given above the permutation (2 4 3 0 1) would become (1 4 0 2 3). This mapping has many applications in the theory of permutations.

int **gsl_permutation_linear_to_canonical**(*gsl_permutation* *q, const *gsl_permutation* *p)
: This function computes the canonical form of the permutation `p` and stores it in the output argument `q`.

int **gsl_permutation_canonical_to_linear**(*gsl_permutation* *p, const *gsl_permutation* *q)
: This function converts a permutation `q` in canonical form back into linear form storing it in the output argument `p`.

size_t **gsl_permutation_inversions**(const *gsl_permutation* *p)
: This function counts the number of inversions in the permutation `p`. An inversion is any pair of elements that are not in order. For example, the permutation 2031 has three inversions, corresponding to the pairs (2,0) (2,1) and (3,1). The identity permutation has no inversions.

size_t **gsl_permutation_linear_cycles**(const *gsl_permutation* *p)
: This function counts the number of cycles in the permutation `p`, given in linear form.

size_t **gsl_permutation_canonical_cycles**(const *gsl_permutation* *q)
: This function counts the number of cycles in the permutation `q`, given in canonical form.

9.9 Examples

The example program below creates a random permutation (by shuffling the elements of the identity) and finds its inverse.

```
#include <stdio.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
```

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```
#include <gsl/gsl_permutation.h>

int
main (void)
{
  const size_t N = 10;
  const gsl_rng_type * T;
  gsl_rng * r;

  gsl_permutation * p = gsl_permutation_alloc (N);
  gsl_permutation * q = gsl_permutation_alloc (N);

  gsl_rng_env_setup();
  T = gsl_rng_default;
  r = gsl_rng_alloc (T);

  printf ("initial permutation:");
  gsl_permutation_init (p);
  gsl_permutation_fprintf (stdout, p, " %u");
  printf ("\n");

  printf (" random permutation:");
  gsl_ran_shuffle (r, p->data, N, sizeof(size_t));
  gsl_permutation_fprintf (stdout, p, " %u");
  printf ("\n");

  printf ("inverse permutation:");
  gsl_permutation_inverse (q, p);
  gsl_permutation_fprintf (stdout, q, " %u");
  printf ("\n");

  gsl_permutation_free (p);
  gsl_permutation_free (q);
  gsl_rng_free (r);

  return 0;
}
```

Here is the output from the program:

```
$ ./a.out
initial permutation: 0 1 2 3 4 5 6 7 8 9
 random permutation: 1 3 5 2 7 6 0 4 9 8
inverse permutation: 6 0 3 1 7 2 5 4 9 8
```

The random permutation `p[i]` and its inverse `q[i]` are related through the identity `p[q[i]] = i`, which can be verified from the output.

The next example program steps forwards through all possible third order permutations, starting from the identity,

```
#include <stdio.h>
#include <gsl/gsl_permutation.h>
```

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```
int
main (void)
{
  gsl_permutation * p = gsl_permutation_alloc (3);

  gsl_permutation_init (p);

  do
   {
      gsl_permutation_fprintf (stdout, p, " %u");
      printf ("\n");
   }
  while (gsl_permutation_next(p) == GSL_SUCCESS);

  gsl_permutation_free (p);

  return 0;
}
```

Here is the output from the program:

```
$ ./a.out
 0 1 2
 0 2 1
 1 0 2
 1 2 0
 2 0 1
 2 1 0
```

The permutations are generated in lexicographic order. To reverse the sequence, begin with the final permutation (which is the reverse of the identity) and replace `gsl_permutation_next()` with `gsl_permutation_prev()`.

9.10 References and Further Reading

The subject of permutations is covered extensively in the following,

- Donald E. Knuth, The Art of Computer Programming: Sorting and Searching (Vol 3, 3rd Ed, 1997), Addison-Wesley, ISBN 0201896850.

For the definition of the *canonical form* see,

- Donald E. Knuth, The Art of Computer Programming: Fundamental Algorithms (Vol 1, 3rd Ed, 1997), Addison-Wesley, ISBN 0201896850. Section 1.3.3, An Unusual Correspondence, p.178–179.

CHAPTER

TEN

COMBINATIONS

This chapter describes functions for creating and manipulating combinations. A combination c is represented by an array of k integers in the range 0 to $n-1$, where each value c_i occurs at most once. The combination c corresponds to indices of k elements chosen from an n element vector. Combinations are useful for iterating over all k-element subsets of a set.

The functions described in this chapter are defined in the header file `gsl_combination.h`.

10.1 The Combination struct

type **`gsl_combination`**

A combination is defined by a structure containing three components, the values of n and k, and a pointer to the combination array. The elements of the combination array are all of type `size_t`, and are stored in increasing order. The *`gsl_combination`* structure looks like this:

```
typedef struct
{
  size_t n;
  size_t k;
  size_t *data;
} gsl_combination;
```

10.2 Combination allocation

gsl_combination ***`gsl_combination_alloc`**(size_t n, size_t k)

This function allocates memory for a new combination with parameters *`n`*, *`k`*. The combination is not initialized and its elements are undefined. Use the function *`gsl_combination_calloc()`* if you want to create a combination which is initialized to the lexicographically first combination. A null pointer is returned if insufficient memory is available to create the combination.

gsl_combination ***`gsl_combination_calloc`**(size_t n, size_t k)

This function allocates memory for a new combination with parameters *`n`*, *`k`* and initializes it to the lexicographically first combination. A null pointer is returned if insufficient memory is available to create the combination.

void **`gsl_combination_init_first`**(*gsl_combination* *c)

This function initializes the combination *`c`* to the lexicographically first combination, i.e. $(0, 1, 2, \ldots, k-1)$.

void **`gsl_combination_init_last`**(*gsl_combination* *c)

This function initializes the combination *`c`* to the lexicographically last combination, i.e. $(n-k, n-k+1, \ldots, n-1)$.

void **gsl_combination_free**(*gsl_combination* *c)

This function frees all the memory used by the combination *c*.

int **gsl_combination_memcpy**(*gsl_combination* *dest, const *gsl_combination* *src)

This function copies the elements of the combination *src* into the combination *dest*. The two combinations must have the same size.

10.3 Accessing combination elements

The following function can be used to access the elements of a combination.

size_t **gsl_combination_get**(const *gsl_combination* *c, const size_t i)

This function returns the value of the *i*-th element of the combination *c*. If *i* lies outside the allowed range of 0 to $k - 1$ then the error handler is invoked and 0 is returned. An inline version of this function is used when `HAVE_INLINE` is defined.

10.4 Combination properties

size_t **gsl_combination_n**(const *gsl_combination* *c)

This function returns the range (n) of the combination c.

size_t **gsl_combination_k**(const *gsl_combination* *c)

This function returns the number of elements (k) in the combination *c*.

size_t ***gsl_combination_data**(const *gsl_combination* *c)

This function returns a pointer to the array of elements in the combination *c*.

int **gsl_combination_valid**(*gsl_combination* *c)

This function checks that the combination *c* is valid. The `k` elements should lie in the range 0 to $n - 1$, with each value occurring once at most and in increasing order.

10.5 Combination functions

int **gsl_combination_next**(*gsl_combination* *c)

This function advances the combination *c* to the next combination in lexicographic order and returns `GSL_SUCCESS`. If no further combinations are available it returns `GSL_FAILURE` and leaves *c* unmodified. Starting with the first combination and repeatedly applying this function will iterate through all possible combinations of a given order.

int **gsl_combination_prev**(*gsl_combination* *c)

This function steps backwards from the combination *c* to the previous combination in lexicographic order, returning `GSL_SUCCESS`. If no previous combination is available it returns `GSL_FAILURE` and leaves *c* unmodified.

10.6 Reading and writing combinations

The library provides functions for reading and writing combinations to a file as binary data or formatted text.

int **gsl_combination_fwrite**(FILE *stream, const *gsl_combination* *c)

This function writes the elements of the combination `c` to the stream `stream` in binary format. The function returns `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

int **gsl_combination_fread**(FILE *stream, *gsl_combination* *c)

This function reads elements from the open stream `stream` into the combination `c` in binary format. The combination `c` must be preallocated with correct values of n and k since the function uses the size of `c` to determine how many bytes to read. The function returns `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

int **gsl_combination_fprintf**(FILE *stream, const *gsl_combination* *c, const char *format)

This function writes the elements of the combination `c` line-by-line to the stream `stream` using the format specifier `format`, which should be suitable for a type of `size_t`. In ISO C99 the type modifier `z` represents `size_t`, so `"%zu\n"` is a suitable format[1]. The function returns `GSL_EFAILED` if there was a problem writing to the file.

int **gsl_combination_fscanf**(FILE *stream, *gsl_combination* *c)

This function reads formatted data from the stream `stream` into the combination `c`. The combination `c` must be preallocated with correct values of n and k since the function uses the size of `c` to determine how many numbers to read. The function returns `GSL_EFAILED` if there was a problem reading from the file.

10.7 Examples

The example program below prints all subsets of the set $0, 1, 2, 3$ ordered by size. Subsets of the same size are ordered lexicographically.

```
#include <stdio.h>
#include <gsl/gsl_combination.h>

int
main (void)
{
  gsl_combination * c;
  size_t i;

  printf ("All subsets of {0,1,2,3} by size:\n") ;
  for (i = 0; i <= 4; i++)
    {
      c = gsl_combination_calloc (4, i);
      do
        {
          printf ("{");
          gsl_combination_fprintf (stdout, c, " %u");
          printf (" }\n");
        }
      while (gsl_combination_next (c) == GSL_SUCCESS);
```

(continues on next page)

[1] In versions of the GNU C library prior to the ISO C99 standard, the type modifier `Z` was used instead.

(continued from previous page)

```
      gsl_combination_free (c);
    }

  return 0;
}
```

Here is the output from the program,

```
All subsets of {0,1,2,3} by size:
{ }
{ 0 }
{ 1 }
{ 2 }
{ 3 }
{ 0 1 }
{ 0 2 }
{ 0 3 }
{ 1 2 }
{ 1 3 }
{ 2 3 }
{ 0 1 2 }
{ 0 1 3 }
{ 0 2 3 }
{ 1 2 3 }
{ 0 1 2 3 }
```

All 16 subsets are generated, and the subsets of each size are sorted lexicographically.

10.8 References and Further Reading

Further information on combinations can be found in,

- Donald L. Kreher, Douglas R. Stinson, Combinatorial Algorithms: Generation, Enumeration and Search, 1998, CRC Press LLC, ISBN 084933988X

CHAPTER ELEVEN

MULTISETS

This chapter describes functions for creating and manipulating multisets. A multiset c is represented by an array of k integers in the range 0 to $n-1$, where each value c_i may occur more than once. The multiset c corresponds to indices of k elements chosen from an n element vector with replacement. In mathematical terms, n is the cardinality of the multiset while k is the maximum multiplicity of any value. Multisets are useful, for example, when iterating over the indices of a k-th order symmetric tensor in n-space.

The functions described in this chapter are defined in the header file `gsl_multiset.h`.

11.1 The Multiset struct

type **`gsl_multiset`**

A multiset is defined by a structure containing three components, the values of n and k, and a pointer to the multiset array. The elements of the multiset array are all of type `size_t`, and are stored in increasing order. The *`gsl_multiset`* structure looks like this:

```
typedef struct
{
  size_t n;
  size_t k;
  size_t *data;
} gsl_multiset;
```

11.2 Multiset allocation

gsl_multiset ***`gsl_multiset_alloc`**(size_t n, size_t k)

This function allocates memory for a new multiset with parameters `n`, `k`. The multiset is not initialized and its elements are undefined. Use the function *`gsl_multiset_calloc()`* if you want to create a multiset which is initialized to the lexicographically first multiset element. A null pointer is returned if insufficient memory is available to create the multiset.

gsl_multiset ***`gsl_multiset_calloc`**(size_t n, size_t k)

This function allocates memory for a new multiset with parameters `n`, `k` and initializes it to the lexicographically first multiset element. A null pointer is returned if insufficient memory is available to create the multiset.

void **`gsl_multiset_init_first`**(*gsl_multiset* *c)

This function initializes the multiset `c` to the lexicographically first multiset element, i.e. 0 repeated k times.

void **`gsl_multiset_init_last`**(*gsl_multiset* *c)

This function initializes the multiset `c` to the lexicographically last multiset element, i.e. $n-1$ repeated k times.

void **gsl_multiset_free**(*gsl_multiset* *c)

This function frees all the memory used by the multiset `c`.

int **gsl_multiset_memcpy**(*gsl_multiset* *dest, const *gsl_multiset* *src)

This function copies the elements of the multiset `src` into the multiset `dest`. The two multisets must have the same size.

11.3 Accessing multiset elements

The following function can be used to access the elements of a multiset.

size_t **gsl_multiset_get**(const *gsl_multiset* *c, const size_t i)

This function returns the value of the `i`-th element of the multiset `c`. If `i` lies outside the allowed range of 0 to $k - 1$ then the error handler is invoked and 0 is returned. An inline version of this function is used when `HAVE_INLINE` is defined.

11.4 Multiset properties

size_t **gsl_multiset_n**(const *gsl_multiset* *c)

This function returns the range (n) of the multiset `c`.

size_t **gsl_multiset_k**(const *gsl_multiset* *c)

This function returns the number of elements (k) in the multiset `c`.

size_t ***gsl_multiset_data**(const *gsl_multiset* *c)

This function returns a pointer to the array of elements in the multiset `c`.

int **gsl_multiset_valid**(*gsl_multiset* *c)

This function checks that the multiset `c` is valid. The `k` elements should lie in the range 0 to $n - 1$, with each value occurring in nondecreasing order.

11.5 Multiset functions

int **gsl_multiset_next**(*gsl_multiset* *c)

This function advances the multiset `c` to the next multiset element in lexicographic order and returns `GSL_SUCCESS`. If no further multisets elements are available it returns `GSL_FAILURE` and leaves `c` unmodified. Starting with the first multiset and repeatedly applying this function will iterate through all possible multisets of a given order.

int **gsl_multiset_prev**(*gsl_multiset* *c)

This function steps backwards from the multiset `c` to the previous multiset element in lexicographic order, returning `GSL_SUCCESS`. If no previous multiset is available it returns `GSL_FAILURE` and leaves `c` unmodified.

11.6 Reading and writing multisets

The library provides functions for reading and writing multisets to a file as binary data or formatted text.

int **gsl_multiset_fwrite**(FILE *stream, const *gsl_multiset* *c)

This function writes the elements of the multiset `c` to the stream `stream` in binary format. The function returns `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

int **gsl_multiset_fread**(FILE *stream, *gsl_multiset* *c)

This function reads elements from the open stream `stream` into the multiset `c` in binary format. The multiset `c` must be preallocated with correct values of n and k since the function uses the size of `c` to determine how many bytes to read. The function returns `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

int **gsl_multiset_fprintf**(FILE *stream, const *gsl_multiset* *c, const char *format)

This function writes the elements of the multiset `c` line-by-line to the stream `stream` using the format specifier `format`, which should be suitable for a type of `size_t`. In ISO C99 the type modifier `z` represents `size_t`, so `"%zu\n"` is a suitable format[1]. The function returns `GSL_EFAILED` if there was a problem writing to the file.

int **gsl_multiset_fscanf**(FILE *stream, *gsl_multiset* *c)

This function reads formatted data from the stream `stream` into the multiset `c`. The multiset `c` must be preallocated with correct values of n and k since the function uses the size of `c` to determine how many numbers to read. The function returns `GSL_EFAILED` if there was a problem reading from the file.

11.7 Examples

The example program below prints all multisets elements containing the values $0, 1, 2, 3$ ordered by size. Multiset elements of the same size are ordered lexicographically.

```
#include <stdio.h>
#include <gsl/gsl_multiset.h>

int
main (void)
{
  gsl_multiset * c;
  size_t i;

  printf ("All multisets of {0,1,2,3} by size:\n") ;
  for (i = 0; i <= 4; i++)
    {
      c = gsl_multiset_calloc (4, i);
      do
        {
          printf ("{");
          gsl_multiset_fprintf (stdout, c, " %u");
          printf (" }\n");
        }
      while (gsl_multiset_next (c) == GSL_SUCCESS);
      gsl_multiset_free (c);
```

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[1] In versions of the GNU C library prior to the ISO C99 standard, the type modifier Z was used instead.

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```
    }

  return 0;
}
```

Here is the output from the program,

```
All multisets of {0,1,2,3} by size:
{ }
{ 0 }
{ 1 }
{ 2 }
{ 3 }
{ 0 0 }
{ 0 1 }
{ 0 2 }
{ 0 3 }
{ 1 1 }
{ 1 2 }
{ 1 3 }
{ 2 2 }
{ 2 3 }
{ 3 3 }
{ 0 0 0 }
{ 0 0 1 }
{ 0 0 2 }
{ 0 0 3 }
{ 0 1 1 }
{ 0 1 2 }
{ 0 1 3 }
{ 0 2 2 }
{ 0 2 3 }
{ 0 3 3 }
{ 1 1 1 }
{ 1 1 2 }
{ 1 1 3 }
{ 1 2 2 }
{ 1 2 3 }
{ 1 3 3 }
{ 2 2 2 }
{ 2 2 3 }
{ 2 3 3 }
{ 3 3 3 }
{ 0 0 0 0 }
{ 0 0 0 1 }
{ 0 0 0 2 }
{ 0 0 0 3 }
{ 0 0 1 1 }
{ 0 0 1 2 }
{ 0 0 1 3 }
{ 0 0 2 2 }
{ 0 0 2 3 }
```

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```
{ 0 0 3 3 }
{ 0 1 1 1 }
{ 0 1 1 2 }
{ 0 1 1 3 }
{ 0 1 2 2 }
{ 0 1 2 3 }
{ 0 1 3 3 }
{ 0 2 2 2 }
{ 0 2 2 3 }
{ 0 2 3 3 }
{ 0 3 3 3 }
{ 1 1 1 1 }
{ 1 1 1 2 }
{ 1 1 1 3 }
{ 1 1 2 2 }
{ 1 1 2 3 }
{ 1 1 3 3 }
{ 1 2 2 2 }
{ 1 2 2 3 }
{ 1 2 3 3 }
{ 1 3 3 3 }
{ 2 2 2 2 }
{ 2 2 2 3 }
{ 2 2 3 3 }
{ 2 3 3 3 }
{ 3 3 3 3 }
```

All 70 multisets are generated and sorted lexicographically.

CHAPTER

TWELVE

SORTING

This chapter describes functions for sorting data, both directly and indirectly (using an index). All the functions use the *heapsort* algorithm. Heapsort is an $O(N \log N)$ algorithm which operates in-place and does not require any additional storage. It also provides consistent performance, the running time for its worst-case (ordered data) being not significantly longer than the average and best cases. Note that the heapsort algorithm does not preserve the relative ordering of equal elements—it is an *unstable* sort. However the resulting order of equal elements will be consistent across different platforms when using these functions.

12.1 Sorting objects

The following function provides a simple alternative to the standard library function `qsort()`. It is intended for systems lacking `qsort()`, not as a replacement for it. The function `qsort()` should be used whenever possible, as it will be faster and can provide stable ordering of equal elements. Documentation for `qsort()` is available in the GNU C Library Reference Manual.

The functions described in this section are defined in the header file `gsl_heapsort.h`.

void **gsl_heapsort**(void *array, size_t count, size_t size, *gsl_comparison_fn_t* compare)

This function sorts the `count` elements of the array `array`, each of size `size`, into ascending order using the comparison function `compare`. The type of the comparison function is defined by

type **gsl_comparison_fn_t**

```
int (*gsl_comparison_fn_t) (const void * a, const void * b)
```

A comparison function should return a negative integer if the first argument is less than the second argument, `0` if the two arguments are equal and a positive integer if the first argument is greater than the second argument.

For example, the following function can be used to sort doubles into ascending numerical order.

```
int
compare_doubles (const double * a, const double * b)
{
  if (*a > *b)
    return 1;
  else if (*a < *b)
    return -1;
  else
    return 0;
}
```

The appropriate function call to perform the sort is:

```
gsl_heapsort (array, count, sizeof(double), compare_doubles);
```

Note that unlike `qsort()` the heapsort algorithm cannot be made into a stable sort by pointer arithmetic. The trick of comparing pointers for equal elements in the comparison function does not work for the heapsort algorithm. The heapsort algorithm performs an internal rearrangement of the data which destroys its initial ordering.

int **gsl_heapsort_index**(size_t *p, const void *array, size_t count, size_t size, gsl_comparison_fn_t compare)

This function indirectly sorts the *count* elements of the array *array*, each of size *size*, into ascending order using the comparison function *compare*. The resulting permutation is stored in *p*, an array of length `n`. The elements of *p* give the index of the array element which would have been stored in that position if the array had been sorted in place. The first element of *p* gives the index of the least element in *array*, and the last element of *p* gives the index of the greatest element in *array*. The array itself is not changed.

12.2 Sorting vectors

The following functions will sort the elements of an array or vector, either directly or indirectly. They are defined for all real and integer types using the normal suffix rules. For example, the `float` versions of the array functions are `gsl_sort_float()` and `gsl_sort_float_index()`. The corresponding vector functions are `gsl_sort_vector_float()` and `gsl_sort_vector_float_index()`. The prototypes are available in the header files `gsl_sort_float.h` `gsl_sort_vector_float.h`. The complete set of prototypes can be included using the header files `gsl_sort.h` and `gsl_sort_vector.h`.

There are no functions for sorting complex arrays or vectors, since the ordering of complex numbers is not uniquely defined. To sort a complex vector by magnitude compute a real vector containing the magnitudes of the complex elements, and sort this vector indirectly. The resulting index gives the appropriate ordering of the original complex vector.

void **gsl_sort**(double *data, const size_t stride, size_t n)

This function sorts the *n* elements of the array *data* with stride *stride* into ascending numerical order.

void **gsl_sort2**(double *data1, const size_t stride1, double *data2, const size_t stride2, size_t n)

This function sorts the *n* elements of the array *data1* with stride *stride1* into ascending numerical order, while making the same rearrangement of the array *data2* with stride *stride2*, also of size *n*.

void **gsl_sort_vector**(*gsl_vector* *v)

This function sorts the elements of the vector *v* into ascending numerical order.

void **gsl_sort_vector2**(*gsl_vector* *v1, *gsl_vector* *v2)

This function sorts the elements of the vector *v1* into ascending numerical order, while making the same rearrangement of the vector *v2*.

void **gsl_sort_index**(size_t *p, const double *data, size_t stride, size_t n)

This function indirectly sorts the *n* elements of the array *data* with stride *stride* into ascending order, storing the resulting permutation in *p*. The array *p* must be allocated with a sufficient length to store the *n* elements of the permutation. The elements of *p* give the index of the array element which would have been stored in that position if the array had been sorted in place. The array *data* is not changed.

int **gsl_sort_vector_index**(*gsl_permutation* *p, const *gsl_vector* *v)

This function indirectly sorts the elements of the vector *v* into ascending order, storing the resulting permutation in *p*. The elements of *p* give the index of the vector element which would have been stored in that position if the vector had been sorted in place. The first element of *p* gives the index of the least element in *v*, and the last element of *p* gives the index of the greatest element in *v*. The vector *v* is not changed.

12.3 Selecting the k smallest or largest elements

The functions described in this section select the k smallest or largest elements of a data set of size N. The routines use an $O(kN)$ direct insertion algorithm which is suited to subsets that are small compared with the total size of the dataset. For example, the routines are useful for selecting the 10 largest values from one million data points, but not for selecting the largest 100,000 values. If the subset is a significant part of the total dataset it may be faster to sort all the elements of the dataset directly with an $O(N \log N)$ algorithm and obtain the smallest or largest values that way.

int **gsl_sort_smallest**(double *dest, size_t k, const double *src, size_t stride, size_t n)

This function copies the `k` smallest elements of the array `src`, of size `n` and stride `stride`, in ascending numerical order into the array `dest`. The size `k` of the subset must be less than or equal to `n`. The data `src` is not modified by this operation.

int **gsl_sort_largest**(double *dest, size_t k, const double *src, size_t stride, size_t n)

This function copies the `k` largest elements of the array `src`, of size `n` and stride `stride`, in descending numerical order into the array `dest`. `k` must be less than or equal to `n`. The data `src` is not modified by this operation.

int **gsl_sort_vector_smallest**(double *dest, size_t k, const *gsl_vector* *v)

int **gsl_sort_vector_largest**(double *dest, size_t k, const *gsl_vector* *v)

These functions copy the `k` smallest or largest elements of the vector `v` into the array `dest`. `k` must be less than or equal to the length of the vector `v`.

The following functions find the indices of the k smallest or largest elements of a dataset.

int **gsl_sort_smallest_index**(size_t *p, size_t k, const double *src, size_t stride, size_t n)

This function stores the indices of the `k` smallest elements of the array `src`, of size `n` and stride `stride`, in the array `p`. The indices are chosen so that the corresponding data is in ascending numerical order. `k` must be less than or equal to `n`. The data `src` is not modified by this operation.

int **gsl_sort_largest_index**(size_t *p, size_t k, const double *src, size_t stride, size_t n)

This function stores the indices of the `k` largest elements of the array `src`, of size `n` and stride `stride`, in the array `p`. The indices are chosen so that the corresponding data is in descending numerical order. `k` must be less than or equal to `n`. The data `src` is not modified by this operation.

int **gsl_sort_vector_smallest_index**(size_t *p, size_t k, const *gsl_vector* *v)

int **gsl_sort_vector_largest_index**(size_t *p, size_t k, const *gsl_vector* *v)

These functions store the indices of the `k` smallest or largest elements of the vector `v` in the array `p`. `k` must be less than or equal to the length of the vector `v`.

12.4 Computing the rank

The *rank* of an element is its order in the sorted data. The rank is the inverse of the index permutation, p. It can be computed using the following algorithm:

```
for (i = 0; i < p->size; i++)
  {
    size_t pi = p->data[i];
    rank->data[pi] = i;
  }
```

This can be computed directly from the function `gsl_permutation_inverse(rank,p)`.

The following function will print the rank of each element of the vector v:

```
void
print_rank (gsl_vector * v)
{
  size_t i;
  size_t n = v->size;
  gsl_permutation * perm = gsl_permutation_alloc(n);
  gsl_permutation * rank = gsl_permutation_alloc(n);

  gsl_sort_vector_index (perm, v);
  gsl_permutation_inverse (rank, perm);

  for (i = 0; i < n; i++)
    {
      double vi = gsl_vector_get(v, i);
      printf ("element = %d, value = %g, rank = %d\n",
                   i, vi, rank->data[i]);
    }

  gsl_permutation_free (perm);
  gsl_permutation_free (rank);
}
```

12.5 Examples

The following example shows how to use the permutation p to print the elements of the vector v in ascending order:

```
gsl_sort_vector_index (p, v);

for (i = 0; i < v->size; i++)
  {
    double vpi = gsl_vector_get (v, p->data[i]);
    printf ("order = %d, value = %g\n", i, vpi);
  }
```

The next example uses the function `gsl_sort_smallest()` to select the 5 smallest numbers from 100000 uniform random variates stored in an array,

```
#include <gsl/gsl_rng.h>
#include <gsl/gsl_sort_double.h>

int
main (void)
{
  const gsl_rng_type * T;
  gsl_rng * r;

  size_t i, k = 5, N = 100000;

  double * x = malloc (N * sizeof(double));
  double * small = malloc (k * sizeof(double));

```

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```
  gsl_rng_env_setup();

  T = gsl_rng_default;
  r = gsl_rng_alloc (T);

  for (i = 0; i < N; i++)
    {
      x[i] = gsl_rng_uniform(r);
    }

  gsl_sort_smallest (small, k, x, 1, N);

  printf ("%zu smallest values from %zu\n", k, N);

  for (i = 0; i < k; i++)
    {
      printf ("%zu: %.18f\n", i, small[i]);
    }

  free (x);
  free (small);
  gsl_rng_free (r);
  return 0;
}
```

The output lists the 5 smallest values, in ascending order,

```
5 smallest values from 100000
0: 0.000003489200025797
1: 0.000008199829608202
2: 0.000008953968062997
3: 0.000010712770745158
4: 0.000033531803637743
```

12.6 References and Further Reading

The subject of sorting is covered extensively in the following,

- Donald E. Knuth, The Art of Computer Programming: Sorting and Searching (Vol 3, 3rd Ed, 1997), Addison-Wesley, ISBN 0201896850.

The Heapsort algorithm is described in the following book,

- Robert Sedgewick, Algorithms in C, Addison-Wesley, ISBN 0201514257.

CHAPTER

THIRTEEN

BLAS SUPPORT

The Basic Linear Algebra Subprograms (BLAS) define a set of fundamental operations on vectors and matrices which can be used to create optimized higher-level linear algebra functionality.

The library provides a low-level layer which corresponds directly to the C-language BLAS standard, referred to here as "CBLAS", and a higher-level interface for operations on GSL vectors and matrices. Users who are interested in simple operations on GSL vector and matrix objects should use the high-level layer described in this chapter. The functions are declared in the file `gsl_blas.h` and should satisfy the needs of most users.

Note that GSL matrices are implemented using dense-storage so the interface only includes the corresponding dense-storage BLAS functions. The full BLAS functionality for band-format and packed-format matrices is available through the low-level CBLAS interface. Similarly, GSL vectors are restricted to positive strides, whereas the low-level CBLAS interface supports negative strides as specified in the BLAS standard[1].

The interface for the `gsl_cblas` layer is specified in the file `gsl_cblas.h`. This interface corresponds to the BLAS Technical Forum's standard for the C interface to legacy BLAS implementations. Users who have access to other conforming CBLAS implementations can use these in place of the version provided by the library. Note that users who have only a Fortran BLAS library can use a CBLAS conformant wrapper to convert it into a CBLAS library. A reference CBLAS wrapper for legacy Fortran implementations exists as part of the CBLAS standard and can be obtained from Netlib. The complete set of CBLAS functions is listed in an *appendix*.

There are three levels of BLAS operations,

Level 1	Vector operations, e.g. $y = \alpha x + y$
Level 2	Matrix-vector operations, e.g. $y = \alpha Ax + \beta y$
Level 3	Matrix-matrix operations, e.g. $C = \alpha AB + C$

Each routine has a name which specifies the operation, the type of matrices involved and their precisions. Some of the most common operations and their names are given below,

DOT	scalar product, $x^T y$
AXPY	vector sum, $\alpha x + y$
MV	matrix-vector product, Ax
SV	matrix-vector solve, $inv(A)x$
MM	matrix-matrix product, AB
SM	matrix-matrix solve, $inv(A)B$

The types of matrices are,

[1] In the low-level CBLAS interface, a negative stride accesses the vector elements in reverse order, i.e. the i-th element is given by $(N-i) * |incx|$ for $incx < 0$.

GE	general
GB	general band
SY	symmetric
SB	symmetric band
SP	symmetric packed
HE	hermitian
HB	hermitian band
HP	hermitian packed
TR	triangular
TB	triangular band
TP	triangular packed

Each operation is defined for four precisions,

S	single real
D	double real
C	single complex
Z	double complex

Thus, for example, the name SGEMM stands for "single-precision general matrix-matrix multiply" and ZGEMM stands for "double-precision complex matrix-matrix multiply".

Note that the vector and matrix arguments to BLAS functions must not be aliased, as the results are undefined when the underlying arrays overlap (*Aliasing of arrays*).

13.1 GSL BLAS Interface

GSL provides dense vector and matrix objects, based on the relevant built-in types. The library provides an interface to the BLAS operations which apply to these objects. The interface to this functionality is given in the file `gsl_blas.h`.

13.1.1 Level 1

int **`gsl_blas_sdsdot`**(float alpha, const gsl_vector_float *x, const gsl_vector_float *y, float *result)

This function computes the sum $\alpha + x^T y$ for the vectors `x` and `y`, returning the result in `result`.

int **`gsl_blas_sdot`**(const gsl_vector_float *x, const gsl_vector_float *y, float *result)

int **`gsl_blas_dsdot`**(const gsl_vector_float *x, const gsl_vector_float *y, double *result)

int **`gsl_blas_ddot`**(const *gsl_vector* *x, const *gsl_vector* *y, double *result)

These functions compute the scalar product $x^T y$ for the vectors `x` and `y`, returning the result in `result`.

int **`gsl_blas_cdotu`**(const gsl_vector_complex_float *x, const gsl_vector_complex_float *y, gsl_complex_float *dotu)

int **`gsl_blas_zdotu`**(const gsl_vector_complex *x, const gsl_vector_complex *y, gsl_complex *dotu)

These functions compute the complex scalar product $x^T y$ for the vectors `x` and `y`, returning the result in `dotu`

int **`gsl_blas_cdotc`**(const gsl_vector_complex_float *x, const gsl_vector_complex_float *y, gsl_complex_float *dotc)

int **gsl_blas_zdotc**(const gsl_vector_complex *x, const gsl_vector_complex *y, gsl_complex *dotc)
: These functions compute the complex conjugate scalar product $x^H y$ for the vectors `x` and `y`, returning the result in `dotc`

float **gsl_blas_snrm2**(const gsl_vector_float *x)

double **gsl_blas_dnrm2**(const *gsl_vector* *x)
: These functions compute the Euclidean norm $||x||_2 = \sqrt{\sum x_i^2}$ of the vector `x`.

float **gsl_blas_scnrm2**(const gsl_vector_complex_float *x)

double **gsl_blas_dznrm2**(const gsl_vector_complex *x)
: These functions compute the Euclidean norm of the complex vector `x`,

$$||x||_2 = \sqrt{\sum (\Re(x_i)^2 + \Im(x_i)^2)}.$$

float **gsl_blas_sasum**(const gsl_vector_float *x)

double **gsl_blas_dasum**(const *gsl_vector* *x)
: These functions compute the absolute sum $\sum |x_i|$ of the elements of the vector `x`.

float **gsl_blas_scasum**(const gsl_vector_complex_float *x)

double **gsl_blas_dzasum**(const gsl_vector_complex *x)
: These functions compute the sum of the magnitudes of the real and imaginary parts of the complex vector `x`, $\sum (|\Re(x_i)| + |\Im(x_i)|)$.

CBLAS_INDEX_t **gsl_blas_isamax**(const gsl_vector_float *x)

CBLAS_INDEX_t **gsl_blas_idamax**(const *gsl_vector* *x)

CBLAS_INDEX_t **gsl_blas_icamax**(const gsl_vector_complex_float *x)

CBLAS_INDEX_t **gsl_blas_izamax**(const gsl_vector_complex *x)
: These functions return the index of the largest element of the vector `x`. The largest element is determined by its absolute magnitude for real vectors and by the sum of the magnitudes of the real and imaginary parts $|\Re(x_i)| + |\Im(x_i)|$ for complex vectors. If the largest value occurs several times then the index of the first occurrence is returned.

int **gsl_blas_sswap**(gsl_vector_float *x, gsl_vector_float *y)

int **gsl_blas_dswap**(*gsl_vector* *x, *gsl_vector* *y)

int **gsl_blas_cswap**(gsl_vector_complex_float *x, gsl_vector_complex_float *y)

int **gsl_blas_zswap**(gsl_vector_complex *x, gsl_vector_complex *y)
: These functions exchange the elements of the vectors `x` and `y`.

int **gsl_blas_scopy**(const gsl_vector_float *x, gsl_vector_float *y)

int **gsl_blas_dcopy**(const *gsl_vector* *x, *gsl_vector* *y)

int **gsl_blas_ccopy**(const gsl_vector_complex_float *x, gsl_vector_complex_float *y) int **gsl_blas_zcopy**(const gsl_vector_complex *x, gsl_vector_complex *y)

These functions copy the elements of the vector `x` into the vector `y`.

int **gsl_blas_saxpy**(float alpha, const gsl_vector_float *x, gsl_vector_float *y)

int **gsl_blas_daxpy**(double alpha, const *gsl_vector* *x, *gsl_vector* *y)

int **gsl_blas_caxpy**(const gsl_complex_float alpha, const gsl_vector_complex_float *x, gsl_vector_complex_float *y)

int **gsl_blas_zaxpy**(const gsl_complex alpha, const gsl_vector_complex *x, gsl_vector_complex *y)

These functions compute the sum $y = \alpha x + y$ for the vectors `x` and `y`.

void **gsl_blas_sscal**(float alpha, gsl_vector_float *x)

void **gsl_blas_dscal**(double alpha, *gsl_vector* *x)

void **gsl_blas_cscal**(const gsl_complex_float alpha, gsl_vector_complex_float *x)

void **gsl_blas_zscal**(const gsl_complex alpha, gsl_vector_complex *x)

void **gsl_blas_csscal**(float alpha, gsl_vector_complex_float *x)

void **gsl_blas_zdscal**(double alpha, gsl_vector_complex *x)

These functions rescale the vector `x` by the multiplicative factor `alpha`.

int **gsl_blas_srotg**(float a[], float b[], float c[], float s[])

int **gsl_blas_drotg**(double a[], double b[], double c[], double s[])

These functions compute a Givens rotation (c, s) which zeroes the vector (a, b),

$$\begin{pmatrix} c & s \\ -s & c \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} r' \\ 0 \end{pmatrix}$$

The variables `a` and `b` are overwritten by the routine.

int **gsl_blas_srot**(gsl_vector_float *x, gsl_vector_float *y, float c, float s)

int **gsl_blas_drot**(*gsl_vector* *x, *gsl_vector* *y, const double c, const double s)

These functions apply a Givens rotation $(x', y') = (cx + sy, -sx + cy)$ to the vectors `x`, `y`.

int **gsl_blas_srotmg**(float d1[], float d2[], float b1[], float b2, float P[])

int **gsl_blas_drotmg**(double d1[], double d2[], double b1[], double b2, double P[])

These functions compute a modified Givens transformation. The modified Givens transformation is defined in the original Level-1 BLAS specification, given in the references.

int **gsl_blas_srotm**(gsl_vector_float *x, gsl_vector_float *y, const float P[])

int **gsl_blas_drotm**(*gsl_vector* *x, *gsl_vector* *y, const double P[])

These functions apply a modified Givens transformation.

13.1.2 Level 2

int **gsl_blas_sgemv**(CBLAS_TRANSPOSE_t TransA, float alpha, const gsl_matrix_float *A, const gsl_vector_float *x, float beta, gsl_vector_float *y)

int **gsl_blas_dgemv**(CBLAS_TRANSPOSE_t TransA, double alpha, const *gsl_matrix* *A, const *gsl_vector* *x, double beta, *gsl_vector* *y)

int **gsl_blas_cgemv**(CBLAS_TRANSPOSE_t TransA, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, const gsl_vector_complex_float *x, const gsl_complex_float beta, gsl_vector_complex_float *y)

int **gsl_blas_zgemv**(CBLAS_TRANSPOSE_t TransA, const gsl_complex alpha, const gsl_matrix_complex *A, const gsl_vector_complex *x, const gsl_complex beta, gsl_vector_complex *y)

These functions compute the matrix-vector product and sum $y = \alpha op(A)x + \beta y$, where $op(A) = A$, A^T, A^H for `TransA` = `CblasNoTrans`, `CblasTrans`, `CblasConjTrans`.

int **gsl_blas_strmv**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_matrix_float *A, gsl_vector_float *x)

int **gsl_blas_dtrmv**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const *gsl_matrix* *A, *gsl_vector* *x)

int **gsl_blas_ctrmv**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_matrix_complex_float *A, gsl_vector_complex_float *x)

int **gsl_blas_ztrmv**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_matrix_complex *A, gsl_vector_complex *x)

These functions compute the matrix-vector product $x = op(A)x$ for the triangular matrix `A`, where $op(A) = A$, A^T, A^H for `TransA` = `CblasNoTrans`, `CblasTrans`, `CblasConjTrans`. When `Uplo` is `CblasUpper` then the upper triangle of `A` is used, and when `Uplo` is `CblasLower` then the lower triangle of `A` is used. If `Diag` is `CblasNonUnit` then the diagonal of the matrix is used, but if `Diag` is `CblasUnit` then the diagonal elements of the matrix `A` are taken as unity and are not referenced.

int **gsl_blas_strsv**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_matrix_float *A, gsl_vector_float *x)

int **gsl_blas_dtrsv**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const *gsl_matrix* *A, *gsl_vector* *x)

int **gsl_blas_ctrsv**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_matrix_complex_float *A, gsl_vector_complex_float *x)

int **gsl_blas_ztrsv**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_matrix_complex *A, gsl_vector_complex *x)

These functions compute $inv(op(A))x$ for `x`, where $op(A) = A$, A^T, A^H for `TransA` = `CblasNoTrans`, `CblasTrans`, `CblasConjTrans`. When `Uplo` is `CblasUpper` then the upper triangle of `A` is used, and when `Uplo` is `CblasLower` then the lower triangle of `A` is used. If `Diag` is `CblasNonUnit` then the diagonal of the matrix is used, but if `Diag` is `CblasUnit` then the diagonal elements of the matrix `A` are taken as unity and are not referenced.

int **gsl_blas_ssymv**(CBLAS_UPLO_t Uplo, float alpha, const gsl_matrix_float *A, const gsl_vector_float *x, float beta, gsl_vector_float *y) int **gsl_blas_dsymv**(CBLAS_UPLO_t Uplo, double alpha, const *gsl_matrix* *A, const *gsl_vector* *x, double beta, *gsl_vector* *y)

These functions compute the matrix-vector product and sum $y = \alpha A x + \beta y$ for the symmetric matrix `A`. Since the matrix `A` is symmetric only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `A` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `A` are used.

int **gsl_blas_chemv**(CBLAS_UPLO_t Uplo, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, const gsl_vector_complex_float *x, const gsl_complex_float beta, gsl_vector_complex_float *y)

int **gsl_blas_zhemv**(CBLAS_UPLO_t Uplo, const gsl_complex alpha, const gsl_matrix_complex *A, const gsl_vector_complex *x, const gsl_complex beta, gsl_vector_complex *y)

These functions compute the matrix-vector product and sum $y = \alpha A x + \beta y$ for the hermitian matrix `A`. Since the matrix `A` is hermitian only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `A` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `A` are used. The imaginary elements of the diagonal are automatically assumed to be zero and are not referenced.

int **gsl_blas_sger**(float alpha, const gsl_vector_float *x, const gsl_vector_float *y, gsl_matrix_float *A)

int **gsl_blas_dger**(double alpha, const *gsl_vector* *x, const *gsl_vector* *y, *gsl_matrix* *A)

int **gsl_blas_cgeru**(const gsl_complex_float alpha, const gsl_vector_complex_float *x, const gsl_vector_complex_float *y, gsl_matrix_complex_float *A)

int **gsl_blas_zgeru**(const gsl_complex alpha, const gsl_vector_complex *x, const gsl_vector_complex *y, gsl_matrix_complex *A)

These functions compute the rank-1 update $A = \alpha x y^T + A$ of the matrix `A`.

int **gsl_blas_cgerc**(const gsl_complex_float alpha, const gsl_vector_complex_float *x, const gsl_vector_complex_float *y, gsl_matrix_complex_float *A)

int **gsl_blas_zgerc**(const gsl_complex alpha, const gsl_vector_complex *x, const gsl_vector_complex *y, gsl_matrix_complex *A)

These functions compute the conjugate rank-1 update $A = \alpha x y^H + A$ of the matrix `A`.

int **gsl_blas_ssyr**(CBLAS_UPLO_t Uplo, float alpha, const gsl_vector_float *x, gsl_matrix_float *A)

int **gsl_blas_dsyr**(CBLAS_UPLO_t Uplo, double alpha, const *gsl_vector* *x, *gsl_matrix* *A)

These functions compute the symmetric rank-1 update $A = \alpha x x^T + A$ of the symmetric matrix `A`. Since the matrix `A` is symmetric only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `A` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `A` are used.

int **gsl_blas_cher**(CBLAS_UPLO_t Uplo, float alpha, const gsl_vector_complex_float *x, gsl_matrix_complex_float *A)

int **gsl_blas_zher**(CBLAS_UPLO_t Uplo, double alpha, const gsl_vector_complex *x, gsl_matrix_complex *A)

These functions compute the hermitian rank-1 update $A = \alpha x x^H + A$ of the hermitian matrix `A`. Since the matrix `A` is hermitian only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `A` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `A` are used. The imaginary elements of the diagonal are automatically set to zero.

int **gsl_blas_ssyr2**(CBLAS_UPLO_t Uplo, float alpha, const gsl_vector_float *x, const gsl_vector_float *y, gsl_matrix_float *A)

int **gsl_blas_dsyr2**(CBLAS_UPLO_t Uplo, double alpha, const *gsl_vector* *x, const *gsl_vector* *y, *gsl_matrix* *A)

These functions compute the symmetric rank-2 update $A = \alpha x y^T + \alpha y x^T + A$ of the symmetric matrix `A`. Since the matrix `A` is symmetric only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `A` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `A` are used.

int **gsl_blas_cher2**(CBLAS_UPLO_t Uplo, const gsl_complex_float alpha, const gsl_vector_complex_float *x, const gsl_vector_complex_float *y, gsl_matrix_complex_float *A)

int **gsl_blas_zher2**(CBLAS_UPLO_t Uplo, const gsl_complex alpha, const gsl_vector_complex *x, const gsl_vector_complex *y, gsl_matrix_complex *A)

These functions compute the hermitian rank-2 update $A = \alpha x y^H + \alpha^* y x^H + A$ of the hermitian matrix `A`. Since the matrix `A` is hermitian only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `A` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `A` are used. The imaginary elements of the diagonal are automatically set to zero.

13.1.3 Level 3

int **gsl_blas_sgemm**(CBLAS_TRANSPOSE_t TransA, CBLAS_TRANSPOSE_t TransB, float alpha, const gsl_matrix_float *A, const gsl_matrix_float *B, float beta, gsl_matrix_float *C)

int **gsl_blas_dgemm**(CBLAS_TRANSPOSE_t TransA, CBLAS_TRANSPOSE_t TransB, double alpha, const *gsl_matrix* *A, const *gsl_matrix* *B, double beta, *gsl_matrix* *C)

int **gsl_blas_cgemm**(CBLAS_TRANSPOSE_t TransA, CBLAS_TRANSPOSE_t TransB, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, const gsl_matrix_complex_float *B, const gsl_complex_float beta, gsl_matrix_complex_float *C)

int **gsl_blas_zgemm**(CBLAS_TRANSPOSE_t TransA, CBLAS_TRANSPOSE_t TransB, const gsl_complex alpha, const gsl_matrix_complex *A, const gsl_matrix_complex *B, const gsl_complex beta, gsl_matrix_complex *C)

These functions compute the matrix-matrix product and sum $C = \alpha op(A) op(B) + \beta C$ where $op(A) = A$, A^T, A^H for `TransA` = `CblasNoTrans`, `CblasTrans`, `CblasConjTrans` and similarly for the parameter `TransB`.

int **gsl_blas_ssymm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, float alpha, const gsl_matrix_float *A, const gsl_matrix_float *B, float beta, gsl_matrix_float *C)

int **gsl_blas_dsymm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, double alpha, const *gsl_matrix* *A, const *gsl_matrix* *B, double beta, *gsl_matrix* *C)

int **gsl_blas_csymm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, const gsl_matrix_complex_float *B, const gsl_complex_float beta, gsl_matrix_complex_float *C)

int **gsl_blas_zsymm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, const gsl_complex alpha, const gsl_matrix_complex *A, const gsl_matrix_complex *B, const gsl_complex beta, gsl_matrix_complex *C)

These functions compute the matrix-matrix product and sum $C = \alpha AB + \beta C$ for `Side` is `CblasLeft` and

$C = \alpha BA + \beta C$ for `Side` is `CblasRight`, where the matrix `A` is symmetric. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `A` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `A` are used.

int **gsl_blas_chemm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, const gsl_matrix_complex_float *B, const gsl_complex_float beta, gsl_matrix_complex_float *C)

int **gsl_blas_zhemm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, const gsl_complex alpha, const gsl_matrix_complex *A, const gsl_matrix_complex *B, const gsl_complex beta, gsl_matrix_complex *C)

These functions compute the matrix-matrix product and sum $C = \alpha AB + \beta C$ for `Side` is `CblasLeft` and $C = \alpha BA + \beta C$ for `Side` is `CblasRight`, where the matrix `A` is hermitian. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `A` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `A` are used. The imaginary elements of the diagonal are automatically set to zero.

int **gsl_blas_strmm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, float alpha, const gsl_matrix_float *A, gsl_matrix_float *B)

int **gsl_blas_dtrmm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, double alpha, const *gsl_matrix* *A, *gsl_matrix* *B)

int **gsl_blas_ctrmm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, gsl_matrix_complex_float *B)

int **gsl_blas_ztrmm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_complex alpha, const gsl_matrix_complex *A, gsl_matrix_complex *B)

These functions compute the matrix-matrix product $B = \alpha op(A)B$ for `Side` is `CblasLeft` and $B = \alpha Bop(A)$ for `Side` is `CblasRight`. The matrix `A` is triangular and $op(A) = A, A^T, A^H$ for `TransA` = `CblasNoTrans`, `CblasTrans`, `CblasConjTrans`. When `Uplo` is `CblasUpper` then the upper triangle of `A` is used, and when `Uplo` is `CblasLower` then the lower triangle of `A` is used. If `Diag` is `CblasNonUnit` then the diagonal of `A` is used, but if `Diag` is `CblasUnit` then the diagonal elements of the matrix `A` are taken as unity and are not referenced.

int **gsl_blas_strsm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, float alpha, const gsl_matrix_float *A, gsl_matrix_float *B)

int **gsl_blas_dtrsm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, double alpha, const *gsl_matrix* *A, *gsl_matrix* *B)

int **gsl_blas_ctrsm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, gsl_matrix_complex_float *B)

int **gsl_blas_ztrsm**(CBLAS_SIDE_t Side, CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t TransA, CBLAS_DIAG_t Diag, const gsl_complex alpha, const gsl_matrix_complex *A, gsl_matrix_complex *B)

These functions compute the inverse-matrix matrix product $B = \alpha op(inv(A))B$ for `Side` is `CblasLeft` and $B = \alpha Bop(inv(A))$ for `Side` is `CblasRight`. The matrix `A` is triangular and $op(A) = A, A^T, A^H$ for `TransA` = `CblasNoTrans`, `CblasTrans`, `CblasConjTrans`. When `Uplo` is `CblasUpper` then the upper triangle of `A` is used, and when `Uplo` is `CblasLower` then the lower triangle of `A` is used. If `Diag` is `CblasNonUnit` then the diagonal of `A` is used, but if `Diag` is `CblasUnit` then the diagonal elements of the matrix `A` are taken as unity and are not referenced.

int **gsl_blas_ssyrk**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, float alpha, const gsl_matrix_float *A, float beta, gsl_matrix_float *C)

int **gsl_blas_dsyrk**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, double alpha, const *gsl_matrix* *A, double beta, *gsl_matrix* *C)

int **gsl_blas_csyrk**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, const gsl_complex_float beta, gsl_matrix_complex_float *C)

int **gsl_blas_zsyrk**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, const gsl_complex alpha, const gsl_matrix_complex *A, const gsl_complex beta, gsl_matrix_complex *C)

These functions compute a rank-k update of the symmetric matrix `C`, $C = \alpha AA^T + \beta C$ when `Trans` is `CblasNoTrans` and $C = \alpha A^T A + \beta C$ when `Trans` is `CblasTrans`. Since the matrix `C` is symmetric only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `C` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `C` are used.

int **gsl_blas_cherk**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, float alpha, const gsl_matrix_complex_float *A, float beta, gsl_matrix_complex_float *C)

int **gsl_blas_zherk**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, double alpha, const gsl_matrix_complex *A, double beta, gsl_matrix_complex *C)

These functions compute a rank-k update of the hermitian matrix `C`, $C = \alpha AA^H + \beta C$ when `Trans` is `CblasNoTrans` and $C = \alpha A^H A + \beta C$ when `Trans` is `CblasConjTrans`. Since the matrix `C` is hermitian only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `C` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `C` are used. The imaginary elements of the diagonal are automatically set to zero.

int **gsl_blas_ssyr2k**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, float alpha, const gsl_matrix_float *A, const gsl_matrix_float *B, float beta, gsl_matrix_float *C)

int **gsl_blas_dsyr2k**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, double alpha, const *gsl_matrix* *A, const *gsl_matrix* *B, double beta, *gsl_matrix* *C)

int **gsl_blas_csyr2k**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, const gsl_matrix_complex_float *B, const gsl_complex_float beta, gsl_matrix_complex_float *C)

int **gsl_blas_zsyr2k**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, const gsl_complex alpha, const gsl_matrix_complex *A, const gsl_matrix_complex *B, const gsl_complex beta, gsl_matrix_complex *C)

These functions compute a rank-2k update of the symmetric matrix `C`, $C = \alpha AB^T + \alpha BA^T + \beta C$ when `Trans` is `CblasNoTrans` and $C = \alpha A^T B + \alpha B^T A + \beta C$ when `Trans` is `CblasTrans`. Since the matrix `C` is symmetric only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `C` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `C` are used.

int **gsl_blas_cher2k**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, const gsl_complex_float alpha, const gsl_matrix_complex_float *A, const gsl_matrix_complex_float *B, float beta, gsl_matrix_complex_float *C) int **gsl_blas_zher2k**(CBLAS_UPLO_t Uplo, CBLAS_TRANSPOSE_t Trans, const gsl_complex alpha, const gsl_matrix_complex *A, const gsl_matrix_complex *B, double beta, gsl_matrix_complex *C)

These functions compute a rank-2k update of the hermitian matrix `C`, $C = \alpha A B^H + \alpha^* B A^H + \beta C$ when `Trans` is `CblasNoTrans` and $C = \alpha A^H B + \alpha^* B^H A + \beta C$ when `Trans` is `CblasConjTrans`. Since the matrix `C` is hermitian only its upper half or lower half need to be stored. When `Uplo` is `CblasUpper` then the upper triangle and diagonal of `C` are used, and when `Uplo` is `CblasLower` then the lower triangle and diagonal of `C` are used. The imaginary elements of the diagonal are automatically set to zero.

13.2 Examples

The following program computes the product of two matrices using the Level-3 BLAS function DGEMM,

$$\begin{pmatrix} 0.11 & 0.12 & 0.13 \\ 0.21 & 0.22 & 0.23 \end{pmatrix} \begin{pmatrix} 1011 & 1012 \\ 1021 & 1022 \\ 1031 & 1031 \end{pmatrix} = \begin{pmatrix} 367.76 & 368.12 \\ 674.06 & 674.72 \end{pmatrix}$$

The matrices are stored in row major order, according to the C convention for arrays.

```
#include <stdio.h>
#include <gsl/gsl_blas.h>

int
main (void)
{
  double a[] = { 0.11, 0.12, 0.13,
                 0.21, 0.22, 0.23 };

  double b[] = { 1011, 1012,
                 1021, 1022,
                 1031, 1032 };

  double c[] = { 0.00, 0.00,
                 0.00, 0.00 };

  gsl_matrix_view A = gsl_matrix_view_array(a, 2, 3);
  gsl_matrix_view B = gsl_matrix_view_array(b, 3, 2);
  gsl_matrix_view C = gsl_matrix_view_array(c, 2, 2);

  /* Compute C = A B */

  gsl_blas_dgemm (CblasNoTrans, CblasNoTrans,
                  1.0, &A.matrix, &B.matrix,
                  0.0, &C.matrix);

  printf ("[ %g, %g\n", c[0], c[1]);
  printf ("  %g, %g ]\n", c[2], c[3]);

  return 0;
}
```

Here is the output from the program,

```
[ 367.76, 368.12
  674.06, 674.72 ]
```

13.3 References and Further Reading

Information on the BLAS standards, including both the legacy and updated interface standards, is available online from the BLAS Homepage and BLAS Technical Forum web-site.

- BLAS Homepage, http://www.netlib.org/blas/
- BLAS Technical Forum, http://www.netlib.org/blas/blast-forum/

The following papers contain the specifications for Level 1, Level 2 and Level 3 BLAS.

- C. Lawson, R. Hanson, D. Kincaid, F. Krogh, "Basic Linear Algebra Subprograms for Fortran Usage", ACM Transactions on Mathematical Software, Vol.: 5 (1979), Pages 308–325.
- J.J. Dongarra, J. DuCroz, S. Hammarling, R. Hanson, "An Extended Set of Fortran Basic Linear Algebra Subprograms", ACM Transactions on Mathematical Software, Vol.: 14, No.: 1 (1988), Pages 1–32.
- J.J. Dongarra, I. Duff, J. DuCroz, S. Hammarling, "A Set of Level 3 Basic Linear Algebra Subprograms", ACM Transactions on Mathematical Software, Vol.: 16 (1990), Pages 1–28.

Postscript versions of the latter two papers are available from http://www.netlib.org/blas/. A CBLAS wrapper for Fortran BLAS libraries is available from the same location.

CHAPTER

FOURTEEN

LINEAR ALGEBRA

This chapter describes functions for solving linear systems. The library provides linear algebra operations which operate directly on the `gsl_vector` and `gsl_matrix` objects. These routines use the standard algorithms from Golub & Van Loan's *Matrix Computations* with Level-1 and Level-2 BLAS calls for efficiency.

The functions described in this chapter are declared in the header file `gsl_linalg.h`.

14.1 LU Decomposition

A general M-by-N matrix A has an LU decomposition

$$PA = LU$$

where P is an M-by-M permutation matrix, L is M-by-$\min(M, N)$ and U is $\min(M, N)$-by-N. For square matrices, L is a lower unit triangular matrix and U is upper triangular. For $M > N$, L is a unit lower trapezoidal matrix of size M-by-N. For $M < N$, U is upper trapezoidal of size M-by-N. For square matrices this decomposition can be used to convert the linear system $Ax = b$ into a pair of triangular systems ($Ly = Pb$, $Ux = y$), which can be solved by forward and back-substitution. Note that the LU decomposition is valid for singular matrices.

int **gsl_linalg_LU_decomp**(*gsl_matrix* *A, *gsl_permutation* *p, int *signum)

int **gsl_linalg_complex_LU_decomp**(gsl_matrix_complex *A, *gsl_permutation* *p, int *signum)

These functions factorize the matrix `A` into the LU decomposition $PA = LU$. On output the diagonal and upper triangular (or trapezoidal) part of the input matrix `A` contain the matrix U. The lower triangular (or trapezoidal) part of the input matrix (excluding the diagonal) contains L. The diagonal elements of L are unity, and are not stored.

The permutation matrix P is encoded in the permutation `p` on output. The j-th column of the matrix P is given by the k-th column of the identity matrix, where $k = p_j$ the j-th element of the permutation vector. The sign of the permutation is given by `signum`. It has the value $(-1)^n$, where n is the number of interchanges in the permutation.

The algorithm used in the decomposition is Gaussian Elimination with partial pivoting (Golub & Van Loan, *Matrix Computations*, Algorithm 3.4.1), combined with a recursive algorithm based on Level 3 BLAS (Peise and Bientinesi, 2016).

int **gsl_linalg_LU_solve**(const *gsl_matrix* *LU, const *gsl_permutation* *p, const *gsl_vector* *b, *gsl_vector* *x)

int **gsl_linalg_complex_LU_solve**(const gsl_matrix_complex *LU, const *gsl_permutation* *p, const gsl_vector_complex *b, gsl_vector_complex *x)

These functions solve the square system $Ax = b$ using the LU decomposition of A into (`LU`, `p`) given by `gsl_linalg_LU_decomp()` or `gsl_linalg_complex_LU_decomp()` as input.

int **gsl_linalg_LU_svx**(const *gsl_matrix* *LU, const *gsl_permutation* *p, *gsl_vector* *x)

int **gsl_linalg_complex_LU_svx**(const gsl_matrix_complex *LU, const *gsl_permutation* *p, gsl_vector_complex *x)

These functions solve the square system $Ax = b$ in-place using the precomputed LU decomposition of A into (`LU`, `p`). On input `x` should contain the right-hand side b, which is replaced by the solution on output.

int **gsl_linalg_LU_refine**(const *gsl_matrix* *A, const *gsl_matrix* *LU, const *gsl_permutation* *p, const *gsl_vector* *b, *gsl_vector* *x, *gsl_vector* *work)

int **gsl_linalg_complex_LU_refine**(const gsl_matrix_complex *A, const gsl_matrix_complex *LU, const *gsl_permutation* *p, const gsl_vector_complex *b, gsl_vector_complex *x, gsl_vector_complex *work)

These functions apply an iterative improvement to `x`, the solution of $Ax = b$, from the precomputed LU decomposition of A into (`LU`, `p`). Additional workspace of length `N` is required in `work`.

int **gsl_linalg_LU_invert**(const *gsl_matrix* *LU, const *gsl_permutation* *p, *gsl_matrix* *inverse)

int **gsl_linalg_complex_LU_invert**(const gsl_matrix_complex *LU, const *gsl_permutation* *p, gsl_matrix_complex *inverse)

These functions compute the inverse of a matrix A from its LU decomposition (`LU`, `p`), storing the result in the matrix `inverse`. The inverse is computed by computing the inverses U^{-1}, L^{-1} and finally forming the product $A^{-1} = U^{-1}L^{-1}P$. Each step is based on Level 3 BLAS calls.

It is preferable to avoid direct use of the inverse whenever possible, as the linear solver functions can obtain the same result more efficiently and reliably (consult any introductory textbook on numerical linear algebra for details).

int **gsl_linalg_LU_invx**(*gsl_matrix* *LU, const *gsl_permutation* *p)

int **gsl_linalg_complex_LU_invx**(gsl_matrix_complex *LU, const *gsl_permutation* *p)

These functions compute the inverse of a matrix A from its LU decomposition (`LU`, `p`), storing the result in-place in the matrix `LU`. The inverse is computed by computing the inverses U^{-1}, L^{-1} and finally forming the product $A^{-1} = U^{-1}L^{-1}P$. Each step is based on Level 3 BLAS calls.

It is preferable to avoid direct use of the inverse whenever possible, as the linear solver functions can obtain the same result more efficiently and reliably (consult any introductory textbook on numerical linear algebra for details).

double **gsl_linalg_LU_det**(*gsl_matrix* *LU, int signum)

gsl_complex **gsl_linalg_complex_LU_det**(gsl_matrix_complex *LU, int signum)

These functions compute the determinant of a matrix A from its LU decomposition, `LU`. The determinant is computed as the product of the diagonal elements of U and the sign of the row permutation `signum`.

double **gsl_linalg_LU_lndet**(*gsl_matrix* *LU)

double **gsl_linalg_complex_LU_lndet**(gsl_matrix_complex *LU)

These functions compute the logarithm of the absolute value of the determinant of a matrix A, $\ln|\det(A)|$, from its LU decomposition, `LU`. This function may be useful if the direct computation of the determinant would overflow or underflow.

int **gsl_linalg_LU_sgndet**(*gsl_matrix* *LU, int signum)

gsl_complex **gsl_linalg_complex_LU_sgndet**(gsl_matrix_complex *LU, int signum)

These functions compute the sign or phase factor of the determinant of a matrix A, $\det(A)/|\det(A)|$, from its LU decomposition, `LU`.

14.2 QR Decomposition

A general rectangular M-by-N matrix A has a QR decomposition into the product of a unitary M-by-M square matrix Q (where $Q^\dagger Q = I$) and an M-by-N right-triangular matrix R,

$$A = QR$$

This decomposition can be used to convert the square linear system $Ax = b$ into the triangular system $Rx = Q^\dagger b$, which can be solved by back-substitution. Another use of the QR decomposition is to compute an orthonormal basis for a set of vectors. The first N columns of Q form an orthonormal basis for the range of A, $ran(A)$, when A has full column rank.

When $M > N$, the bottom $M - N$ rows of R are zero, and so A can be naturally partioned as

$$A = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 R_1$$

where R_1 is N-by-N upper triangular, Q_1 is M-by-N, and Q_2 is M-by-$(M - N)$. $Q_1 R_1$ is sometimes called the *thin* or *reduced* QR decomposition. The solution of the least squares problem $\min_x ||b - Ax||^2$ when A has full rank is:

$$x = R_1^{-1} c_1$$

where c_1 is the first N elements of $Q^\dagger b$. If A is rank deficient, see *QR Decomposition with Column Pivoting* and *Complete Orthogonal Decomposition*.

GSL offers two interfaces for the QR decomposition. The first proceeds by zeroing out columns below the diagonal of A, one column at a time using Householder transforms. In this method, the factor Q is represented as a product of Householder reflectors:

$$Q = H_n \cdots H_2 H_1$$

where each $H_i = I - \tau_i v_i v_i^\dagger$ for a scalar τ_i and column vector v_i. In this method, functions which compute the full matrix Q or apply $Q^\dagger$ to a right hand side vector operate by applying the Householder matrices one at a time using Level 2 BLAS.

The second interface is based on a Level 3 BLAS block recursive algorithm developed by Elmroth and Gustavson. In this case, Q is written in block form as

$$Q = I - VTV^\dagger$$

where V is an M-by-N matrix of the column vectors v_i and T is an N-by-N upper triangular matrix, whose diagonal elements are the τ_i. Computing the full T, while requiring more flops than the Level 2 approach, offers the advantage that all standard operations can take advantage of cache efficient Level 3 BLAS operations, and so this method often performs faster than the Level 2 approach. The functions for the recursive block algorithm have a `_r` suffix, and it is recommended to use this interface for performance critical applications.

int **gsl_linalg_QR_decomp_r**(*gsl_matrix* *A, *gsl_matrix* *T)

int **gsl_linalg_complex_QR_decomp_r**(gsl_matrix_complex *A, gsl_matrix_complex *T)

These functions factor the M-by-N matrix `A` into the QR decomposition $A = QR$ using the recursive Level 3 BLAS algorithm of Elmroth and Gustavson. On output the diagonal and upper triangular part of `A` contain the matrix R. The N-by-N matrix `T` stores the upper triangular factor appearing in Q. The matrix Q is given by $Q = I - VTV^\dagger$, where the elements below the diagonal of `A` contain the columns of V on output.

This algorithm requires $M \geq N$ and performs best for "tall-skinny" matrices, i.e. $M \gg N$.

int **gsl_linalg_QR_solve_r**(const *gsl_matrix* *QR, const *gsl_matrix* *T, const *gsl_vector* *b, *gsl_vector* *x) int **gsl_linalg_complex_QR_solve_r**(const gsl_matrix_complex *QR, const gsl_matrix_complex *T, const gsl_vector_complex *b, gsl_vector_complex *x)

These functions solve the square system $Ax = b$ using the QR decomposition of A held in (`QR`, `T`). The least-squares solution for rectangular systems can be found using `gsl_linalg_QR_lssolve_r()` or `gsl_linalg_complex_QR_lssolve_r()`.

int **gsl_linalg_QR_lssolve_r**(const *gsl_matrix* *QR, const *gsl_matrix* *T, const *gsl_vector* *b, *gsl_vector* *x, *gsl_vector* *work)

int **gsl_linalg_complex_QR_lssolve_r**(const gsl_matrix_complex *QR, const gsl_matrix_complex *T, const gsl_vector_complex *b, gsl_vector_complex *x, gsl_vector_complex *work)

These functions find the least squares solution to the overdetermined system $Ax = b$ where the matrix `A` has more rows than columns. The least squares solution minimizes the Euclidean norm of the residual, $||b - Ax||$. The routine requires as input the QR decomposition of A into (`QR`, `T`) given by `gsl_linalg_QR_decomp_r()` or `gsl_linalg_complex_QR_decomp_r()`. The parameter `x` is of length M. The solution x is returned in the first N rows of `x`, i.e. $x =$ `x[0], x[1], ..., x[N-1]`. The last $M - N$ rows of `x` contain a vector whose norm is equal to the residual norm $||b - Ax||$. This similar to the behavior of LAPACK DGELS. Additional workspace of length N is required in `work`.

int **gsl_linalg_QR_QTvec_r**(const *gsl_matrix* *QR, const *gsl_matrix* *T, *gsl_vector* *v, *gsl_vector* *work)

int **gsl_linalg_complex_QR_QHvec_r**(const gsl_matrix_complex *QR, const gsl_matrix_complex *T, gsl_vector_complex *v, gsl_vector_complex *work)

These functions apply the matrix Q^T (or $Q^\dagger$) encoded in the decomposition (`QR`, `T`) to the vector `v`, storing the result $Q^T v$ (or $Q^\dagger v$) in `v`. The matrix multiplication is carried out directly using the encoding of the Householder vectors without needing to form the full matrix Q^T (or $Q^\dagger$). Additional workspace of size N is required in `work`.

int **gsl_linalg_QR_QTmat_r**(const *gsl_matrix* *QR, const *gsl_matrix* *T, *gsl_matrix* *B, *gsl_matrix* *work)

This function applies the matrix Q^T encoded in the decomposition (`QR`, `T`) to the M-by-K matrix `B`, storing the result $Q^T B$ in `B`. The matrix multiplication is carried out directly using the encoding of the Householder vectors without needing to form the full matrix Q^T. Additional workspace of size N-by-K is required in `work`.

int **gsl_linalg_QR_unpack_r**(const *gsl_matrix* *QR, const *gsl_matrix* *T, *gsl_matrix* *Q, *gsl_matrix* *R)

int **gsl_linalg_complex_QR_unpack_r**(const gsl_matrix_complex *QR, const gsl_matrix_complex *T, gsl_matrix_complex *Q, gsl_matrix_complex *R)

These functions unpack the encoded QR decomposition (`QR`, `T`) as output from `gsl_linalg_QR_decomp_r()` or `gsl_linalg_complex_QR_decomp_r()` into the matrices `Q` and `R`, where `Q` is M-by-M and `R` is N-by-N. Note that the full R matrix is M-by-N, however the lower trapezoidal portion is zero, so only the upper triangular factor is stored.

int **gsl_linalg_QR_rcond**(const *gsl_matrix* *QR, double *rcond, *gsl_vector* *work)

This function estimates the reciprocal condition number (using the 1-norm) of the R factor, stored in the upper triangle of `QR`. The reciprocal condition number estimate, defined as $1/(||R||_1 \cdot ||R^{-1}||_1)$, is stored in `rcond`. Additional workspace of size $3N$ is required in `work`.

14.2.1 Level 2 Interface

The functions below are for the slower Level 2 interface to the QR decomposition. It is recommended to use these functions only for $M < N$, since the Level 3 interface above performs much faster for $M \geq N$.

int **gsl_linalg_QR_decomp**(*gsl_matrix* *A, *gsl_vector* *tau)

int **gsl_linalg_complex_QR_decomp**(gsl_matrix_complex *A, gsl_vector_complex *tau)

These functions factor the M-by-N matrix `A` into the QR decomposition $A = QR$. On output the diagonal and upper triangular part of the input matrix contain the matrix R. The vector `tau` and the columns of the lower triangular part of the matrix `A` contain the Householder coefficients and Householder vectors which encode the orthogonal matrix `Q`. The vector `tau` must be of length N. The matrix Q is related to these components by the product of $k = min(M, N)$ reflector matrices, $Q = H_k...H_2H_1$ where $H_i = I - \tau_i v_i v_i^\dagger$ and v_i is the Householder vector $v_i = (0, ..., 1, A(i+1, i), A(i+2, i), ..., A(m, i))$. This is the same storage scheme as used by LAPACK.

The algorithm used to perform the decomposition is Householder QR (Golub & Van Loan, "Matrix Computations", Algorithm 5.2.1).

int **gsl_linalg_QR_solve**(const *gsl_matrix* *QR, const *gsl_vector* *tau, const *gsl_vector* *b, *gsl_vector* *x)

int **gsl_linalg_complex_QR_solve**(const gsl_matrix_complex *QR, const gsl_vector_complex *tau, const gsl_vector_complex *b, gsl_vector_complex *x)

These functions solve the square system $Ax = b$ using the QR decomposition of A held in (`QR`, `tau`). The least-squares solution for rectangular systems can be found using `gsl_linalg_QR_lssolve()`.

int **gsl_linalg_QR_svx**(const *gsl_matrix* *QR, const *gsl_vector* *tau, *gsl_vector* *x)

int **gsl_linalg_complex_QR_svx**(const gsl_matrix_complex *QR, const gsl_vector_complex *tau, gsl_vector_complex *x)

These functions solve the square system $Ax = b$ in-place using the QR decomposition of A held in (`QR`, `tau`). On input `x` should contain the right-hand side b, which is replaced by the solution on output.

int **gsl_linalg_QR_lssolve**(const *gsl_matrix* *QR, const *gsl_vector* *tau, const *gsl_vector* *b, *gsl_vector* *x, *gsl_vector* *residual)

int **gsl_linalg_complex_QR_lssolve**(const gsl_matrix_complex *QR, const gsl_vector_complex *tau, const gsl_vector_complex *b, gsl_vector_complex *x, gsl_vector_complex *residual)

These functions find the least squares solution to the overdetermined system $Ax = b$ where the matrix `A` has more rows than columns. The least squares solution minimizes the Euclidean norm of the residual, $||Ax - b||$.The routine requires as input the QR decomposition of A into (`QR`, `tau`) given by `gsl_linalg_QR_decomp()` or `gsl_linalg_complex_QR_decomp()`. The solution is returned in `x`. The residual is computed as a by-product and stored in `residual`.

int **gsl_linalg_QR_QTvec**(const *gsl_matrix* *QR, const *gsl_vector* *tau, *gsl_vector* *v)

int **gsl_linalg_complex_QR_QHvec**(const gsl_matrix_complex *QR, const gsl_vector_complex *tau, gsl_vector_complex *v)

These functions apply the matrix Q^T (or $Q^\dagger$) encoded in the decomposition (`QR`, `tau`) to the vector `v`, storing the result $Q^T v$ (or $Q^\dagger v$) in `v`. The matrix multiplication is carried out directly using the encoding of the Householder vectors without needing to form the full matrix Q^T (or $Q^\dagger$).

int **gsl_linalg_QR_Qvec**(const *gsl_matrix* *QR, const *gsl_vector* *tau, *gsl_vector* *v) int **gsl_linalg_complex_QR_Qvec**(const gsl_matrix_complex *QR, const gsl_vector_complex *tau, gsl_vector_complex *v)

These functions apply the matrix Q encoded in the decomposition (`QR`, `tau`) to the vector `v`, storing the result Qv in `v`. The matrix multiplication is carried out directly using the encoding of the Householder vectors without needing to form the full matrix Q.

int **gsl_linalg_QR_QTmat**(const *gsl_matrix* *QR, const *gsl_vector* *tau, *gsl_matrix* *B)

This function applies the matrix Q^T encoded in the decomposition (`QR`, `tau`) to the M-by-K matrix `B`, storing the result $Q^T B$ in `B`. The matrix multiplication is carried out directly using the encoding of the Householder vectors without needing to form the full matrix Q^T.

int **gsl_linalg_QR_Rsolve**(const *gsl_matrix* *QR, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the triangular system $Rx = b$ for `x`. It may be useful if the product $b' = Q^T b$ has already been computed using `gsl_linalg_QR_QTvec()`.

int **gsl_linalg_QR_Rsvx**(const *gsl_matrix* *QR, *gsl_vector* *x)

This function solves the triangular system $Rx = b$ for `x` in-place. On input `x` should contain the right-hand side b and is replaced by the solution on output. This function may be useful if the product $b' = Q^T b$ has already been computed using `gsl_linalg_QR_QTvec()`.

int **gsl_linalg_QR_unpack**(const *gsl_matrix* *QR, const *gsl_vector* *tau, *gsl_matrix* *Q, *gsl_matrix* *R)

This function unpacks the encoded QR decomposition (`QR`, `tau`) into the matrices `Q` and `R`, where `Q` is M-by-M and `R` is M-by-N.

int **gsl_linalg_QR_QRsolve**(*gsl_matrix* *Q, *gsl_matrix* *R, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the system $Rx = Q^T b$ for `x`. It can be used when the QR decomposition of a matrix is available in unpacked form as (`Q`, `R`).

int **gsl_linalg_QR_update**(*gsl_matrix* *Q, *gsl_matrix* *R, *gsl_vector* *w, const *gsl_vector* *v)

This function performs a rank-1 update wv^T of the QR decomposition (`Q`, `R`). The update is given by $Q'R' = Q(R+wv^T)$ where the output matrices Q and R are also orthogonal and right triangular. Note that `w` is destroyed by the update.

int **gsl_linalg_R_solve**(const *gsl_matrix* *R, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the triangular system $Rx = b$ for the N-by-N matrix `R`.

int **gsl_linalg_R_svx**(const *gsl_matrix* *R, *gsl_vector* *x)

This function solves the triangular system $Rx = b$ in-place. On input `x` should contain the right-hand side b, which is replaced by the solution on output.

14.2.2 Triangle on Top of Rectangle

This section provides routines for computing the QR decomposition of the specialized matrix

$$\begin{pmatrix} U \\ A \end{pmatrix} = QR$$

where U is an N-by-N upper triangular matrix, and A is an M-by-N dense matrix. This type of matrix arises, for example, in the sequential TSQR algorithm. The Elmroth and Gustavson algorithm is used to efficiently factor this matrix. Due to the upper triangular factor, the Q matrix takes the form

$$Q = I - VTV^T$$

with

$$V = \begin{pmatrix} I \\ Y \end{pmatrix}$$

and Y is dense and of the same dimensions as A.

int **gsl_linalg_QR_UR_decomp**(*gsl_matrix* *U, *gsl_matrix* *A, *gsl_matrix* *T)

This function computes the QR decomposition of the matrix $(U; A)$, where U is N-by-N upper triangular and A is M-by-N dense. On output, U is replaced by the R factor, and A is replaced by Y. The N-by-N upper triangular block reflector is stored in `T` on output.

14.2.3 Triangle on Top of Triangle

This section provides routines for computing the QR decomposition of the specialized matrix

$$\begin{pmatrix} U_1 \\ U_2 \end{pmatrix} = QR$$

where U_1, U_2 are N-by-N upper triangular matrices. The Elmroth and Gustavson algorithm is used to efficiently factor this matrix. The Q matrix takes the form

$$Q = I - VTV^T$$

with

$$V = \begin{pmatrix} I \\ Y \end{pmatrix}$$

and Y is N-by-N upper triangular.

int **gsl_linalg_QR_UU_decomp**(*gsl_matrix* *U1, *gsl_matrix* *U2, *gsl_matrix* *T)

This function computes the QR decomposition of the matrix $(U_1; U_2)$, where U_1, U_2 are N-by-N upper triangular. On output, `U1` is replaced by the R factor, and `U2` is replaced by Y. The N-by-N upper triangular block reflector is stored in `T` on output.

int **gsl_linalg_QR_UU_lssolve**(const *gsl_matrix* *R, const *gsl_matrix* *Y, const *gsl_matrix* *T, const *gsl_vector* *b, *gsl_vector* *x, *gsl_vector* *work)

This function find the least squares solution to the overdetermined system,

$$\min_x \left|\left| b - \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} x \right|\right|^2$$

where U_1, U_2 are N-by-N upper triangular matrices. The routine requires as input the QR decomposition of $(U_1; U_2)$ into (`R`, `Y`, `T`) given by `gsl_linalg_QR_UU_decomp()`. The parameter `x` is of length $2N$. The solution x is returned in the first N rows of `x`, i.e. $x =$ `x[0], x[1], ..., x[N-1]`. The last N rows of `x` contain a vector whose norm is equal to the residual norm $||b - (U_1; U_2)x||$. This similar to the behavior of LAPACK DGELS. Additional workspace of length N is required in `work`.

int **gsl_linalg_QR_UU_QTec**(const *gsl_matrix* *Y, const *gsl_matrix* *T, *gsl_vector* *b, *gsl_vector* *work)

This function computes $Q^T b$ using the decomposition (`Y`, `T`) previously computed by `gsl_linalg_QR_UU_decomp()`. On input, `b` contains the vector b, and on output it will contain $Q^T b$. Additional workspace of length N is required in `work`.

14.2.4 Triangle on Top of Trapezoidal

This section provides routines for computing the QR decomposition of the specialized matrix

$$\begin{pmatrix} U \\ A \end{pmatrix} = QR$$

where U is an N-by-N upper triangular matrix, and A is an M-by-N upper trapezoidal matrix with $M \geq N$. A has the structure,

$$A = \begin{pmatrix} A_d \\ A_u \end{pmatrix}$$

where A_d is $(M - N)$-by-N dense, and A_u is N-by-N upper triangular. The Elmroth and Gustavson algorithm is used to efficiently factor this matrix. The Q matrix takes the form

$$Q = I - VTV^T$$

with

$$V = \begin{pmatrix} I \\ Y \end{pmatrix}$$

and Y is upper trapezoidal and of the same dimensions as A.

int **gsl_linalg_QR_UZ_decomp**(*gsl_matrix* *U, *gsl_matrix* *A, *gsl_matrix* *T)

This function computes the QR decomposition of the matrix $(U; A)$, where U is N-by-N upper triangular and A is M-by-N upper trapezoidal. On output, U is replaced by the R factor, and A is replaced by Y. The N-by-N upper triangular block reflector is stored in `T` on output.

14.2.5 Triangle on Top of Diagonal

This section provides routines for computing the QR decomposition of the specialized matrix

$$\begin{pmatrix} U \\ D \end{pmatrix} = QR$$

where U is an N-by-N upper triangular matrix and D is an N-by-N diagonal matrix. This type of matrix arises in regularized least squares problems. The Elmroth and Gustavson algorithm is used to efficiently factor this matrix. The Q matrix takes the form

$$Q = I - VTV^T$$

with

$$V = \begin{pmatrix} I \\ Y \end{pmatrix}$$

and Y is N-by-N upper triangular.

int **gsl_linalg_QR_UD_decomp**(*gsl_matrix* *U, const *gsl_vector* *D, *gsl_matrix* *Y, *gsl_matrix* *T)

This function computes the QR decomposition of the matrix $(U; D)$, where U is N-by-N upper triangular and D is N-by-N diagonal. On output, `U` is replaced by the R factor and Y is stored in `Y`. The N-by-N upper triangular block reflector is stored in `T` on output.

int **gsl_linalg_QR_UD_lssolve**(const *gsl_matrix* *R, const *gsl_matrix* *Y, const *gsl_matrix* *T, const *gsl_vector* *b, *gsl_vector* *x, *gsl_vector* *work)

This function find the least squares solution to the overdetermined system,

$$\min_x \left|\left| b - \begin{pmatrix} U \\ D \end{pmatrix} x \right|\right|^2$$

where U is N-by-N upper triangular and D is N-by-N diagonal. The routine requires as input the QR decomposition of $(U; D)$ into (`R`, `Y`, `T`) given by `gsl_linalg_QR_UD_decomp()`. The parameter `x` is of length $2N$. The solution x is returned in the first N rows of `x`, i.e. $x =$ `x[0], x[1], ..., x[N-1]`. The last N rows of `x` contain a vector whose norm is equal to the residual norm $||b - (U; D)x||$. This similar to the behavior of LAPACK DGELS. Additional workspace of length N is required in `work`.

14.3 QR Decomposition with Column Pivoting

The QR decomposition of an M-by-N matrix A can be extended to the rank deficient case by introducing a column permutation P,

$$AP = QR$$

The first r columns of Q form an orthonormal basis for the range of A for a matrix with column rank r. This decomposition can also be used to convert the square linear system $Ax = b$ into the triangular system $Ry = Q^T b, x = Py$, which can be solved by back-substitution and permutation. We denote the QR decomposition with column pivoting by QRP^T since $A = QRP^T$. When A is rank deficient with $r = \text{rank}(A)$, the matrix R can be partitioned as

$$R = \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{pmatrix} \approx \begin{pmatrix} R_{11} & R_{12} \\ 0 & 0 \end{pmatrix}$$

where R_{11} is r-by-r and nonsingular. In this case, a *basic* least squares solution for the overdetermined system $Ax = b$ can be obtained as

$$x = P \begin{pmatrix} R_{11}^{-1} c_1 \\ 0 \end{pmatrix}$$

where c_1 consists of the first r elements of $Q^T b$. This basic solution is not guaranteed to be the minimum norm solution unless $R_{12} = 0$ (see *Complete Orthogonal Decomposition*).

int **gsl_linalg_QRPT_decomp**(*gsl_matrix* *A, *gsl_vector* *tau, *gsl_permutation* *p, int *signum, *gsl_vector* *norm)

This function factorizes the M-by-N matrix `A` into the QRP^T decomposition $A = QRP^T$. On output the diagonal and upper triangular part of the input matrix contain the matrix R. The permutation matrix P is stored in the permutation `p`. The sign of the permutation is given by `signum`. It has the value $(-1)^n$, where n is the number of interchanges in the permutation. The vector `tau` and the columns of the lower triangular part of the matrix `A` contain the Householder coefficients and vectors which encode the orthogonal matrix `Q`. The vector `tau` must be of length $k = \min(M, N)$. The matrix Q is related to these components by, $Q = Q_k ... Q_2 Q_1$ where $Q_i = I - \tau_i v_i v_i^T$ and v_i is the Householder vector

$$v_i = (0, ..., 1, A(i+1, i), A(i+2, i), ..., A(m, i))$$

This is the same storage scheme as used by LAPACK. The vector `norm` is a workspace of length `N` used for column pivoting.

The algorithm used to perform the decomposition is Householder QR with column pivoting (Golub & Van Loan, "Matrix Computations", Algorithm 5.4.1).

int **gsl_linalg_QRPT_decomp2**(const *gsl_matrix* *A, *gsl_matrix* *q, *gsl_matrix* *r, *gsl_vector* *tau, *gsl_permutation* *p, int *signum, *gsl_vector* *norm)

This function factorizes the matrix `A` into the decomposition $A = QRP^T$ without modifying `A` itself and storing the output in the separate matrices `q` and `r`.

int **gsl_linalg_QRPT_solve**(const *gsl_matrix* *QR, const *gsl_vector* *tau, const *gsl_permutation* *p, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the square system $Ax = b$ using the QRP^T decomposition of A held in (`QR`, `tau`, `p`) which must have been computed previously by `gsl_linalg_QRPT_decomp()`.

int **gsl_linalg_QRPT_svx**(const *gsl_matrix* *QR, const *gsl_vector* *tau, const *gsl_permutation* *p, *gsl_vector* *x)

This function solves the square system $Ax = b$ in-place using the QRP^T decomposition of A held in (`QR`, `tau`, `p`). On input `x` should contain the right-hand side b, which is replaced by the solution on output.

int **gsl_linalg_QRPT_lssolve**(const *gsl_matrix* *QR, const *gsl_vector* *tau, const *gsl_permutation* *p, const *gsl_vector* *b, *gsl_vector* *x, *gsl_vector* *residual)

This function finds the least squares solution to the overdetermined system $Ax = b$ where the matrix `A` has more rows than columns and is assumed to have full rank. The least squares solution minimizes the Euclidean norm of the residual, $||b - Ax||$. The routine requires as input the QR decomposition of A into (`QR`, `tau`, `p`) given by `gsl_linalg_QRPT_decomp()`. The solution is returned in `x`. The residual is computed as a by-product and stored in `residual`. For rank deficient matrices, `gsl_linalg_QRPT_lssolve2()` should be used instead.

int **gsl_linalg_QRPT_lssolve2**(const *gsl_matrix* *QR, const *gsl_vector* *tau, const *gsl_permutation* *p, const *gsl_vector* *b, const size_t rank, *gsl_vector* *x, *gsl_vector* *residual)

This function finds the least squares solution to the overdetermined system $Ax = b$ where the matrix `A` has more rows than columns and has rank given by the input `rank`. If the user does not know the rank of A, the routine `gsl_linalg_QRPT_rank()` can be called to estimate it. The least squares solution is the so-called "basic" solution discussed above and may not be the minimum norm solution. The routine requires as input the QR decomposition of A into (`QR`, `tau`, `p`) given by `gsl_linalg_QRPT_decomp()`. The solution is returned in `x`. The residual is computed as a by-product and stored in `residual`.

int **gsl_linalg_QRPT_QRsolve**(const *gsl_matrix* *Q, const *gsl_matrix* *R, const *gsl_permutation* *p, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the square system $RP^Tx = Q^Tb$ for `x`. It can be used when the QR decomposition of a matrix is available in unpacked form as (`Q`, `R`).

int **gsl_linalg_QRPT_update**(*gsl_matrix* *Q, *gsl_matrix* *R, const *gsl_permutation* *p, *gsl_vector* *w, const *gsl_vector* *v)

This function performs a rank-1 update wv^T of the QRP^T decomposition (`Q`, `R`, `p`). The update is given by $Q'R' = Q(R + wv^TP)$ where the output matrices Q' and R' are also orthogonal and right triangular. Note that `w` is destroyed by the update. The permutation `p` is not changed.

int **gsl_linalg_QRPT_Rsolve**(const *gsl_matrix* *QR, const *gsl_permutation* *p, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the triangular system $RP^Tx = b$ for the N-by-N matrix R contained in `QR`.

int **gsl_linalg_QRPT_Rsvx**(const *gsl_matrix* *QR, const *gsl_permutation* *p, *gsl_vector* *x)

This function solves the triangular system $RP^Tx = b$ in-place for the N-by-N matrix R contained in `QR`. On input `x` should contain the right-hand side b, which is replaced by the solution on output.

size_t **gsl_linalg_QRPT_rank**(const *gsl_matrix* *QR, const double tol)

This function estimates the rank of the triangular matrix R contained in `QR`. The algorithm simply counts the number of diagonal elements of R whose absolute value is greater than the specified tolerance `tol`. If the input `tol` is negative, a default value of $20(M + N)eps(max(|diag(R)|))$ is used.

int **gsl_linalg_QRPT_rcond**(const *gsl_matrix* *QR, double *rcond, *gsl_vector* *work)

This function estimates the reciprocal condition number (using the 1-norm) of the R factor, stored in the upper triangle of `QR`. The reciprocal condition number estimate, defined as $1/(||R||_1 \cdot ||R^{-1}||_1)$, is stored in `rcond`. Additional workspace of size $3N$ is required in `work`.

14.4 LQ Decomposition

A general rectangular M-by-N matrix A has a LQ decomposition into the product of a lower trapezoidal M-by-N matrix L and an orthogonal N-by-N square matrix Q:

$$A = LQ$$

If $M \le N$, then L can be written as $L = (L_1 \quad 0)$ where L_1 is M-by-M lower triangular, and

$$A = \begin{pmatrix} L_1 & 0 \end{pmatrix} \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} = L_1 Q_1$$

where Q_1 consists of the first M rows of Q, and Q_2 contains the remaining $N - M$ rows. The LQ factorization of A is essentially the same as the *QR factorization* of A^T.

The LQ factorization may be used to find the minimum norm solution of an underdetermined system of equations $Ax = b$, where A is M-by-N and $M \leq N$. The solution is

$$x = Q^T \begin{pmatrix} L_1^{-1} b \\ 0 \end{pmatrix}$$

int **gsl_linalg_LQ_decomp**(*gsl_matrix* *A, *gsl_vector* *tau)

This function factorizes the M-by-N matrix `A` into the LQ decomposition $A = LQ$. On output the diagonal and lower trapezoidal part of the input matrix contain the matrix L. The vector `tau` and the elements above the diagonal of the matrix `A` contain the Householder coefficients and Householder vectors which encode the orthogonal matrix `Q`. The vector `tau` must be of length $k = \min(M, N)$. The matrix Q is related to these components by, $Q = Q_k ... Q_2 Q_1$ where $Q_i = I - \tau_i v_i v_i^T$ and v_i is the Householder vector $v_i = (0, ..., 1, A(i, i+1), A(i, i+2), ..., A(i, N))$. This is the same storage scheme as used by LAPACK.

int **gsl_linalg_LQ_lssolve**(const *gsl_matrix* *LQ, const *gsl_vector* *tau, const *gsl_vector* *b, *gsl_vector* *x, *gsl_vector* *residual)

This function finds the minimum norm least squares solution to the underdetermined system $Ax = b$, where the M-by-N matrix `A` has $M \leq N$. The routine requires as input the LQ decomposition of A into (`LQ`, `tau`) given by `gsl_linalg_LQ_decomp()`. The solution is returned in `x`. The residual, $b - Ax$, is computed as a by-product and stored in `residual`.

int **gsl_linalg_LQ_unpack**(const *gsl_matrix* *LQ, const *gsl_vector* *tau, *gsl_matrix* *Q, *gsl_matrix* *L)

This function unpacks the encoded LQ decomposition (`LQ`, `tau`) into the matrices `Q` and `L`, where `Q` is N-by-N and `L` is M-by-N.

int **gsl_linalg_LQ_QTvec**(const *gsl_matrix* *LQ, const *gsl_vector* *tau, *gsl_vector* *v)

This function applies Q^T to the vector `v`, storing the result $Q^T v$ in `v` on output.

14.5 QL Decomposition

A general rectangular M-by-N matrix A has a QL decomposition into the product of an orthogonal M-by-M square matrix Q (where $Q^T Q = I$) and an M-by-N left-triangular matrix L.

When $M \geq N$, the decomposition is given by

$$A = Q \begin{pmatrix} 0 \\ L_1 \end{pmatrix}$$

where L_1 is N-by-N lower triangular. When $M \leq N$, the decomposition is given by

$$A = Q \begin{pmatrix} L_1 & L_2 \end{pmatrix}$$

where L_1 is a dense M-by-$N - M$ matrix and L_2 is a lower triangular M-by-M matrix.

int **gsl_linalg_QL_decomp**(*gsl_matrix* *A, *gsl_vector* *tau)

This function factorizes the M-by-N matrix `A` into the QL decomposition $A = QL$. The vector `tau` must be of length N and contains the Householder coefficients on output. The matrix Q is stored in packed form in `A` on output, using the same storage scheme as LAPACK.

int **gsl_linalg_QL_unpack**(const *gsl_matrix* *QL, const *gsl_vector* *tau, *gsl_matrix* *Q, *gsl_matrix* *L)

This function unpacks the encoded QL decomposition (`QL`, `tau`) into the matrices `Q` and `L`, where `Q` is M-by-M and `L` is M-by-N.

14.6 Complete Orthogonal Decomposition

The complete orthogonal decomposition of a M-by-N matrix A is a generalization of the QR decomposition with column pivoting, given by

$$AP = Q \begin{pmatrix} R_{11} & 0 \\ 0 & 0 \end{pmatrix} Z^T$$

where P is a N-by-N permutation matrix, Q is M-by-M orthogonal, R_{11} is r-by-r upper triangular, with $r = \mathrm{rank}(A)$, and Z is N-by-N orthogonal. If A has full rank, then $R_{11} = R$, $Z = I$ and this reduces to the QR decomposition with column pivoting.

For a rank deficient least squares problem, $\min_x ||b - Ax||^2$, the solution vector x is not unique. However if we further require that $||x||^2$ is minimized, then the complete orthogonal decomposition gives us the ability to compute the unique minimum norm solution, which is given by

$$x = PZ \begin{pmatrix} R_{11}^{-1} c_1 \\ 0 \end{pmatrix}$$

and the vector c_1 is the first r elements of $Q^T b$.

The COD also enables a straightforward solution of regularized least squares problems in Tikhonov standard form, written as

$$\min_x ||b - Ax||^2 + \lambda^2 ||x||^2$$

where $\lambda > 0$ is a regularization parameter which represents a tradeoff between minimizing the residual norm $||b - Ax||$ and the solution norm $||x||$. For this system, the solution is given by

$$x = PZ \begin{pmatrix} y_1 \\ 0 \end{pmatrix}$$

where y_1 is a vector of length r which is found by solving

$$\begin{pmatrix} R_{11} \\ \lambda I_r \end{pmatrix} y_1 = \begin{pmatrix} c_1 \\ 0 \end{pmatrix}$$

and c_1 is defined above. The equation above can be solved efficiently for different values of λ using QR factorizations of the left hand side matrix.

int **gsl_linalg_COD_decomp**(*gsl_matrix* *A, *gsl_vector* *tau_Q, *gsl_vector* *tau_Z, *gsl_permutation* *p, size_t *rank, *gsl_vector* *work)

int **gsl_linalg_COD_decomp_e**(*gsl_matrix* *A, *gsl_vector* *tau_Q, *gsl_vector* *tau_Z, *gsl_permutation* *p, double tol, size_t *rank, *gsl_vector* *work)

These functions factor the M-by-N matrix `A` into the decomposition $A = QRZP^T$. The rank of `A` is computed as the number of diagonal elements of R greater than the tolerance `tol` and output in `rank`. If `tol` is not specified, a default value is used (see `gsl_linalg_QRPT_rank()`). On output, the permutation matrix P is stored in `p`. The matrix R_{11} is stored in the upper `rank`-by-`rank` block of `A`. The matrices Q and Z are encoded in packed storage in `A` on output. The vectors `tau_Q` and `tau_Z` contain the Householder scalars corresponding to the matrices Q and Z respectively and must be of length $k = \min(M, N)$. The vector `work` is additional workspace of length N.

int **gsl_linalg_COD_lssolve**(const *gsl_matrix* *QRZT, const *gsl_vector* *tau_Q, const *gsl_vector* *tau_Z, const *gsl_permutation* *p, const size_t rank, const *gsl_vector* *b, *gsl_vector* *x, *gsl_vector* *residual)

This function finds the unique minimum norm least squares solution to the overdetermined system $Ax = b$ where the matrix `A` has more rows than columns. The least squares solution minimizes the Euclidean norm of the residual, $||b - Ax||$ as well as the norm of the solution $||x||$. The routine requires as input the $QRZT$ decomposition of A into (`QRZT`, `tau_Q`, `tau_Z`, `p`, `rank`) given by `gsl_linalg_COD_decomp()`. The solution is returned in `x`. The residual, $b - Ax$, is computed as a by-product and stored in `residual`.

int **gsl_linalg_COD_lssolve2**(const double lambda, const *gsl_matrix* *QRZT, const *gsl_vector* *tau_Q, const *gsl_vector* *tau_Z, const *gsl_permutation* *p, const size_t rank, const *gsl_vector* *b, *gsl_vector* *x, *gsl_vector* *residual, *gsl_matrix* *S, *gsl_vector* *work)

This function finds the solution to the regularized least squares problem in Tikhonov standard form, $\min_x ||b - Ax||^2 + \lambda^2 ||x||^2$. The routine requires as input the $QRZT$ decomposition of A into (`QRZT`, `tau_Q`, `tau_Z`, `p`, `rank`) given by `gsl_linalg_COD_decomp()`. The parameter λ is supplied in `lambda`. The solution is returned in `x`. The residual, $b - Ax$, is stored in `residual` on output. `S` is additional workspace of size `rank`-by-`rank`. `work` is additional workspace of length `rank`.

int **gsl_linalg_COD_unpack**(const *gsl_matrix* *QRZT, const *gsl_vector* *tau_Q, const *gsl_vector* *tau_Z, const size_t rank, *gsl_matrix* *Q, *gsl_matrix* *R, *gsl_matrix* *Z)

This function unpacks the encoded $QRZT$ decomposition (`QRZT`, `tau_Q`, `tau_Z`, `rank`) into the matrices `Q`, `R`, and `Z`, where `Q` is M-by-M, `R` is M-by-N, and `Z` is N-by-N.

int **gsl_linalg_COD_matZ**(const *gsl_matrix* *QRZT, const *gsl_vector* *tau_Z, const size_t rank, *gsl_matrix* *A, *gsl_vector* *work)

This function multiplies the input matrix `A` on the right by `Z`, $A' = AZ$ using the encoded $QRZT$ decomposition (`QRZT`, `tau_Z`, `rank`). `A` must have N columns but may have any number of rows. Additional workspace of length M is provided in `work`.

14.7 Singular Value Decomposition

A general rectangular M-by-N matrix A has a singular value decomposition (SVD) into the product of an M-by-N orthogonal matrix U, an N-by-N diagonal matrix of singular values S and the transpose of an N-by-N orthogonal square matrix V,

$$A = USV^T$$

The singular values $\sigma_i = S_{ii}$ are all non-negative and are generally chosen to form a non-increasing sequence

$$\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_N \geq 0$$

The singular value decomposition of a matrix has many practical uses. The condition number of the matrix is given by the ratio of the largest singular value to the smallest singular value. The presence of a zero singular value indicates that the matrix is singular. The number of non-zero singular values indicates the rank of the matrix. In practice singular value decomposition of a rank-deficient matrix will not produce exact zeroes for singular values, due to finite numerical precision. Small singular values should be edited by choosing a suitable tolerance.

For a rank-deficient matrix, the null space of A is given by the columns of V corresponding to the zero singular values. Similarly, the range of A is given by columns of U corresponding to the non-zero singular values.

Note that the routines here compute the "thin" version of the SVD with U as M-by-N orthogonal matrix. This allows in-place computation and is the most commonly-used form in practice. Mathematically, the "full" SVD is defined with U as an M-by-M orthogonal matrix and S as an M-by-N diagonal matrix (with additional rows of zeros).

int **gsl_linalg_SV_decomp**(*gsl_matrix* *A, *gsl_matrix* *V, *gsl_vector* *S, *gsl_vector* *work)

This function factorizes the M-by-N matrix `A` into the singular value decomposition $A = USV^T$ for $M \geq N$. On output the matrix `A` is replaced by U. The diagonal elements of the singular value matrix S are stored in the vector `S`. The singular values are non-negative and form a non-increasing sequence from S_1 to S_N. The matrix `V` contains the elements of V in untransposed form. To form the product USV^T it is necessary to take the transpose of `V`. A workspace of length `N` is required in `work`.

This routine uses the Golub-Reinsch SVD algorithm.

int **gsl_linalg_SV_decomp_mod**(*gsl_matrix* *A, *gsl_matrix* *X, *gsl_matrix* *V, *gsl_vector* *S, *gsl_vector* *work)

This function computes the SVD using the modified Golub-Reinsch algorithm, which is faster for $M \gg N$. It requires the vector `work` of length `N` and the N-by-N matrix `X` as additional working space.

int **gsl_linalg_SV_decomp_jacobi**(*gsl_matrix* *A, *gsl_matrix* *V, *gsl_vector* *S)

This function computes the SVD of the M-by-N matrix `A` using one-sided Jacobi orthogonalization for $M \geq N$. The Jacobi method can compute singular values to higher relative accuracy than Golub-Reinsch algorithms (see references for details).

int **gsl_linalg_SV_solve**(const *gsl_matrix* *U, const *gsl_matrix* *V, const *gsl_vector* *S, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the system $Ax = b$ using the singular value decomposition (`U`, `S`, `V`) of A which must have been computed previously with `gsl_linalg_SV_decomp()`.

Only non-zero singular values are used in computing the solution. The parts of the solution corresponding to singular values of zero are ignored. Other singular values can be edited out by setting them to zero before calling this function.

In the over-determined case where `A` has more rows than columns the system is solved in the least squares sense, returning the solution `x` which minimizes $||Ax - b||_2$.

int **gsl_linalg_SV_leverage**(const *gsl_matrix* *U, *gsl_vector* *h)

This function computes the statistical leverage values h_i of a matrix A using its singular value decomposition (`U`, `S`, `V`) previously computed with `gsl_linalg_SV_decomp()`. h_i are the diagonal values of the matrix $A(A^TA)^{-1}A^T$ and depend only on the matrix `U` which is the input to this function.

14.8 Cholesky Decomposition

A symmetric, positive definite square matrix A has a Cholesky decomposition into a product of a lower triangular matrix L and its transpose L^T,

$$A = LL^T$$

This is sometimes referred to as taking the square-root of a matrix. The Cholesky decomposition can only be carried out when all the eigenvalues of the matrix are positive. This decomposition can be used to convert the linear system $Ax = b$ into a pair of triangular systems ($Ly = b$, $L^Tx = y$), which can be solved by forward and back-substitution.

If the matrix A is near singular, it is sometimes possible to reduce the condition number and recover a more accurate solution vector x by scaling as

$$(SAS)\left(S^{-1}x\right) = Sb$$

where S is a diagonal matrix whose elements are given by $S_{ii} = 1/\sqrt{A_{ii}}$. This scaling is also known as Jacobi preconditioning. There are routines below to solve both the scaled and unscaled systems.

int **gsl_linalg_cholesky_decomp1**(*gsl_matrix* *A)

int **gsl_linalg_complex_cholesky_decomp**(gsl_matrix_complex *A)

These functions factorize the symmetric, positive-definite square matrix `A` into the Cholesky decomposition $A = LL^T$ (or $A = LL^\dagger$ for the complex case). On input, the values from the diagonal and lower-triangular part of the matrix `A` are used (the upper triangular part is ignored). On output the diagonal and lower triangular part of the input matrix `A` contain the matrix L, while the upper triangular part contains the original matrix. If the matrix is not positive-definite then the decomposition will fail, returning the error code `GSL_EDOM`.

When testing whether a matrix is positive-definite, disable the error handler first to avoid triggering an error. These functions use Level 3 BLAS to compute the Cholesky factorization (Peise and Bientinesi, 2016).

int **gsl_linalg_cholesky_decomp**(*gsl_matrix* *A)

This function is now deprecated and is provided only for backward compatibility.

int **gsl_linalg_cholesky_solve**(const *gsl_matrix* *cholesky, const *gsl_vector* *b, *gsl_vector* *x)

int **gsl_linalg_complex_cholesky_solve**(const gsl_matrix_complex *cholesky, const gsl_vector_complex *b, gsl_vector_complex *x)

These functions solve the system $Ax = b$ using the Cholesky decomposition of A held in the matrix `cholesky` which must have been previously computed by `gsl_linalg_cholesky_decomp()` or `gsl_linalg_complex_cholesky_decomp()`.

int **gsl_linalg_cholesky_svx**(const *gsl_matrix* *cholesky, *gsl_vector* *x)

int **gsl_linalg_complex_cholesky_svx**(const gsl_matrix_complex *cholesky, gsl_vector_complex *x)

These functions solve the system $Ax = b$ in-place using the Cholesky decomposition of A held in the matrix `cholesky` which must have been previously computed by `gsl_linalg_cholesky_decomp()` or `gsl_linalg_complex_cholesky_decomp()`. On input `x` should contain the right-hand side b, which is replaced by the solution on output.

int **gsl_linalg_cholesky_invert**(*gsl_matrix* *cholesky)

int **gsl_linalg_complex_cholesky_invert**(gsl_matrix_complex *cholesky)

These functions compute the inverse of a matrix from its Cholesky decomposition `cholesky`, which must have been previously computed by `gsl_linalg_cholesky_decomp()` or `gsl_linalg_complex_cholesky_decomp()`. On output, the inverse is stored in-place in `cholesky`.

int **gsl_linalg_cholesky_decomp2**(*gsl_matrix* *A, *gsl_vector* *S)

This function calculates a diagonal scaling transformation S for the symmetric, positive-definite square matrix `A`, and then computes the Cholesky decomposition $SAS = LL^T$. On input, the values from the diagonal and lower-triangular part of the matrix `A` are used (the upper triangular part is ignored). On output the diagonal and lower triangular part of the input matrix `A` contain the matrix L, while the upper triangular part of the input matrix is overwritten with L^T (the diagonal terms being identical for both L and L^T). If the matrix is not positive-definite then the decomposition will fail, returning the error code `GSL_EDOM`. The diagonal scale factors are stored in `S` on output.

When testing whether a matrix is positive-definite, disable the error handler first to avoid triggering an error.

int **gsl_linalg_cholesky_solve2**(const *gsl_matrix* *cholesky, const *gsl_vector* *S, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the system $(SAS)(S^{-1}x) = Sb$ using the Cholesky decomposition of SAS held in the matrix `cholesky` which must have been previously computed by `gsl_linalg_cholesky_decomp2()`.

int **gsl_linalg_cholesky_svx2**(const *gsl_matrix* *cholesky, const *gsl_vector* *S, *gsl_vector* *x)

This function solves the system $(SAS)(S^{-1}x) = Sb$ in-place using the Cholesky decomposition of SAS held in the matrix `cholesky` which must have been previously computed by `gsl_linalg_cholesky_decomp2()`. On input `x` should contain the right-hand side b, which is replaced by the solution on output.

int **gsl_linalg_cholesky_scale**(const *gsl_matrix* *A, *gsl_vector* *S)

This function calculates a diagonal scaling transformation of the symmetric, positive definite matrix `A`, such that SAS has a condition number within a factor of N of the matrix of smallest possible condition number over all possible diagonal scalings. On output, `S` contains the scale factors, given by $S_i = 1/\sqrt{A_{ii}}$. For any $A_{ii} \leq 0$, the corresponding scale factor S_i is set to 1.

int **gsl_linalg_cholesky_scale_apply**(*gsl_matrix* *A, const *gsl_vector* *S)

This function applies the scaling transformation `S` to the matrix `A`. On output, `A` is replaced by SAS.

int **gsl_linalg_cholesky_rcond**(const *gsl_matrix* *cholesky, double *rcond, *gsl_vector* *work)

This function estimates the reciprocal condition number (using the 1-norm) of the symmetric positive definite matrix A, using its Cholesky decomposition provided in `cholesky`. The reciprocal condition number estimate, defined as $1/(||A||_1 \cdot ||A^{-1}||_1)$, is stored in `rcond`. Additional workspace of size $3N$ is required in `work`.

14.9 Pivoted Cholesky Decomposition

A symmetric positive semi-definite square matrix A has an alternate Cholesky decomposition into a product of a lower unit triangular matrix L, a diagonal matrix D and L^T, given by LDL^T. For postive definite matrices, this is equivalent to the Cholesky formulation discussed above, with the standard Cholesky lower triangular factor given by $LD^{\frac{1}{2}}$. For ill-conditioned matrices, it can help to use a pivoting strategy to prevent the entries of D and L from growing too large, and also ensure $D_1 \geq D_2 \geq \cdots \geq D_n > 0$, where D_i are the diagonal entries of D. The final decomposition is given by

$$PAP^T = LDL^T$$

where P is a permutation matrix.

int **gsl_linalg_pcholesky_decomp**(*gsl_matrix* *A, *gsl_permutation* *p)
This function factors the symmetric, positive-definite square matrix `A` into the Pivoted Cholesky decomposition $PAP^T = LDL^T$. On input, the values from the diagonal and lower-triangular part of the matrix `A` are used to construct the factorization. On output the diagonal of the input matrix `A` stores the diagonal elements of D, and the lower triangular portion of `A` contains the matrix L. Since L has ones on its diagonal these do not need to be explicitely stored. The upper triangular portion of `A` is unmodified. The permutation matrix P is stored in `p` on output.

int **gsl_linalg_pcholesky_solve**(const *gsl_matrix* *LDLT, const *gsl_permutation* *p, const *gsl_vector* *b, *gsl_vector* *x)
This function solves the system $Ax = b$ using the Pivoted Cholesky decomposition of A held in the matrix `LDLT` and permutation `p` which must have been previously computed by `gsl_linalg_pcholesky_decomp()`.

int **gsl_linalg_pcholesky_svx**(const *gsl_matrix* *LDLT, const *gsl_permutation* *p, *gsl_vector* *x)
This function solves the system $Ax = b$ in-place using the Pivoted Cholesky decomposition of A held in the matrix `LDLT` and permutation `p` which must have been previously computed by `gsl_linalg_pcholesky_decomp()`. On input, `x` contains the right hand side vector b which is replaced by the solution vector on output.

int **gsl_linalg_pcholesky_decomp2**(*gsl_matrix* *A, *gsl_permutation* *p, *gsl_vector* *S)
This function computes the pivoted Cholesky factorization of the matrix SAS, where the input matrix `A` is symmetric and positive definite, and the diagonal scaling matrix `S` is computed to reduce the condition number of `A` as much as possible. See *Cholesky Decomposition* for more information on the matrix `S`. The Pivoted Cholesky decomposition satisfies $PSASP^T = LDL^T$. On input, the values from the diagonal and lower-triangular part of the matrix `A` are used to construct the factorization. On output the diagonal of the input matrix `A` stores the diagonal elements of D, and the lower triangular portion of `A` contains the matrix L. Since L has ones on its diagonal these do not need to be explicitely stored. The upper triangular portion of `A` is unmodified. The permutation matrix P is stored in `p` on output. The diagonal scaling transformation is stored in `S` on output.

int **gsl_linalg_pcholesky_solve2**(const *gsl_matrix* *LDLT, const *gsl_permutation* *p, const *gsl_vector* *S, const *gsl_vector* *b, *gsl_vector* *x)
This function solves the system $(SAS)(S^{-1}x) = Sb$ using the Pivoted Cholesky decomposition of SAS held in the matrix `LDLT`, permutation `p`, and vector `S`, which must have been previously computed by `gsl_linalg_pcholesky_decomp2()`.

int **gsl_linalg_pcholesky_svx2**(const *gsl_matrix* *LDLT, const *gsl_permutation* *p, const *gsl_vector* *S, *gsl_vector* *x)
This function solves the system $(SAS)(S^{-1}x) = Sb$ in-place using the Pivoted Cholesky decomposition of SAS held in the matrix `LDLT`, permutation `p` and vector `S`, which must have been previously computed by

`gsl_linalg_pcholesky_decomp2()`. On input, `x` contains the right hand side vector b which is replaced by the solution vector on output.

int **gsl_linalg_pcholesky_invert**(const *gsl_matrix* *LDLT, const *gsl_permutation* *p, *gsl_matrix* *Ainv)
This function computes the inverse of the matrix A, using the Pivoted Cholesky decomposition stored in `LDLT` and `p`. On output, the matrix `Ainv` contains A^{-1}.

int **gsl_linalg_pcholesky_rcond**(const *gsl_matrix* *LDLT, const *gsl_permutation* *p, double *rcond, *gsl_vector* *work)
This function estimates the reciprocal condition number (using the 1-norm) of the symmetric positive definite matrix A, using its pivoted Cholesky decomposition provided in `LDLT`. The reciprocal condition number estimate, defined as $1/(||A||_1 \cdot ||A^{-1}||_1)$, is stored in `rcond`. Additional workspace of size $3N$ is required in `work`.

14.10 Modified Cholesky Decomposition

The modified Cholesky decomposition is suitable for solving systems $Ax = b$ where A is a symmetric indefinite matrix. Such matrices arise in nonlinear optimization algorithms. The standard Cholesky decomposition requires a positive definite matrix and would fail in this case. Instead of resorting to a method like QR or SVD, which do not take into account the symmetry of the matrix, we can instead introduce a small perturbation to the matrix A to make it positive definite, and then use a Cholesky decomposition on the perturbed matrix. The resulting decomposition satisfies

$$P(A+E)P^T = LDL^T$$

where P is a permutation matrix, E is a diagonal perturbation matrix, L is unit lower triangular, and D is diagonal. If A is sufficiently positive definite, then the perturbation matrix E will be zero and this method is equivalent to the pivoted Cholesky algorithm. For indefinite matrices, the perturbation matrix E is computed to ensure that $A + E$ is positive definite and well conditioned.

int **gsl_linalg_mcholesky_decomp**(*gsl_matrix* *A, *gsl_permutation* *p, *gsl_vector* *E)
This function factors the symmetric, indefinite square matrix `A` into the Modified Cholesky decomposition $P(A+E)P^T = LDL^T$. On input, the values from the diagonal and lower-triangular part of the matrix `A` are used to construct the factorization. On output the diagonal of the input matrix `A` stores the diagonal elements of D, and the lower triangular portion of `A` contains the matrix L. Since L has ones on its diagonal these do not need to be explicitely stored. The upper triangular portion of `A` is unmodified. The permutation matrix P is stored in `p` on output. The diagonal perturbation matrix is stored in `E` on output. The parameter `E` may be set to NULL if it is not required.

int **gsl_linalg_mcholesky_solve**(const *gsl_matrix* *LDLT, const *gsl_permutation* *p, const *gsl_vector* *b, *gsl_vector* *x)
This function solves the perturbed system $(A + E)x = b$ using the Cholesky decomposition of $A + E$ held in the matrix `LDLT` and permutation `p` which must have been previously computed by `gsl_linalg_mcholesky_decomp()`.

int **gsl_linalg_mcholesky_svx**(const *gsl_matrix* *LDLT, const *gsl_permutation* *p, *gsl_vector* *x)
This function solves the perturbed system $(A + E)x = b$ in-place using the Cholesky decomposition of $A + E$ held in the matrix `LDLT` and permutation `p` which must have been previously computed by `gsl_linalg_mcholesky_decomp()`. On input, `x` contains the right hand side vector b which is replaced by the solution vector on output.

int **gsl_linalg_mcholesky_rcond**(const *gsl_matrix* *LDLT, const *gsl_permutation* *p, double *rcond, *gsl_vector* *work)
This function estimates the reciprocal condition number (using the 1-norm) of the perturbed matrix $A + E$, using its pivoted Cholesky decomposition provided in `LDLT`. The reciprocal condition number estimate, defined as $1/(||A + E||_1 \cdot ||(A + E)^{-1}||_1)$, is stored in `rcond`. Additional workspace of size $3N$ is required in `work`.

14.11 LDLT Decomposition

If A is a symmetric, nonsingular square matrix, then it has a unique factorization of the form

$$A = LDL^T$$

where L is a unit lower triangular matrix and D is diagonal. If A is positive definite, then this factorization is equivalent to the Cholesky factorization, where the lower triangular Cholesky factor is $LD^{\frac{1}{2}}$. Some indefinite matrices for which no Cholesky decomposition exists have an LDL^T decomposition with negative entries in D. The LDL^T algorithm is sometimes referred to as the *square root free* Cholesky decomposition, as the algorithm does not require the computation of square roots. The algorithm is stable for positive definite matrices, but is not guaranteed to be stable for indefinite matrices.

int **gsl_linalg_ldlt_decomp**(*gsl_matrix* *A)

This function factorizes the symmetric, non-singular square matrix `A` into the decomposition $A = LDL^T$. On input, the values from the diagonal and lower-triangular part of the matrix `A` are used. The upper triangle of `A` is used as temporary workspace. On output the diagonal of `A` contains the matrix D and the lower triangle of `A` contains the unit lower triangular matrix L. The matrix 1-norm, $||A||_1$ is stored in the upper right corner on output, for later use by `gsl_linalg_ldlt_rcond()`.

If the matrix is detected to be singular, the function returns the error code `GSL_EDOM`.

int **gsl_linalg_ldlt_solve**(const *gsl_matrix* *LDLT, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the system $Ax = b$ using the LDL^T decomposition of A held in the matrix `LDLT` which must have been previously computed by `gsl_linalg_ldlt_decomp()`.

int **gsl_linalg_ldlt_svx**(const *gsl_matrix* *LDLT, *gsl_vector* *x)

This function solves the system $Ax = b$ in-place using the LDL^T decomposition of A held in the matrix `LDLT` which must have been previously computed by `gsl_linalg_ldlt_decomp()`. On input `x` should contain the right-hand side b, which is replaced by the solution on output.

int **gsl_linalg_ldlt_rcond**(const *gsl_matrix* *LDLT, double *rcond, *gsl_vector* *work)

This function estimates the reciprocal condition number (using the 1-norm) of the symmetric nonsingular matrix A, using its LDL^T decomposition provided in `LDLT`. The reciprocal condition number estimate, defined as $1/(||A||_1 \cdot ||A^{-1}||_1)$, is stored in `rcond`. Additional workspace of size $3N$ is required in `work`.

14.12 Tridiagonal Decomposition of Real Symmetric Matrices

A symmetric matrix A can be factorized by similarity transformations into the form,

$$A = QTQ^T$$

where Q is an orthogonal matrix and T is a symmetric tridiagonal matrix.

int **gsl_linalg_symmtd_decomp**(*gsl_matrix* *A, *gsl_vector* *tau)

This function factorizes the symmetric square matrix `A` into the symmetric tridiagonal decomposition QTQ^T. On output the diagonal and subdiagonal part of the input matrix `A` contain the tridiagonal matrix T. The remaining lower triangular part of the input matrix contains the Householder vectors which, together with the Householder coefficients `tau`, encode the orthogonal matrix Q. This storage scheme is the same as used by LAPACK. The upper triangular part of `A` is not referenced.

int **gsl_linalg_symmtd_unpack**(const *gsl_matrix* *A, const *gsl_vector* *tau, *gsl_matrix* *Q, *gsl_vector* *diag, *gsl_vector* *subdiag)

This function unpacks the encoded symmetric tridiagonal decomposition (`A`, `tau`) obtained from `gsl_linalg_symmtd_decomp()` into the orthogonal matrix `Q`, the vector of diagonal elements `diag` and the vector of subdiagonal elements `subdiag`.

int **gsl_linalg_symmtd_unpack_T**(const *gsl_matrix* *A, *gsl_vector* *diag, *gsl_vector* *subdiag)

This function unpacks the diagonal and subdiagonal of the encoded symmetric tridiagonal decomposition (`A`, `tau`) obtained from `gsl_linalg_symmtd_decomp()` into the vectors `diag` and `subdiag`.

14.13 Tridiagonal Decomposition of Hermitian Matrices

A hermitian matrix A can be factorized by similarity transformations into the form,

$$A = UTU^T$$

where U is a unitary matrix and T is a real symmetric tridiagonal matrix.

int **gsl_linalg_hermtd_decomp**(gsl_matrix_complex *A, gsl_vector_complex *tau)

This function factorizes the hermitian matrix `A` into the symmetric tridiagonal decomposition UTU^T. On output the real parts of the diagonal and subdiagonal part of the input matrix `A` contain the tridiagonal matrix T. The remaining lower triangular part of the input matrix contains the Householder vectors which, together with the Householder coefficients `tau`, encode the unitary matrix U. This storage scheme is the same as used by LAPACK. The upper triangular part of `A` and imaginary parts of the diagonal are not referenced.

int **gsl_linalg_hermtd_unpack**(const gsl_matrix_complex *A, const gsl_vector_complex *tau, gsl_matrix_complex *U, *gsl_vector* *diag, *gsl_vector* *subdiag)

This function unpacks the encoded tridiagonal decomposition (`A`, `tau`) obtained from `gsl_linalg_hermtd_decomp()` into the unitary matrix `U`, the real vector of diagonal elements `diag` and the real vector of subdiagonal elements `subdiag`.

int **gsl_linalg_hermtd_unpack_T**(const gsl_matrix_complex *A, *gsl_vector* *diag, *gsl_vector* *subdiag)

This function unpacks the diagonal and subdiagonal of the encoded tridiagonal decomposition (`A`, `tau`) obtained from the `gsl_linalg_hermtd_decomp()` into the real vectors `diag` and `subdiag`.

14.14 Hessenberg Decomposition of Real Matrices

A general real matrix A can be decomposed by orthogonal similarity transformations into the form

$$A = UHU^T$$

where U is orthogonal and H is an upper Hessenberg matrix, meaning that it has zeros below the first subdiagonal. The Hessenberg reduction is the first step in the Schur decomposition for the nonsymmetric eigenvalue problem, but has applications in other areas as well.

int **gsl_linalg_hessenberg_decomp**(*gsl_matrix* *A, *gsl_vector* *tau)

This function computes the Hessenberg decomposition of the matrix `A` by applying the similarity transformation $H = U^T AU$. On output, H is stored in the upper portion of `A`. The information required to construct the matrix U is stored in the lower triangular portion of `A`. U is a product of $N - 2$ Householder matrices. The Householder vectors are stored in the lower portion of `A` (below the subdiagonal) and the Householder coefficients are stored in the vector `tau`. `tau` must be of length `N`.

int **gsl_linalg_hessenberg_unpack**(*gsl_matrix* *H, *gsl_vector* *tau, *gsl_matrix* *U)

This function constructs the orthogonal matrix U from the information stored in the Hessenberg matrix `H` along with the vector `tau`. `H` and `tau` are outputs from `gsl_linalg_hessenberg_decomp()`.

int **gsl_linalg_hessenberg_unpack_accum**(*gsl_matrix* *H, *gsl_vector* *tau, *gsl_matrix* *V)

This function is similar to `gsl_linalg_hessenberg_unpack()`, except it accumulates the matrix `U` into `V`, so that $V' = VU$. The matrix `V` must be initialized prior to calling this function. Setting `V` to the identity matrix provides the same result as `gsl_linalg_hessenberg_unpack()`. If `H` is order `N`, then `V` must have `N` columns but may have any number of rows.

int **gsl_linalg_hessenberg_set_zero**(*gsl_matrix* *H)

This function sets the lower triangular portion of `H`, below the subdiagonal, to zero. It is useful for clearing out the Householder vectors after calling `gsl_linalg_hessenberg_decomp()`.

14.15 Hessenberg-Triangular Decomposition of Real Matrices

A general real matrix pair (A, B) can be decomposed by orthogonal similarity transformations into the form

$$A = UHV^T$$
$$B = URV^T$$

where U and V are orthogonal, H is an upper Hessenberg matrix, and R is upper triangular. The Hessenberg-Triangular reduction is the first step in the generalized Schur decomposition for the generalized eigenvalue problem.

int **gsl_linalg_hesstri_decomp**(*gsl_matrix* *A, *gsl_matrix* *B, *gsl_matrix* *U, *gsl_matrix* *V, *gsl_vector* *work)

This function computes the Hessenberg-Triangular decomposition of the matrix pair (`A`, `B`). On output, H is stored in `A`, and R is stored in `B`. If `U` and `V` are provided (they may be null), the similarity transformations are stored in them. Additional workspace of length N is needed in `work`.

14.16 Bidiagonalization

A general matrix A can be factorized by similarity transformations into the form,

$$A = UBV^T$$

where U and V are orthogonal matrices and B is a N-by-N bidiagonal matrix with non-zero entries only on the diagonal and superdiagonal. The size of `U` is M-by-N and the size of `V` is N-by-N.

int **gsl_linalg_bidiag_decomp**(*gsl_matrix* *A, *gsl_vector* *tau_U, *gsl_vector* *tau_V)

This function factorizes the M-by-N matrix `A` into bidiagonal form UBV^T. The diagonal and superdiagonal of the matrix B are stored in the diagonal and superdiagonal of `A`. The orthogonal matrices U and `V` are stored as compressed Householder vectors in the remaining elements of `A`. The Householder coefficients are stored in the vectors `tau_U` and `tau_V`. The length of `tau_U` must equal the number of elements in the diagonal of `A` and the length of `tau_V` should be one element shorter.

int **gsl_linalg_bidiag_unpack**(const *gsl_matrix* *A, const *gsl_vector* *tau_U, *gsl_matrix* *U, const *gsl_vector* *tau_V, *gsl_matrix* *V, *gsl_vector* *diag, *gsl_vector* *superdiag)

This function unpacks the bidiagonal decomposition of `A` produced by `gsl_linalg_bidiag_decomp()`, (`A`, `tau_U`, `tau_V`) into the separate orthogonal matrices `U`, `V` and the diagonal vector `diag` and superdiagonal `superdiag`. Note that `U` is stored as a compact M-by-N orthogonal matrix satisfying $U^T U = I$ for efficiency.

int **gsl_linalg_bidiag_unpack2**(*gsl_matrix* *A, *gsl_vector* *tau_U, *gsl_vector* *tau_V, *gsl_matrix* *V)

This function unpacks the bidiagonal decomposition of `A` produced by `gsl_linalg_bidiag_decomp()`, (`A`, `tau_U`, `tau_V`) into the separate orthogonal matrices `U`, `V` and the diagonal vector `diag` and superdiagonal `superdiag`. The matrix `U` is stored in-place in `A`.

int **gsl_linalg_bidiag_unpack_B**(const *gsl_matrix* *A, *gsl_vector* *diag, *gsl_vector* *superdiag)

This function unpacks the diagonal and superdiagonal of the bidiagonal decomposition of `A` from `gsl_linalg_bidiag_decomp()`, into the diagonal vector `diag` and superdiagonal vector `superdiag`.

14.17 Givens Rotations

A Givens rotation is a rotation in the plane acting on two elements of a given vector. It can be represented in matrix form as

$$G(i,j,\theta) = \begin{pmatrix} 1 & \ldots & 0 & \ldots & 0 & \ldots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \ldots & \cos\theta & \ldots & -\sin\theta & \ldots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \ldots & \sin\theta & \ldots & \cos\theta & \ldots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \ldots & 0 & \ldots & 0 & \ldots & 1 \end{pmatrix}$$

where the $\cos\theta$ and $\sin\theta$ appear at the intersection of the i-th and j-th rows and columns. When acting on a vector x, $G(i,j,\theta)x$ performs a rotation of the (i,j) elements of x. Givens rotations are typically used to introduce zeros in vectors, such as during the QR decomposition of a matrix. In this case, it is typically desired to find c and s such that

$$\begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} r \\ 0 \end{pmatrix}$$

with $r = \sqrt{a^2 + b^2}$.

void **gsl_linalg_givens**(const double a, const double b, double *c, double *s)

This function computes $c = \cos\theta$ and $s = \sin\theta$ so that the Givens matrix $G(\theta)$ acting on the vector (a,b) produces $(r,0)$, with $r = \sqrt{a^2 + b^2}$.

void **gsl_linalg_givens_gv**(*gsl_vector* *v, const size_t i, const size_t j, const double c, const double s)

This function applies the Givens rotation defined by $c = \cos\theta$ and $s = \sin\theta$ to the `i` and `j` elements of `v`. On output, $(v(i), v(j)) \leftarrow G(\theta)(v(i), v(j))$.

14.18 Householder Transformations

A Householder transformation is a rank-1 modification of the identity matrix which can be used to zero out selected elements of a vector. A Householder matrix H takes the form,

$$H = I - \tau v v^T$$

where v is a vector (called the *Householder vector*) and $\tau = 2/(v^T v)$. The functions described in this section use the rank-1 structure of the Householder matrix to create and apply Householder transformations efficiently.

double **gsl_linalg_householder_transform**(*gsl_vector* *w)

gsl_complex **gsl_linalg_complex_householder_transform**(gsl_vector_complex *w)

This function prepares a Householder transformation $H = I - \tau v v^T$ which can be used to zero all the elements of the input vector `w` except the first. On output the Householder vector `v` is stored in `w` and the scalar τ is returned. The householder vector `v` is normalized so that `v[0] = 1`, however this 1 is not stored in the output vector. Instead, `w[0]` is set to the first element of the transformed vector, so that if $u = Hw$, `w[0] = u[0]` on output and the remainder of u is zero.

int **gsl_linalg_householder_hm**(double tau, const *gsl_vector* *v, *gsl_matrix* *A) int **gsl_linalg_complex_householder_hm**(gsl_complex tau, const gsl_vector_complex *v, gsl_matrix_complex *A)

This function applies the Householder matrix H defined by the scalar `tau` and the vector `v` to the left-hand side of the matrix `A`. On output the result HA is stored in `A`.

int **gsl_linalg_householder_mh**(double tau, const *gsl_vector* *v, *gsl_matrix* *A)

int **gsl_linalg_complex_householder_mh**(gsl_complex tau, const gsl_vector_complex *v, gsl_matrix_complex *A)

This function applies the Householder matrix H defined by the scalar `tau` and the vector `v` to the right-hand side of the matrix `A`. On output the result AH is stored in `A`.

int **gsl_linalg_householder_hv**(double tau, const *gsl_vector* *v, *gsl_vector* *w)

int **gsl_linalg_complex_householder_hv**(gsl_complex tau, const gsl_vector_complex *v, gsl_vector_complex *w)

This function applies the Householder transformation H defined by the scalar `tau` and the vector `v` to the vector `w`. On output the result Hw is stored in `w`.

14.19 Householder solver for linear systems

int **gsl_linalg_HH_solve**(*gsl_matrix* *A, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the system $Ax = b$ directly using Householder transformations. On output the solution is stored in `x` and `b` is not modified. The matrix `A` is destroyed by the Householder transformations.

int **gsl_linalg_HH_svx**(*gsl_matrix* *A, *gsl_vector* *x)

This function solves the system $Ax = b$ in-place using Householder transformations. On input `x` should contain the right-hand side b, which is replaced by the solution on output. The matrix `A` is destroyed by the Householder transformations.

14.20 Tridiagonal Systems

The functions described in this section efficiently solve symmetric, non-symmetric and cyclic tridiagonal systems with minimal storage. Note that the current implementations of these functions use a variant of Cholesky decomposition, so the tridiagonal matrix must be positive definite. For non-positive definite matrices, the functions return the error code `GSL_ESING`.

int **gsl_linalg_solve_tridiag**(const *gsl_vector* *diag, const *gsl_vector* *e, const *gsl_vector* *f, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the general N-by-N system $Ax = b$ where `A` is tridiagonal ($N \geq 2$). The super-diagonal and sub-diagonal vectors `e` and `f` must be one element shorter than the diagonal vector `diag`. The form of `A` for the 4-by-4 case is shown below,

$$A = \begin{pmatrix} d_0 & e_0 & 0 & 0 \\ f_0 & d_1 & e_1 & 0 \\ 0 & f_1 & d_2 & e_2 \\ 0 & 0 & f_2 & d_3 \end{pmatrix}$$

int **gsl_linalg_solve_symm_tridiag**(const *gsl_vector* *diag, const *gsl_vector* *e, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the general N-by-N system $Ax = b$ where `A` is symmetric tridiagonal ($N \geq 2$). The off-diagonal vector `e` must be one element shorter than the diagonal vector `diag`. The form of `A` for the 4-by-4 case is shown below,

$$A = \begin{pmatrix} d_0 & e_0 & 0 & 0 \\ e_0 & d_1 & e_1 & 0 \\ 0 & e_1 & d_2 & e_2 \\ 0 & 0 & e_2 & d_3 \end{pmatrix}$$

int **gsl_linalg_solve_cyc_tridiag**(const *gsl_vector* *diag, const *gsl_vector* *e, const *gsl_vector* *f, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the general N-by-N system $Ax = b$ where `A` is cyclic tridiagonal ($N \geq 3$). The cyclic super-diagonal and sub-diagonal vectors `e` and `f` must have the same number of elements as the diagonal vector `diag`. The form of `A` for the 4-by-4 case is shown below,

$$A = \begin{pmatrix} d_0 & e_0 & 0 & f_3 \\ f_0 & d_1 & e_1 & 0 \\ 0 & f_1 & d_2 & e_2 \\ e_3 & 0 & f_2 & d_3 \end{pmatrix}$$

int **gsl_linalg_solve_symm_cyc_tridiag**(const *gsl_vector* *diag, const *gsl_vector* *e, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the general N-by-N system $Ax = b$ where `A` is symmetric cyclic tridiagonal ($N \geq 3$). The cyclic off-diagonal vector `e` must have the same number of elements as the diagonal vector `diag`. The form of `A` for the 4-by-4 case is shown below,

$$A = \begin{pmatrix} d_0 & e_0 & 0 & e_3 \\ e_0 & d_1 & e_1 & 0 \\ 0 & e_1 & d_2 & e_2 \\ e_3 & 0 & e_2 & d_3 \end{pmatrix}$$

14.21 Triangular Systems

int **gsl_linalg_tri_invert**(CBLAS_UPLO_t Uplo, CBLAS_DIAG_t Diag, *gsl_matrix* *T)

int **gsl_linalg_complex_tri_invert**(CBLAS_UPLO_t Uplo, CBLAS_DIAG_t Diag, gsl_matrix_complex *T)

These functions compute the in-place inverse of the triangular matrix `T`, stored in the lower triangle when `Uplo` = `CblasLower` and upper triangle when `Uplo` = `CblasUpper`. The parameter `Diag` = `CblasUnit`, `CblasNonUnit` specifies whether the matrix is unit triangular.

int **gsl_linalg_tri_LTL**(*gsl_matrix* *L)

int **gsl_linalg_complex_tri_LHL**(gsl_matrix_complex *L)

These functions compute the product $L^T L$ (or $L^\dagger L$) in-place and stores it in the lower triangle of `L` on output.

int **gsl_linalg_tri_UL**(*gsl_matrix* *LU)

int **gsl_linalg_complex_tri_UL**(gsl_matrix_complex *LU)

These functions compute the product UL where U is upper triangular and L is unit lower triangular, stored in `LU`, as computed by `gsl_linalg_LU_decomp()` or `gsl_linalg_complex_LU_decomp()`. The product is computed in-place using Level 3 BLAS.

int **gsl_linalg_tri_rcond**(CBLAS_UPLO_t Uplo, const *gsl_matrix* *A, double *rcond, *gsl_vector* *work)

This function estimates the 1-norm reciprocal condition number of the triangular matrix `A`, using the lower triangle when `Uplo` is `CblasLower` and upper triangle when `Uplo` is `CblasUpper`. The reciprocal condition number $1/\left(||A||_1 \, ||A^{-1}||_1\right)$ is stored in `rcond` on output. Additional workspace of size $3N$ is required in `work`.

14.22 Banded Systems

Band matrices are sparse matrices whose non-zero entries are confined to a diagonal *band*. From a storage point of view, significant savings can be achieved by storing only the non-zero diagonals of a banded matrix. Algorithms such as LU and Cholesky factorizations preserve the band structure of these matrices. Computationally, working with compact banded matrices is preferable to working on the full dense matrix with many zero entries.

14.22.1 General Banded Format

An example of a general banded matrix is given below.

$$A = \begin{pmatrix} \alpha_1 & \beta_1 & \gamma_1 & 0 & 0 & 0 \\ \delta_1 & \alpha_2 & \beta_2 & \gamma_2 & 0 & 0 \\ 0 & \delta_2 & \alpha_3 & \beta_3 & \gamma_3 & 0 \\ 0 & 0 & \delta_3 & \alpha_4 & \beta_4 & \gamma_4 \\ 0 & 0 & 0 & \delta_4 & \alpha_5 & \beta_5 \\ 0 & 0 & 0 & 0 & \delta_5 & \alpha_6 \end{pmatrix}$$

This matrix has a *lower bandwidth* of 1 and an *upper bandwidth* of 2. The lower bandwidth is the number of non-zero subdiagonals, and the upper bandwidth is the number of non-zero superdiagonals. A (p, q) banded matrix has a lower bandwidth p and upper bandwidth q. For example, diagonal matrices are $(0, 0)$, tridiagonal matrices are $(1, 1)$, and upper triangular matrices are $(0, N - 1)$ banded matrices.

The corresponding 6-by-4 packed banded matrix looks like

$$AB = \begin{pmatrix} * & * & \alpha_1 & \delta_1 \\ * & \beta_1 & \alpha_2 & \delta_2 \\ \gamma_1 & \beta_2 & \alpha_3 & \delta_3 \\ \gamma_2 & \beta_3 & \alpha_4 & \delta_4 \\ \gamma_3 & \beta_4 & \alpha_5 & \delta_5 \\ \gamma_4 & \beta_5 & \alpha_6 & * \end{pmatrix}$$

where the superdiagonals are stored in columns, followed by the diagonal, followed by the subdiagonals. The entries marked by $*$ are not referenced by the banded routines. With this format, each row of AB corresponds to the non-zero entries of the corresponding column of A. For an N-by-N matrix A, the dimension of AB will be N-by-$(p + q + 1)$.

14.22.2 Symmetric Banded Format

Symmetric banded matrices allow for additional storage savings. As an example, consider the following 6×6 symmetric banded matrix with lower bandwidth $p = 2$:

$$A = \begin{pmatrix} \alpha_1 & \beta_1 & \gamma_1 & 0 & 0 & 0 \\ \beta_1 & \alpha_2 & \beta_2 & \gamma_2 & 0 & 0 \\ \gamma_1 & \beta_2 & \alpha_3 & \beta_3 & \gamma_3 & 0 \\ 0 & \gamma_2 & \beta_3 & \alpha_4 & \beta_4 & \gamma_4 \\ 0 & 0 & \gamma_3 & \beta_4 & \alpha_5 & \beta_5 \\ 0 & 0 & 0 & \gamma_4 & \beta_5 & \alpha_6 \end{pmatrix}$$

The packed symmetric banded 6×3 matrix will look like:

$$AB = \begin{pmatrix} \alpha_1 & \beta_1 & \gamma_1 \\ \alpha_2 & \beta_2 & \gamma_2 \\ \alpha_3 & \beta_3 & \gamma_3 \\ \alpha_4 & \beta_4 & \gamma_4 \\ \alpha_5 & \beta_5 & * \\ \alpha_6 & * & * \end{pmatrix}$$

The entries marked by $*$ are not referenced by the symmetric banded routines. The relationship between the packed format and original matrix is,

$$AB(i,j) = A(i,i+j) = A(i+j,i)$$

for $i = 0,\dots,N-1, j = 0,\dots,p$. Conversely,

$$A(i,j) = AB(j,i-j)$$

for $i = 0,\dots,N-1, j = \max(0,i-p),\dots,i$.

Warning: Note that this format is the transpose of the symmetric banded format used by LAPACK. In order to develop efficient routines for symmetric banded matrices, it helps to have the nonzero elements in each column in contiguous memory locations. Since C uses row-major order, GSL stores the columns in the rows of the packed banded format, while LAPACK, written in Fortran, uses the transposed format.

14.22.3 Banded LU Decomposition

The routines in this section are designed to factor banded M-by-N matrices with an LU factorization, $PA = LU$. The matrix A is banded of type (p,q), i.e. a lower bandwidth of p and an upper bandwidth of q. See *LU Decomposition* for more information on the factorization. For banded (p,q) matrices, the U factor will have an upper bandwidth of $p+q$, while the L factor will have a lower bandwidth of at most p. Therefore, additional storage is needed to store the p additional bands of U.

As an example, consider the $M = N = 7$ matrix with lower bandwidth $p = 3$ and upper bandwidth $q = 2$,

$$A = \begin{pmatrix} \alpha_1 & \beta_1 & \gamma_1 & 0 & 0 & 0 & 0 \\ \delta_1 & \alpha_2 & \beta_2 & \gamma_2 & 0 & 0 & 0 \\ \epsilon_1 & \delta_2 & \alpha_3 & \beta_3 & \gamma_3 & 0 & 0 \\ \zeta_1 & \epsilon_2 & \delta_3 & \alpha_4 & \beta_4 & \gamma_4 & 0 \\ 0 & \zeta_2 & \epsilon_3 & \delta_4 & \alpha_5 & \beta_5 & \gamma_5 \\ 0 & 0 & \zeta_3 & \epsilon_4 & \delta_5 & \alpha_6 & \beta_6 \\ 0 & 0 & 0 & \zeta_4 & \epsilon_5 & \delta_6 & \alpha_7 \end{pmatrix}$$

The corresponding N-by-$2p+q+1$ packed banded matrix looks like

$$AB = \left(\begin{array}{ccccccccc} * & * & * & * & * & \alpha_1 & \delta_1 & \epsilon_1 & \zeta_1 \\ * & * & * & * & \beta_1 & \alpha_2 & \delta_2 & \epsilon_2 & \zeta_2 \\ * & * & * & \gamma_1 & \beta_2 & \alpha_3 & \delta_3 & \epsilon_3 & \zeta_3 \\ * & * & - & \gamma_2 & \beta_3 & \alpha_4 & \delta_4 & \epsilon_4 & \zeta_4 \\ * & - & - & \gamma_3 & \beta_4 & \alpha_5 & \delta_5 & \epsilon_5 & * \\ - & - & - & \gamma_4 & \beta_5 & \alpha_6 & \delta_6 & * & * \\ - & - & - & \gamma_5 & \beta_6 & \alpha_7 & * & * & * \\ \multicolumn{3}{c}{\underbrace{\qquad\qquad}_{p}} & \multicolumn{2}{c}{\underbrace{\qquad}_{q}} & & \multicolumn{3}{c}{\underbrace{\qquad\qquad}_{p}} \end{array}\right)$$

Entries marked with $-$ are used to store the additional p diagonals of the U factor. Entries marked with $*$ are not referenced by the banded routines.

int **gsl_linalg_LU_band_decomp**(const size_t M, const size_t lb, const size_t ub, *gsl_matrix* *AB, gsl_vector_uint *piv)

This function computes the LU factorization of the banded matrix `AB` which is stored in packed band format (see above) and has dimension N-by-$2p+q+1$. The number of rows M of the original matrix is provided in `M`. The lower bandwidth p is provided in `lb` and the upper bandwidth q is provided in `ub`. The vector `piv` has length $\min(M,N)$ and stores the pivot indices on output (for $0 \le i < \min(M,N)$, row i of the matrix was interchanged with row `piv[i]`). On output, `AB` contains both the L and U factors in packed format.

int **gsl_linalg_LU_band_solve**(const size_t lb, const size_t ub, const *gsl_matrix* *LUB, const gsl_vector_uint *piv, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the square system $Ax = b$ using the banded LU factorization (`LUB`, `piv`) computed by `gsl_linalg_LU_band_decomp()`. The lower and upper bandwidths are provided in `lb` and `ub` respectively. The right hand side vector is provided in `b`. The solution vector is stored in `x` on output.

int **gsl_linalg_LU_band_svx**(const size_t lb, const size_t ub, const *gsl_matrix* *LUB, const gsl_vector_uint *piv, *gsl_vector* *x)

This function solves the square system $Ax = b$ in-place, using the banded LU factorization (`LUB`, `piv`) computed by `gsl_linalg_LU_band_decomp()`. The lower and upper bandwidths are provided in `lb` and `ub` respectively. On input, the right hand side vector b is provided in `x`, which is replaced by the solution vector x on output.

int **gsl_linalg_LU_band_unpack**(const size_t M, const size_t lb, const size_t ub, const *gsl_matrix* *LUB, const gsl_vector_uint *piv, *gsl_matrix* *L, *gsl_matrix* *U)

This function unpacks the banded LU factorization (`LUB`, `piv`) previously computed by `gsl_linalg_LU_band_decomp()` into the matrices `L` and `U`. The matrix `U` has dimension min(M, N)-by-N and stores the upper triangular factor on output. The matrix `L` has dimension M-by-min(M, N) and stores the matrix $P^T L$ on output.

14.22.4 Banded Cholesky Decomposition

The routines in this section are designed to factor and solve N-by-N linear systems of the form $Ax = b$ where A is a banded, symmetric, and positive definite matrix with lower bandwidth p. See *Cholesky Decomposition* for more information on the factorization. The lower triangular factor of the Cholesky decomposition preserves the same banded structure as the matrix A, enabling an efficient algorithm which overwrites the original matrix with the L factor.

int **gsl_linalg_cholesky_band_decomp**(*gsl_matrix* *A)

This function factorizes the symmetric, positive-definite square matrix `A` into the Cholesky decomposition $A = LL^T$. The input matrix `A` is given in *symmetric banded format*, and has dimensions N-by-$(p + 1)$, where p is the lower bandwidth of the matrix. On output, the entries of `A` are replaced by the entries of the matrix L in the same format. In addition, the lower right element of `A` is used to store the matrix 1-norm, used later by `gsl_linalg_cholesky_band_rcond()` to calculate the reciprocal condition number.

If the matrix is not positive-definite then the decomposition will fail, returning the error code `GSL_EDOM`. When testing whether a matrix is positive-definite, disable the error handler first to avoid triggering an error.

int **gsl_linalg_cholesky_band_solve**(const *gsl_matrix* *LLT, const *gsl_vector* *b, *gsl_vector* *x)

int **gsl_linalg_cholesky_band_solvem**(const *gsl_matrix* *LLT, const *gsl_matrix* *B, *gsl_matrix* *X)

This function solves the symmetric banded system $Ax = b$ (or $AX = B$) using the Cholesky decomposition of A held in the matrix `LLT` which must have been previously computed by `gsl_linalg_cholesky_band_decomp()`.

int **gsl_linalg_cholesky_band_svx**(const *gsl_matrix* *LLT, *gsl_vector* *x)

int **gsl_linalg_cholesky_band_svxm**(const *gsl_matrix* *LLT, *gsl_matrix* *X)

This function solves the symmetric banded system $Ax = b$ (or $AX = B$) in-place using the Cholesky decomposition of A held in the matrix `LLT` which must have been previously computed by `gsl_linalg_cholesky_band_decomp()`. On input `x` (or `X`) should contain the right-hand side b (or B), which is replaced by the solution on output.

int **gsl_linalg_cholesky_band_invert**(const *gsl_matrix* *LLT, *gsl_matrix* *Ainv)

This function computes the inverse of a symmetric banded matrix from its Cholesky decomposition `LLT`, which must have been previously computed by `gsl_linalg_cholesky_band_decomp()`. On output, the inverse is stored in `Ainv`, using both the lower and upper portions.

int **gsl_linalg_cholesky_band_unpack**(const *gsl_matrix* *LLT, *gsl_matrix* *L)

This function unpacks the lower triangular Cholesky factor from `LLT` and stores it in the lower triangular portion of the N-by-N matrix `L`. The upper triangular portion of `L` is not referenced.

int **gsl_linalg_cholesky_band_scale**(const *gsl_matrix* *A, *gsl_vector* *S)

This function calculates a diagonal scaling transformation of the symmetric, positive definite banded matrix `A`, such that SAS has a condition number within a factor of N of the matrix of smallest possible condition number over all possible diagonal scalings. On output, `S` contains the scale factors, given by $S_i = 1/\sqrt{A_{ii}}$. For any $A_{ii} \le 0$, the corresponding scale factor S_i is set to 1.

int **gsl_linalg_cholesky_band_scale_apply**(*gsl_matrix* *A, const *gsl_vector* *S)

This function applies the scaling transformation `S` to the banded symmetric positive definite matrix `A`. On output, `A` is replaced by SAS.

int **gsl_linalg_cholesky_band_rcond**(const *gsl_matrix* *LLT, double *rcond, *gsl_vector* *work)

This function estimates the reciprocal condition number (using the 1-norm) of the symmetric banded positive definite matrix A, using its Cholesky decomposition provided in `LLT`. The reciprocal condition number estimate, defined as $1/(||A||_1 \cdot ||A^{-1}||_1)$, is stored in `rcond`. Additional workspace of size $3N$ is required in `work`.

14.22.5 Banded LDLT Decomposition

The routines in this section are designed to factor and solve N-by-N linear systems of the form $Ax = b$ where A is a banded, symmetric, and non-singular matrix with lower bandwidth p. See *LDLT Decomposition* for more information on the factorization. The lower triangular factor of the LDL^T decomposition preserves the same banded structure as the matrix A, enabling an efficient algorithm which overwrites the original matrix with the L and D factors.

int **gsl_linalg_ldlt_band_decomp**(*gsl_matrix* *A)

This function factorizes the symmetric, non-singular square matrix `A` into the decomposition $A = LDL^T$. The input matrix `A` is given in *symmetric banded format*, and has dimensions N-by-$(p+1)$, where p is the lower bandwidth of the matrix. On output, the entries of `A` are replaced by the entries of the matrices D and L in the same format.

If the matrix is singular then the decomposition will fail, returning the error code `GSL_EDOM`.

int **gsl_linalg_ldlt_band_solve**(const *gsl_matrix* *LDLT, const *gsl_vector* *b, *gsl_vector* *x)

This function solves the symmetric banded system $Ax = b$ using the LDL^T decomposition of A held in the matrix `LDLT` which must have been previously computed by `gsl_linalg_ldlt_band_decomp()`.

int **gsl_linalg_ldlt_band_svx**(const *gsl_matrix* *LDLT, *gsl_vector* *x)

This function solves the symmetric banded system $Ax = b$ in-place using the LDL^T decomposition of A held in the matrix `LDLT` which must have been previously computed by `gsl_linalg_ldlt_band_decomp()`. On input `x` should contain the right-hand side b, which is replaced by the solution on output.

int **gsl_linalg_ldlt_band_unpack**(const *gsl_matrix* *LDLT, *gsl_matrix* *L, *gsl_vector* *D)

This function unpacks the unit lower triangular factor L from `LDLT` and stores it in the lower triangular portion of the N-by-N matrix `L`. The upper triangular portion of `L` is not referenced. The diagonal matrix D is stored in the vector `D`.

int **gsl_linalg_ldlt_band_rcond**(const *gsl_matrix* *LDLT, double *rcond, *gsl_vector* *work)

This function estimates the reciprocal condition number (using the 1-norm) of the symmetric banded nonsingular matrix A, using its LDL^T decomposition provided in `LDLT`. The reciprocal condition number estimate, defined as $1/(||A||_1 \cdot ||A^{-1}||_1)$, is stored in `rcond`. Additional workspace of size $3N$ is required in `work`.

14.23 Balancing

The process of balancing a matrix applies similarity transformations to make the rows and columns have comparable norms. This is useful, for example, to reduce roundoff errors in the solution of eigenvalue problems. Balancing a matrix A consists of replacing A with a similar matrix

$$A' = D^{-1}AD$$

where D is a diagonal matrix whose entries are powers of the floating point radix.

int **gsl_linalg_balance_matrix**(*gsl_matrix* *A, *gsl_vector* *D)

This function replaces the matrix `A` with its balanced counterpart and stores the diagonal elements of the similarity transformation into the vector `D`.

14.24 Examples

The following program solves the linear system $Ax = b$. The system to be solved is,

$$\begin{pmatrix} 0.18 & 0.60 & 0.57 & 0.96 \\ 0.41 & 0.24 & 0.99 & 0.58 \\ 0.14 & 0.30 & 0.97 & 0.66 \\ 0.51 & 0.13 & 0.19 & 0.85 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1.0 \\ 2.0 \\ 3.0 \\ 4.0 \end{pmatrix}$$

and the solution is found using LU decomposition of the matrix A.

```
#include <stdio.h>
#include <gsl/gsl_linalg.h>

int
main (void)
{
  double a_data[] = { 0.18, 0.60, 0.57, 0.96,
                      0.41, 0.24, 0.99, 0.58,
                      0.14, 0.30, 0.97, 0.66,
                      0.51, 0.13, 0.19, 0.85 };

  double b_data[] = { 1.0, 2.0, 3.0, 4.0 };

  gsl_matrix_view m
    = gsl_matrix_view_array (a_data, 4, 4);

  gsl_vector_view b
    = gsl_vector_view_array (b_data, 4);

  gsl_vector *x = gsl_vector_alloc (4);

  int s;

  gsl_permutation * p = gsl_permutation_alloc (4);

  gsl_linalg_LU_decomp (&m.matrix, p, &s);

```

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```
  gsl_linalg_LU_solve (&m.matrix, p, &b.vector, x);

  printf ("x = \n");
  gsl_vector_fprintf (stdout, x, "%g");

  gsl_permutation_free (p);
  gsl_vector_free (x);
  return 0;
}
```

Here is the output from the program,

```
x =
-4.05205
-12.6056
1.66091
8.69377
```

This can be verified by multiplying the solution x by the original matrix A using GNU octave,

```
octave> A = [ 0.18, 0.60, 0.57, 0.96;
              0.41, 0.24, 0.99, 0.58;
              0.14, 0.30, 0.97, 0.66;
              0.51, 0.13, 0.19, 0.85 ];

octave> x = [ -4.05205; -12.6056; 1.66091; 8.69377];

octave> A * x
ans =
  1.0000
  2.0000
  3.0000
  4.0000
```

This reproduces the original right-hand side vector, b, in accordance with the equation $Ax = b$.

14.25 References and Further Reading

Further information on the algorithms described in this section can be found in the following book,

- G. H. Golub, C. F. Van Loan, "Matrix Computations" (3rd Ed, 1996), Johns Hopkins University Press, ISBN 0-8018-5414-8.

The LAPACK library is described in the following manual,

- *LAPACK Users' Guide* (Third Edition, 1999), Published by SIAM, ISBN 0-89871-447-8

The LAPACK source code can be found at http://www.netlib.org/lapack, along with an online copy of the users guide.

Further information on recursive Level 3 BLAS algorithms may be found in the following paper,

- E. Peise and P. Bientinesi, "Recursive algorithms for dense linear algebra: the ReLAPACK collection", http://arxiv.org/abs/1602.06763, 2016.

The recursive Level 3 BLAS QR decomposition is described in the following paper,

- E. Elmroth and F. G. Gustavson, 2000. Applying recursion to serial and parallel QR factorization leads to better performance. IBM Journal of Research and Development, 44(4), pp.605-624.

The Modified Golub-Reinsch algorithm is described in the following paper,

- T.F. Chan, "An Improved Algorithm for Computing the Singular Value Decomposition", ACM Transactions on Mathematical Software, 8 (1982), pp 72–83.

The Jacobi algorithm for singular value decomposition is described in the following papers,

- J.C. Nash, "A one-sided transformation method for the singular value decomposition and algebraic eigenproblem", Computer Journal, Volume 18, Number 1 (1975), p 74–76
- J.C. Nash and S. Shlien "Simple algorithms for the partial singular value decomposition", Computer Journal, Volume 30 (1987), p 268–275.
- J. Demmel, K. Veselic, "Jacobi's Method is more accurate than QR", Lapack Working Note 15 (LAWN-15), October 1989. Available from netlib, http://www.netlib.org/lapack/ in the `lawns` or `lawnspdf` directories.

The algorithm for estimating a matrix condition number is described in the following paper,

- N. J. Higham, "FORTRAN codes for estimating the one-norm of a real or complex matrix, with applications to condition estimation", ACM Trans. Math. Soft., vol. 14, no. 4, pp. 381-396, December 1988.

CHAPTER

FIFTEEN

EIGENSYSTEMS

This chapter describes functions for computing eigenvalues and eigenvectors of matrices. There are routines for real symmetric, real nonsymmetric, complex hermitian, real generalized symmetric-definite, complex generalized hermitian-definite, and real generalized nonsymmetric eigensystems. Eigenvalues can be computed with or without eigenvectors. The hermitian and real symmetric matrix algorithms are symmetric bidiagonalization followed by QR reduction. The nonsymmetric algorithm is the Francis QR double-shift. The generalized nonsymmetric algorithm is the QZ method due to Moler and Stewart.

The functions described in this chapter are declared in the header file `gsl_eigen.h`.

15.1 Real Symmetric Matrices

For real symmetric matrices, the library uses the symmetric bidiagonalization and QR reduction method. This is described in Golub & van Loan, section 8.3. The computed eigenvalues are accurate to an absolute accuracy of $\epsilon||A||_2$, where ϵ is the machine precision.

type **gsl_eigen_symm_workspace**

This workspace contains internal parameters used for solving symmetric eigenvalue problems.

gsl_eigen_symm_workspace ***gsl_eigen_symm_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues of `n`-by-`n` real symmetric matrices. The size of the workspace is $O(2n)$.

void **gsl_eigen_symm_free**(*gsl_eigen_symm_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_eigen_symm**(*gsl_matrix* *A, *gsl_vector* *eval, *gsl_eigen_symm_workspace* *w)

This function computes the eigenvalues of the real symmetric matrix `A`. Additional workspace of the appropriate size must be provided in `w`. The diagonal and lower triangular part of `A` are destroyed during the computation, but the strict upper triangular part is not referenced. The eigenvalues are stored in the vector `eval` and are unordered.

type **gsl_eigen_symmv_workspace**

This workspace contains internal parameters used for solving symmetric eigenvalue and eigenvector problems.

gsl_eigen_symmv_workspace ***gsl_eigen_symmv_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues and eigenvectors of `n`-by-`n` real symmetric matrices. The size of the workspace is $O(4n)$.

void **gsl_eigen_symmv_free**(*gsl_eigen_symmv_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_eigen_symmv**(*gsl_matrix* *A, *gsl_vector* *eval, *gsl_matrix* *evec, *gsl_eigen_symmv_workspace* *w)

This function computes the eigenvalues and eigenvectors of the real symmetric matrix `A`. Additional workspace of the appropriate size must be provided in `w`. The diagonal and lower triangular part of `A` are destroyed during the computation, but the strict upper triangular part is not referenced. The eigenvalues are stored in the vector `eval` and are unordered. The corresponding eigenvectors are stored in the columns of the matrix `evec`. For example, the eigenvector in the first column corresponds to the first eigenvalue. The eigenvectors are guaranteed to be mutually orthogonal and normalised to unit magnitude.

15.2 Complex Hermitian Matrices

For hermitian matrices, the library uses the complex form of the symmetric bidiagonalization and QR reduction method.

type **gsl_eigen_herm_workspace**

This workspace contains internal parameters used for solving hermitian eigenvalue problems.

gsl_eigen_herm_workspace ***gsl_eigen_herm_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues of `n`-by-`n` complex hermitian matrices. The size of the workspace is $O(3n)$.

void **gsl_eigen_herm_free**(*gsl_eigen_herm_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_eigen_herm**(gsl_matrix_complex *A, *gsl_vector* *eval, *gsl_eigen_herm_workspace* *w)

This function computes the eigenvalues of the complex hermitian matrix `A`. Additional workspace of the appropriate size must be provided in `w`. The diagonal and lower triangular part of `A` are destroyed during the computation, but the strict upper triangular part is not referenced. The imaginary parts of the diagonal are assumed to be zero and are not referenced. The eigenvalues are stored in the vector `eval` and are unordered.

type **gsl_eigen_hermv_workspace**

This workspace contains internal parameters used for solving hermitian eigenvalue and eigenvector problems.

gsl_eigen_hermv_workspace ***gsl_eigen_hermv_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues and eigenvectors of `n`-by-`n` complex hermitian matrices. The size of the workspace is $O(5n)$.

void **gsl_eigen_hermv_free**(*gsl_eigen_hermv_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_eigen_hermv**(gsl_matrix_complex *A, *gsl_vector* *eval, gsl_matrix_complex *evec, *gsl_eigen_hermv_workspace* *w)

This function computes the eigenvalues and eigenvectors of the complex hermitian matrix `A`. Additional workspace of the appropriate size must be provided in `w`. The diagonal and lower triangular part of `A` are destroyed during the computation, but the strict upper triangular part is not referenced. The imaginary parts of the diagonal are assumed to be zero and are not referenced. The eigenvalues are stored in the vector `eval` and are unordered. The corresponding complex eigenvectors are stored in the columns of the matrix `evec`. For example, the eigenvector in the first column corresponds to the first eigenvalue. The eigenvectors are guaranteed to be mutually orthogonal and normalised to unit magnitude.

15.3 Real Nonsymmetric Matrices

The solution of the real nonsymmetric eigensystem problem for a matrix A involves computing the Schur decomposition

$$A = ZTZ^T$$

where Z is an orthogonal matrix of Schur vectors and T, the Schur form, is quasi upper triangular with diagonal 1-by-1 blocks which are real eigenvalues of A, and diagonal 2-by-2 blocks whose eigenvalues are complex conjugate eigenvalues of A. The algorithm used is the double-shift Francis method.

type **gsl_eigen_nonsymm_workspace**

This workspace contains internal parameters used for solving nonsymmetric eigenvalue problems.

gsl_eigen_nonsymm_workspace ***gsl_eigen_nonsymm_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues of `n`-by-`n` real nonsymmetric matrices. The size of the workspace is $O(2n)$.

void **gsl_eigen_nonsymm_free**(*gsl_eigen_nonsymm_workspace* *w)

This function frees the memory associated with the workspace `w`.

void **gsl_eigen_nonsymm_params**(const int compute_t, const int balance, *gsl_eigen_nonsymm_workspace* *w)

This function sets some parameters which determine how the eigenvalue problem is solved in subsequent calls to `gsl_eigen_nonsymm()`.

If `compute_t` is set to 1, the full Schur form T will be computed by `gsl_eigen_nonsymm()`. If it is set to 0, T will not be computed (this is the default setting). Computing the full Schur form T requires approximately 1.5–2 times the number of flops.

If `balance` is set to 1, a balancing transformation is applied to the matrix prior to computing eigenvalues. This transformation is designed to make the rows and columns of the matrix have comparable norms, and can result in more accurate eigenvalues for matrices whose entries vary widely in magnitude. See *Balancing* for more information. Note that the balancing transformation does not preserve the orthogonality of the Schur vectors, so if you wish to compute the Schur vectors with `gsl_eigen_nonsymm_Z()` you will obtain the Schur vectors of the balanced matrix instead of the original matrix. The relationship will be

$$T = Q^T D^{-1} A D Q$$

where `Q` is the matrix of Schur vectors for the balanced matrix, and `D` is the balancing transformation. Then `gsl_eigen_nonsymm_Z()` will compute a matrix `Z` which satisfies

$$T = Z^{-1} A Z$$

with $Z = DQ$. Note that `Z` will not be orthogonal. For this reason, balancing is not performed by default.

int **gsl_eigen_nonsymm**(*gsl_matrix* *A, gsl_vector_complex *eval, *gsl_eigen_nonsymm_workspace* *w)

This function computes the eigenvalues of the real nonsymmetric matrix `A` and stores them in the vector `eval`. If T is desired, it is stored in the upper portion of `A` on output. Otherwise, on output, the diagonal of `A` will contain the 1-by-1 real eigenvalues and 2-by-2 complex conjugate eigenvalue systems, and the rest of `A` is destroyed. In rare cases, this function may fail to find all eigenvalues. If this happens, an error code is returned and the number of converged eigenvalues is stored in `w->n_evals`. The converged eigenvalues are stored in the beginning of `eval`.

int **gsl_eigen_nonsymm_Z**(*gsl_matrix* *A, gsl_vector_complex *eval, *gsl_matrix* *Z, *gsl_eigen_nonsymm_workspace* *w)

This function is identical to `gsl_eigen_nonsymm()` except that it also computes the Schur vectors and stores them into `Z`.

type **gsl_eigen_nonsymmv_workspace**

This workspace contains internal parameters used for solving nonsymmetric eigenvalue and eigenvector problems.

gsl_eigen_nonsymmv_workspace ***gsl_eigen_nonsymmv_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues and eigenvectors of `n`-by-`n` real nonsymmetric matrices. The size of the workspace is $O(5n)$.

void **gsl_eigen_nonsymmv_free**(*gsl_eigen_nonsymmv_workspace* *w)

This function frees the memory associated with the workspace `w`.

void **gsl_eigen_nonsymmv_params**(const int balance, *gsl_eigen_nonsymm_workspace* *w)

This function sets parameters which determine how the eigenvalue problem is solved in subsequent calls to `gsl_eigen_nonsymmv()`. If `balance` is set to 1, a balancing transformation is applied to the matrix. See `gsl_eigen_nonsymm_params()` for more information. Balancing is turned off by default since it does not preserve the orthogonality of the Schur vectors.

int **gsl_eigen_nonsymmv**(*gsl_matrix* *A, gsl_vector_complex *eval, gsl_matrix_complex *evec, *gsl_eigen_nonsymmv_workspace* *w)

This function computes eigenvalues and right eigenvectors of the `n`-by-`n` real nonsymmetric matrix `A`. It first calls `gsl_eigen_nonsymm()` to compute the eigenvalues, Schur form T, and Schur vectors. Then it finds eigenvectors of T and backtransforms them using the Schur vectors. The Schur vectors are destroyed in the process, but can be saved by using `gsl_eigen_nonsymmv_Z()`. The computed eigenvectors are normalized to have unit magnitude. On output, the upper portion of `A` contains the Schur form T. If `gsl_eigen_nonsymm()` fails, no eigenvectors are computed, and an error code is returned.

int **gsl_eigen_nonsymmv_Z**(*gsl_matrix* *A, gsl_vector_complex *eval, gsl_matrix_complex *evec, *gsl_matrix* *Z, *gsl_eigen_nonsymmv_workspace* *w)

This function is identical to `gsl_eigen_nonsymmv()` except that it also saves the Schur vectors into `Z`.

15.4 Real Generalized Symmetric-Definite Eigensystems

The real generalized symmetric-definite eigenvalue problem is to find eigenvalues λ and eigenvectors x such that

$$Ax = \lambda Bx$$

where A and B are symmetric matrices, and B is positive-definite. This problem reduces to the standard symmetric eigenvalue problem by applying the Cholesky decomposition to B:

$$\begin{aligned} Ax &= \lambda Bx \\ Ax &= \lambda LL^T x \\ \left(L^{-1}AL^{-T}\right) L^T x &= \lambda L^T x \end{aligned}$$

Therefore, the problem becomes $Cy = \lambda y$ where $C = L^{-1}AL^{-T}$ is symmetric, and $y = L^T x$. The standard symmetric eigensolver can be applied to the matrix C. The resulting eigenvectors are backtransformed to find the vectors of the original problem. The eigenvalues and eigenvectors of the generalized symmetric-definite eigenproblem are always real.

type **gsl_eigen_gensymm_workspace**

This workspace contains internal parameters used for solving generalized symmetric eigenvalue problems.

gsl_eigen_gensymm_workspace ***gsl_eigen_gensymm_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues of `n`-by-`n` real generalized symmetric-definite eigensystems. The size of the workspace is $O(2n)$.

void **gsl_eigen_gensymm_free**(*gsl_eigen_gensymm_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_eigen_gensymm**(*gsl_matrix* *A, *gsl_matrix* *B, *gsl_vector* *eval, *gsl_eigen_gensymm_workspace* *w)

This function computes the eigenvalues of the real generalized symmetric-definite matrix pair (`A`, `B`), and stores them in `eval`, using the method outlined above. On output, `B` contains its Cholesky decomposition and `A` is destroyed.

type **gsl_eigen_gensymmv_workspace**

This workspace contains internal parameters used for solving generalized symmetric eigenvalue and eigenvector problems.

gsl_eigen_gensymmv_workspace ***gsl_eigen_gensymmv_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues and eigenvectors of `n`-by-`n` real generalized symmetric-definite eigensystems. The size of the workspace is $O(4n)$.

void **gsl_eigen_gensymmv_free**(*gsl_eigen_gensymmv_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_eigen_gensymmv**(*gsl_matrix* *A, *gsl_matrix* *B, *gsl_vector* *eval, *gsl_matrix* *evec, *gsl_eigen_gensymmv_workspace* *w)

This function computes the eigenvalues and eigenvectors of the real generalized symmetric-definite matrix pair (`A`, `B`), and stores them in `eval` and `evec` respectively. The computed eigenvectors are normalized to have unit magnitude. On output, `B` contains its Cholesky decomposition and `A` is destroyed.

15.5 Complex Generalized Hermitian-Definite Eigensystems

The complex generalized hermitian-definite eigenvalue problem is to find eigenvalues λ and eigenvectors x such that

$$Ax = \lambda Bx$$

where A and B are hermitian matrices, and B is positive-definite. Similarly to the real case, this can be reduced to $Cy = \lambda y$ where $C = L^{-1}AL^{-\dagger}$ is hermitian, and $y = L^{\dagger}x$. The standard hermitian eigensolver can be applied to the matrix C. The resulting eigenvectors are backtransformed to find the vectors of the original problem. The eigenvalues of the generalized hermitian-definite eigenproblem are always real.

type **gsl_eigen_genherm_workspace**

This workspace contains internal parameters used for solving generalized hermitian eigenvalue problems.

gsl_eigen_genherm_workspace ***gsl_eigen_genherm_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues of `n`-by-`n` complex generalized hermitian-definite eigensystems. The size of the workspace is $O(3n)$.

void **gsl_eigen_genherm_free**(*gsl_eigen_genherm_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_eigen_genherm**(gsl_matrix_complex *A, gsl_matrix_complex *B, *gsl_vector* *eval, *gsl_eigen_genherm_workspace* *w)

This function computes the eigenvalues of the complex generalized hermitian-definite matrix pair (`A`, `B`), and stores them in `eval`, using the method outlined above. On output, `B` contains its Cholesky decomposition and `A` is destroyed.

type **gsl_eigen_genhermv_workspace**

This workspace contains internal parameters used for solving generalized hermitian eigenvalue and eigenvector problems.

gsl_eigen_genhermv_workspace ***gsl_eigen_genhermv_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues and eigenvectors of `n`-by-`n` complex generalized hermitian-definite eigensystems. The size of the workspace is $O(5n)$.

void **gsl_eigen_genhermv_free**(*gsl_eigen_genhermv_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_eigen_genhermv**(gsl_matrix_complex *A, gsl_matrix_complex *B, *gsl_vector* *eval, gsl_matrix_complex *evec, *gsl_eigen_genhermv_workspace* *w)

This function computes the eigenvalues and eigenvectors of the complex generalized hermitian-definite matrix pair (`A`, `B`), and stores them in `eval` and `evec` respectively. The computed eigenvectors are normalized to have unit magnitude. On output, `B` contains its Cholesky decomposition and `A` is destroyed.

15.6 Real Generalized Nonsymmetric Eigensystems

Given two square matrices (A, B), the generalized nonsymmetric eigenvalue problem is to find eigenvalues λ and eigenvectors x such that

$$Ax = \lambda Bx$$

We may also define the problem as finding eigenvalues μ and eigenvectors y such that

$$\mu Ay = By$$

Note that these two problems are equivalent (with $\lambda = 1/\mu$) if neither λ nor μ is zero. If say, λ is zero, then it is still a well defined eigenproblem, but its alternate problem involving μ is not. Therefore, to allow for zero (and infinite) eigenvalues, the problem which is actually solved is

$$\beta Ax = \alpha Bx$$

The eigensolver routines below will return two values α and β and leave it to the user to perform the divisions $\lambda = \alpha/\beta$ and $\mu = \beta/\alpha$.

If the determinant of the matrix pencil $A - \lambda B$ is zero for all λ, the problem is said to be singular; otherwise it is called regular. Singularity normally leads to some $\alpha = \beta = 0$ which means the eigenproblem is ill-conditioned and generally does not have well defined eigenvalue solutions. The routines below are intended for regular matrix pencils and could yield unpredictable results when applied to singular pencils.

The solution of the real generalized nonsymmetric eigensystem problem for a matrix pair (A, B) involves computing the generalized Schur decomposition

$$A = QSZ^T$$
$$B = QTZ^T$$

where Q and Z are orthogonal matrices of left and right Schur vectors respectively, and (S, T) is the generalized Schur form whose diagonal elements give the α and β values. The algorithm used is the QZ method due to Moler and Stewart (see references).

type **gsl_eigen_gen_workspace**

This workspace contains internal parameters used for solving generalized eigenvalue problems.

gsl_eigen_gen_workspace ***gsl_eigen_gen_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues of `n`-by-`n` real generalized nonsymmetric eigensystems. The size of the workspace is $O(n)$.

void **gsl_eigen_gen_free**(*gsl_eigen_gen_workspace* *w)

This function frees the memory associated with the workspace `w`.

void **gsl_eigen_gen_params**(const int compute_s, const int compute_t, const int balance, *gsl_eigen_gen_workspace* *w)

This function sets some parameters which determine how the eigenvalue problem is solved in subsequent calls to `gsl_eigen_gen()`.

If `compute_s` is set to 1, the full Schur form S will be computed by `gsl_eigen_gen()`. If it is set to 0, S will not be computed (this is the default setting). S is a quasi upper triangular matrix with 1-by-1 and 2-by-2 blocks on its diagonal. 1-by-1 blocks correspond to real eigenvalues, and 2-by-2 blocks correspond to complex eigenvalues.

If `compute_t` is set to 1, the full Schur form T will be computed by `gsl_eigen_gen()`. If it is set to 0, T will not be computed (this is the default setting). T is an upper triangular matrix with non-negative elements on its diagonal. Any 2-by-2 blocks in S will correspond to a 2-by-2 diagonal block in T.

The `balance` parameter is currently ignored, since generalized balancing is not yet implemented.

int **gsl_eigen_gen**(*gsl_matrix* *A, *gsl_matrix* *B, gsl_vector_complex *alpha, *gsl_vector* *beta, *gsl_eigen_gen_workspace* *w)

This function computes the eigenvalues of the real generalized nonsymmetric matrix pair (`A`, `B`), and stores them as pairs in (`alpha`, `beta`), where `alpha` is complex and `beta` is real. If β_i is non-zero, then $\lambda = \alpha_i/\beta_i$ is an eigenvalue. Likewise, if α_i is non-zero, then $\mu = \beta_i/\alpha_i$ is an eigenvalue of the alternate problem $\mu Ay = By$. The elements of `beta` are normalized to be non-negative.

If S is desired, it is stored in `A` on output. If T is desired, it is stored in `B` on output. The ordering of eigenvalues in (`alpha`, `beta`) follows the ordering of the diagonal blocks in the Schur forms S and T. In rare cases, this function may fail to find all eigenvalues. If this occurs, an error code is returned.

int **gsl_eigen_gen_QZ**(*gsl_matrix* *A, *gsl_matrix* *B, gsl_vector_complex *alpha, *gsl_vector* *beta, *gsl_matrix* *Q, *gsl_matrix* *Z, *gsl_eigen_gen_workspace* *w)

This function is identical to `gsl_eigen_gen()` except that it also computes the left and right Schur vectors and stores them into `Q` and `Z` respectively.

type **gsl_eigen_genv_workspace**

This workspace contains internal parameters used for solving generalized eigenvalue and eigenvector problems.

gsl_eigen_genv_workspace ***gsl_eigen_genv_alloc**(const size_t n)

This function allocates a workspace for computing eigenvalues and eigenvectors of `n`-by-`n` real generalized nonsymmetric eigensystems. The size of the workspace is $O(7n)$.

void **gsl_eigen_genv_free**(*gsl_eigen_genv_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_eigen_genv**(*gsl_matrix* *A, *gsl_matrix* *B, gsl_vector_complex *alpha, *gsl_vector* *beta, gsl_matrix_complex *evec, *gsl_eigen_genv_workspace* *w)

This function computes eigenvalues and right eigenvectors of the n-by-n real generalized nonsymmetric matrix pair (`A`, `B`). The eigenvalues are stored in (`alpha`, `beta`) and the eigenvectors are stored in `evec`. It first calls `gsl_eigen_gen()` to compute the eigenvalues, Schur forms, and Schur vectors. Then it finds eigenvectors of the Schur forms and backtransforms them using the Schur vectors. The Schur vectors are destroyed in the process, but can be saved by using `gsl_eigen_genv_QZ()`. The computed eigenvectors are normalized to have unit magnitude. On output, (`A`, `B`) contains the generalized Schur form (S, T). If `gsl_eigen_gen()` fails, no eigenvectors are computed, and an error code is returned.

int **gsl_eigen_genv_QZ**(*gsl_matrix* *A, *gsl_matrix* *B, gsl_vector_complex *alpha, *gsl_vector* *beta, gsl_matrix_complex *evec, *gsl_matrix* *Q, *gsl_matrix* *Z, *gsl_eigen_genv_workspace* *w)

This function is identical to `gsl_eigen_genv()` except that it also computes the left and right Schur vectors and stores them into `Q` and `Z` respectively.

15.7 Sorting Eigenvalues and Eigenvectors

int **gsl_eigen_symmv_sort**(*gsl_vector* *eval, *gsl_matrix* *evec, *gsl_eigen_sort_t* sort_type)

This function simultaneously sorts the eigenvalues stored in the vector `eval` and the corresponding real eigenvectors stored in the columns of the matrix `evec` into ascending or descending order according to the value of the parameter `sort_type`,

type **gsl_eigen_sort_t**

GSL_EIGEN_SORT_VAL_ASC	ascending order in numerical value
GSL_EIGEN_SORT_VAL_DESC	descending order in numerical value
GSL_EIGEN_SORT_ABS_ASC	ascending order in magnitude
GSL_EIGEN_SORT_ABS_DESC	descending order in magnitude

int **gsl_eigen_hermv_sort**(*gsl_vector* *eval, gsl_matrix_complex *evec, gsl_eigen_sort_t sort_type)
: This function simultaneously sorts the eigenvalues stored in the vector `eval` and the corresponding complex eigenvectors stored in the columns of the matrix `evec` into ascending or descending order according to the value of the parameter `sort_type` as shown above.

int **gsl_eigen_nonsymmv_sort**(gsl_vector_complex *eval, gsl_matrix_complex *evec, gsl_eigen_sort_t sort_type)
: This function simultaneously sorts the eigenvalues stored in the vector `eval` and the corresponding complex eigenvectors stored in the columns of the matrix `evec` into ascending or descending order according to the value of the parameter `sort_type` as shown above. Only `GSL_EIGEN_SORT_ABS_ASC` and `GSL_EIGEN_SORT_ABS_DESC` are supported due to the eigenvalues being complex.

int **gsl_eigen_gensymmv_sort**(*gsl_vector* *eval, *gsl_matrix* *evec, gsl_eigen_sort_t sort_type)
: This function simultaneously sorts the eigenvalues stored in the vector `eval` and the corresponding real eigenvectors stored in the columns of the matrix `evec` into ascending or descending order according to the value of the parameter `sort_type` as shown above.

int **gsl_eigen_genhermv_sort**(*gsl_vector* *eval, gsl_matrix_complex *evec, gsl_eigen_sort_t sort_type)
: This function simultaneously sorts the eigenvalues stored in the vector `eval` and the corresponding complex eigenvectors stored in the columns of the matrix `evec` into ascending or descending order according to the value of the parameter `sort_type` as shown above.

int **gsl_eigen_genv_sort**(gsl_vector_complex *alpha, *gsl_vector* *beta, gsl_matrix_complex *evec, gsl_eigen_sort_t sort_type)
: This function simultaneously sorts the eigenvalues stored in the vectors (`alpha`, `beta`) and the corresponding complex eigenvectors stored in the columns of the matrix `evec` into ascending or descending order according to the value of the parameter `sort_type` as shown above. Only `GSL_EIGEN_SORT_ABS_ASC` and `GSL_EIGEN_SORT_ABS_DESC` are supported due to the eigenvalues being complex.

15.8 Examples

The following program computes the eigenvalues and eigenvectors of the 4-th order Hilbert matrix, $H(i,j) = 1/(i + j + 1)$.

```
#include <stdio.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_eigen.h>

int
main (void)
{
  double data[] = { 1.0  , 1/2.0, 1/3.0, 1/4.0,
                    1/2.0, 1/3.0, 1/4.0, 1/5.0,
                    1/3.0, 1/4.0, 1/5.0, 1/6.0,
                    1/4.0, 1/5.0, 1/6.0, 1/7.0 };

  gsl_matrix_view m
    = gsl_matrix_view_array (data, 4, 4);

  gsl_vector *eval = gsl_vector_alloc (4);
  gsl_matrix *evec = gsl_matrix_alloc (4, 4);

  gsl_eigen_symmv_workspace * w =
    gsl_eigen_symmv_alloc (4);
```

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```
  gsl_eigen_symmv (&m.matrix, eval, evec, w);

  gsl_eigen_symmv_free (w);

  gsl_eigen_symmv_sort (eval, evec,
                        GSL_EIGEN_SORT_ABS_ASC);

  {
    int i;

    for (i = 0; i < 4; i++)
      {
        double eval_i
           = gsl_vector_get (eval, i);
        gsl_vector_view evec_i
           = gsl_matrix_column (evec, i);

        printf ("eigenvalue = %g\n", eval_i);
        printf ("eigenvector = \n");
        gsl_vector_fprintf (stdout,
                            &evec_i.vector, "%g");
      }
  }

  gsl_vector_free (eval);
  gsl_matrix_free (evec);

  return 0;
}
```

Here is the beginning of the output from the program:

```
$ ./a.out
eigenvalue = 9.67023e-05
eigenvector =
-0.0291933
0.328712
-0.791411
0.514553
...
```

This can be compared with the corresponding output from GNU octave:

```
octave> [v,d] = eig(hilb(4));
octave> diag(d)
ans =

   9.6702e-05
   6.7383e-03
   1.6914e-01
   1.5002e+00
```

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```
octave> v
v =

   0.029193   0.179186  -0.582076   0.792608
  -0.328712  -0.741918   0.370502   0.451923
   0.791411   0.100228   0.509579   0.322416
  -0.514553   0.638283   0.514048   0.252161
```

Note that the eigenvectors can differ by a change of sign, since the sign of an eigenvector is arbitrary.

The following program illustrates the use of the nonsymmetric eigensolver, by computing the eigenvalues and eigenvectors of the Vandermonde matrix $V(x;i,j) = x_i^{n-j}$ with $x = (-1,-2,3,4)$.

```
#include <stdio.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_eigen.h>

int
main (void)
{
  double data[] = { -1.0, 1.0, -1.0, 1.0,
                    -8.0, 4.0, -2.0, 1.0,
                    27.0, 9.0, 3.0, 1.0,
                    64.0, 16.0, 4.0, 1.0 };

  gsl_matrix_view m
    = gsl_matrix_view_array (data, 4, 4);

  gsl_vector_complex *eval = gsl_vector_complex_alloc (4);
  gsl_matrix_complex *evec = gsl_matrix_complex_alloc (4, 4);

  gsl_eigen_nonsymmv_workspace * w =
    gsl_eigen_nonsymmv_alloc (4);

  gsl_eigen_nonsymmv (&m.matrix, eval, evec, w);

  gsl_eigen_nonsymmv_free (w);

  gsl_eigen_nonsymmv_sort (eval, evec,
                           GSL_EIGEN_SORT_ABS_DESC);

  {
    int i, j;

    for (i = 0; i < 4; i++)
      {
        gsl_complex eval_i
           = gsl_vector_complex_get (eval, i);
        gsl_vector_complex_view evec_i
           = gsl_matrix_complex_column (evec, i);

        printf ("eigenvalue = %g + %gi\n",
```

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```
                GSL_REAL(eval_i), GSL_IMAG(eval_i));
        printf ("eigenvector = \n");
        for (j = 0; j < 4; ++j)
          {
            gsl_complex z =
              gsl_vector_complex_get(&evec_i.vector, j);
            printf("%g + %gi\n", GSL_REAL(z), GSL_IMAG(z));
          }
      }
  }

  gsl_vector_complex_free(eval);
  gsl_matrix_complex_free(evec);

  return 0;
}
```

Here is the beginning of the output from the program:

```
$ ./a.out
eigenvalue = -6.41391 + 0i
eigenvector =
-0.0998822 + 0i
-0.111251 + 0i
0.292501 + 0i
0.944505 + 0i
eigenvalue = 5.54555 + 3.08545i
eigenvector =
-0.043487 + -0.0076308i
0.0642377 + -0.142127i
-0.515253 + 0.0405118i
-0.840592 + -0.00148565i
...
```

This can be compared with the corresponding output from GNU octave:

```
octave> [v,d] = eig(vander([-1 -2 3 4]));
octave> diag(d)
ans =

  -6.4139 + 0.0000i
   5.5456 + 3.0854i
   5.5456 - 3.0854i
   2.3228 + 0.0000i

octave> v
v =

 Columns 1 through 3:

  -0.09988 + 0.00000i  -0.04350 - 0.00755i  -0.04350 + 0.00755i
  -0.11125 + 0.00000i   0.06399 - 0.14224i   0.06399 + 0.14224i
```

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```
   0.29250 + 0.00000i  -0.51518 + 0.04142i  -0.51518 - 0.04142i
   0.94451 + 0.00000i  -0.84059 + 0.00000i  -0.84059 - 0.00000i

 Column 4:

  -0.14493 + 0.00000i
   0.35660 + 0.00000i
   0.91937 + 0.00000i
   0.08118 + 0.00000i
```

Note that the eigenvectors corresponding to the eigenvalue $5.54555 + 3.08545i$ differ by the multiplicative constant $0.9999984 + 0.0017674i$ which is an arbitrary phase factor of magnitude 1.

15.9 References and Further Reading

Further information on the algorithms described in this section can be found in the following book,

- G. H. Golub, C. F. Van Loan, "Matrix Computations" (3rd Ed, 1996), Johns Hopkins University Press, ISBN 0-8018-5414-8.

Further information on the generalized eigensystems QZ algorithm can be found in this paper,

- C. Moler, G. Stewart, "An Algorithm for Generalized Matrix Eigenvalue Problems", SIAM J. Numer. Anal., Vol 10, No 2, 1973.

Eigensystem routines for very large matrices can be found in the Fortran library LAPACK. The LAPACK library is described in,

- LAPACK Users' Guide (Third Edition, 1999), Published by SIAM, ISBN 0-89871-447-8.

The LAPACK source code can be found at the website http://www.netlib.org/lapack along with an online copy of the users guide.

CHAPTER

SIXTEEN

FAST FOURIER TRANSFORMS (FFTS)

This chapter describes functions for performing Fast Fourier Transforms (FFTs). The library includes radix-2 routines (for lengths which are a power of two) and mixed-radix routines (which work for any length). For efficiency there are separate versions of the routines for real data and for complex data. The mixed-radix routines are a reimplementation of the FFTPACK library of Paul Swarztrauber. Fortran code for FFTPACK is available on Netlib (FFTPACK also includes some routines for sine and cosine transforms but these are currently not available in GSL). For details and derivations of the underlying algorithms consult the document "GSL FFT Algorithms" (see *References and Further Reading*)

16.1 Mathematical Definitions

Fast Fourier Transforms are efficient algorithms for calculating the discrete Fourier transform (DFT),

$$x_j = \sum_{k=0}^{n-1} z_k \exp(-2\pi i jk/n)$$

The DFT usually arises as an approximation to the continuous Fourier transform when functions are sampled at discrete intervals in space or time. The naive evaluation of the discrete Fourier transform is a matrix-vector multiplication $W\vec{z}$. A general matrix-vector multiplication takes $O(n^2)$ operations for n data-points. Fast Fourier transform algorithms use a divide-and-conquer strategy to factorize the matrix W into smaller sub-matrices, corresponding to the integer factors of the length n. If n can be factorized into a product of integers $f_1 f_2 \ldots f_m$ then the DFT can be computed in $O(n \sum f_i)$ operations. For a radix-2 FFT this gives an operation count of $O(n \log_2 n)$.

All the FFT functions offer three types of transform: forwards, inverse and backwards, based on the same mathematical definitions. The definition of the *forward Fourier transform*, $x = \mathrm{FFT}(z)$, is,

$$x_j = \sum_{k=0}^{n-1} z_k \exp(-2\pi i jk/n)$$

and the definition of the *inverse Fourier transform*, $x = \mathrm{IFFT}(z)$, is,

$$z_j = \frac{1}{n} \sum_{k=0}^{n-1} x_k \exp(2\pi i jk/n).$$

The factor of $1/n$ makes this a true inverse. For example, a call to `gsl_fft_complex_forward()` followed by a call to `gsl_fft_complex_inverse()` should return the original data (within numerical errors).

In general there are two possible choices for the sign of the exponential in the transform/ inverse-transform pair. GSL follows the same convention as FFTPACK, using a negative exponential for the forward transform. The advantage of this convention is that the inverse transform recreates the original function with simple Fourier synthesis. Numerical Recipes uses the opposite convention, a positive exponential in the forward transform.

The *backwards FFT* is simply our terminology for an unscaled version of the inverse FFT,

$$z_j^{backwards} = \sum_{k=0}^{n-1} x_k \exp(2\pi ijk/n)$$

When the overall scale of the result is unimportant it is often convenient to use the backwards FFT instead of the inverse to save unnecessary divisions.

16.2 Overview of complex data FFTs

The inputs and outputs for the complex FFT routines are *packed arrays* of floating point numbers. In a packed array the real and imaginary parts of each complex number are placed in alternate neighboring elements. For example, the following definition of a packed array of length 6:

```
double x[3*2];
gsl_complex_packed_array data = x;
```

can be used to hold an array of three complex numbers, `z[3]`, in the following way:

```
data[0] = Re(z[0])
data[1] = Im(z[0])
data[2] = Re(z[1])
data[3] = Im(z[1])
data[4] = Re(z[2])
data[5] = Im(z[2])
```

The array indices for the data have the same ordering as those in the definition of the DFT—i.e. there are no index transformations or permutations of the data.

A *stride* parameter allows the user to perform transforms on the elements `z[stride*i]` instead of `z[i]`. A stride greater than 1 can be used to take an in-place FFT of the column of a matrix. A stride of 1 accesses the array without any additional spacing between elements.

To perform an FFT on a vector argument, such as `gsl_vector_complex * v`, use the following definitions (or their equivalents) when calling the functions described in this chapter:

```
gsl_complex_packed_array data = v->data;
size_t stride = v->stride;
size_t n = v->size;
```

For physical applications it is important to remember that the index appearing in the DFT does not correspond directly to a physical frequency. If the time-step of the DFT is Δ then the frequency-domain includes both positive and negative frequencies, ranging from $-1/(2\Delta)$ through 0 to $+1/(2\Delta)$. The positive frequencies are stored from the beginning of the array up to the middle, and the negative frequencies are stored backwards from the end of the array.

Here is a table which shows the layout of the array `data`, and the correspondence between the time-domain data z, and the frequency-domain data x:

```
index    z               x = FFT(z)

0        z(t = 0)        x(f = 0)
1        z(t = 1)        x(f = 1/(n Delta))
2        z(t = 2)        x(f = 2/(n Delta))
.        ........        ..................
```

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```
n/2       z(t = n/2)       x(f = +1/(2 Delta),
                                 -1/(2 Delta))
.         ........         ..................
n-3       z(t = n-3)       x(f = -3/(n Delta))
n-2       z(t = n-2)       x(f = -2/(n Delta))
n-1       z(t = n-1)       x(f = -1/(n Delta))
```

When n is even the location $n/2$ contains the most positive and negative frequencies ($+1/(2\Delta)$, $-1/(2\Delta)$) which are equivalent. If n is odd then general structure of the table above still applies, but $n/2$ does not appear.

16.3 Radix-2 FFT routines for complex data

The radix-2 algorithms described in this section are simple and compact, although not necessarily the most efficient. They use the Cooley-Tukey algorithm to compute in-place complex FFTs for lengths which are a power of 2—no additional storage is required. The corresponding self-sorting mixed-radix routines offer better performance at the expense of requiring additional working space.

All the functions described in this section are declared in the header file `gsl_fft_complex.h`.

int **gsl_fft_complex_radix2_forward**(gsl_complex_packed_array data, size_t stride, size_t n)

int **gsl_fft_complex_radix2_transform**(gsl_complex_packed_array data, size_t stride, size_t n, gsl_fft_direction sign)

int **gsl_fft_complex_radix2_backward**(gsl_complex_packed_array data, size_t stride, size_t n)

int **gsl_fft_complex_radix2_inverse**(gsl_complex_packed_array data, size_t stride, size_t n)

These functions compute forward, backward and inverse FFTs of length *n* with stride *stride*, on the packed complex array *data* using an in-place radix-2 decimation-in-time algorithm. The length of the transform *n* is restricted to powers of two. For the `transform` version of the function the `sign` argument can be either `forward` (-1) or `backward` ($+1$).

The functions return a value of `GSL_SUCCESS` if no errors were detected, or *GSL_EDOM* if the length of the data *n* is not a power of two.

int **gsl_fft_complex_radix2_dif_forward**(gsl_complex_packed_array data, size_t stride, size_t n)

int **gsl_fft_complex_radix2_dif_transform**(gsl_complex_packed_array data, size_t stride, size_t n, gsl_fft_direction sign)

int **gsl_fft_complex_radix2_dif_backward**(gsl_complex_packed_array data, size_t stride, size_t n)

int **gsl_fft_complex_radix2_dif_inverse**(gsl_complex_packed_array data, size_t stride, size_t n)

These are decimation-in-frequency versions of the radix-2 FFT functions.

Here is an example program which computes the FFT of a short pulse in a sample of length 128. To make the resulting Fourier transform real the pulse is defined for equal positive and negative times ($-10 \ldots 10$), where the negative times wrap around the end of the array.

```
#include <stdio.h>
#include <math.h>
#include <gsl/gsl_errno.h>
```

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```
#include <gsl/gsl_fft_complex.h>

#define REAL(z,i) ((z)[2*(i)])
#define IMAG(z,i) ((z)[2*(i)+1])

int
main (void)
{
  int i; double data[2*128];

  for (i = 0; i < 128; i++)
    {
       REAL(data,i) = 0.0; IMAG(data,i) = 0.0;
    }

  REAL(data,0) = 1.0;

  for (i = 1; i <= 10; i++)
    {
       REAL(data,i) = REAL(data,128-i) = 1.0;
    }

  for (i = 0; i < 128; i++)
    {
      printf ("%d %e %e\n", i,
              REAL(data,i), IMAG(data,i));
    }
  printf ("\n\n");

  gsl_fft_complex_radix2_forward (data, 1, 128);

  for (i = 0; i < 128; i++)
    {
      printf ("%d %e %e\n", i,
              REAL(data,i)/sqrt(128),
              IMAG(data,i)/sqrt(128));
    }

  return 0;
}
```

Note that we have assumed that the program is using the default error handler (which calls `abort()` for any errors). If you are not using a safe error handler you would need to check the return status of *gsl_fft_complex_radix2_forward()*.

The transformed data is rescaled by $1/\sqrt{n}$ so that it fits on the same plot as the input. Only the real part is shown, by the choice of the input data the imaginary part is zero. Allowing for the wrap-around of negative times at $t = 128$, and working in units of k/n, the DFT approximates the continuum Fourier transform, giving a modulated sine function.

$$\int_{-a}^{+a} e^{-2\pi ikx} dx = \frac{\sin(2\pi ka)}{\pi k}$$

The output of the example program is plotted in Fig. 16.1.

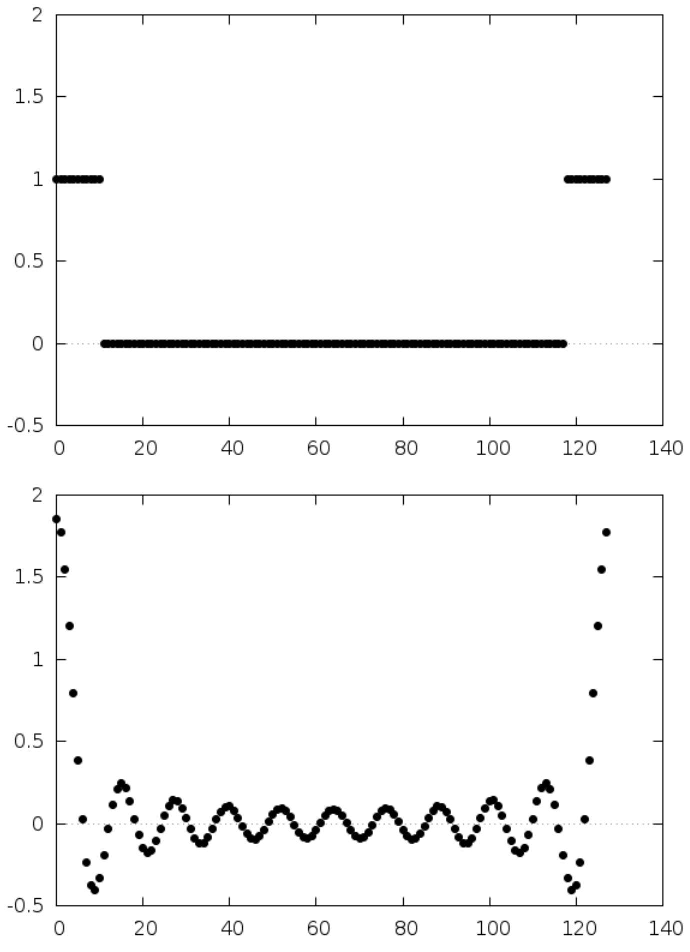

Fig. 16.1: A pulse and its discrete Fourier transform, output from the example program.

16.4 Mixed-radix FFT routines for complex data

This section describes mixed-radix FFT algorithms for complex data. The mixed-radix functions work for FFTs of any length. They are a reimplementation of Paul Swarztrauber's Fortran FFTPACK library. The theory is explained in the review article "Self-sorting Mixed-radix FFTs" by Clive Temperton. The routines here use the same indexing scheme and basic algorithms as FFTPACK.

The mixed-radix algorithm is based on sub-transform modules—highly optimized small length FFTs which are combined to create larger FFTs. There are efficient modules for factors of 2, 3, 4, 5, 6 and 7. The modules for the composite factors of 4 and 6 are faster than combining the modules for $2 * 2$ and $2 * 3$.

For factors which are not implemented as modules there is a fall-back to a general length-n module which uses Singleton's method for efficiently computing a DFT. This module is $O(n^2)$, and slower than a dedicated module would be but works for any length n. Of course, lengths which use the general length-n module will still be factorized as much as possible. For example, a length of 143 will be factorized into $11 * 13$. Large prime factors are the worst case scenario, e.g. as found in $n = 2 * 3 * 99991$, and should be avoided because their $O(n^2)$ scaling will dominate the run-time (consult the document "GSL FFT Algorithms" included in the GSL distribution if you encounter this problem).

The mixed-radix initialization function `gsl_fft_complex_wavetable_alloc()` returns the list of factors chosen by the library for a given length n. It can be used to check how well the length has been factorized, and estimate the run-time. To a first approximation the run-time scales as $n \sum f_i$, where the f_i are the factors of n. For programs under user control you may wish to issue a warning that the transform will be slow when the length is poorly factorized. If you frequently encounter data lengths which cannot be factorized using the existing small-prime modules consult "GSL FFT Algorithms" for details on adding support for other factors.

All the functions described in this section are declared in the header file `gsl_fft_complex.h`.

gsl_fft_complex_wavetable ***gsl_fft_complex_wavetable_alloc**(size_t n)

This function prepares a trigonometric lookup table for a complex FFT of length `n`. The function returns a pointer to the newly allocated `gsl_fft_complex_wavetable` if no errors were detected, and a null pointer in the case of error. The length `n` is factorized into a product of subtransforms, and the factors and their trigonometric coefficients are stored in the wavetable. The trigonometric coefficients are computed using direct calls to `sin` and `cos`, for accuracy. Recursion relations could be used to compute the lookup table faster, but if an application performs many FFTs of the same length then this computation is a one-off overhead which does not affect the final throughput.

The wavetable structure can be used repeatedly for any transform of the same length. The table is not modified by calls to any of the other FFT functions. The same wavetable can be used for both forward and backward (or inverse) transforms of a given length.

void **gsl_fft_complex_wavetable_free**(*gsl_fft_complex_wavetable* *wavetable)

This function frees the memory associated with the wavetable `wavetable`. The wavetable can be freed if no further FFTs of the same length will be needed.

These functions operate on a `gsl_fft_complex_wavetable` structure which contains internal parameters for the FFT. It is not necessary to set any of the components directly but it can sometimes be useful to examine them. For example, the chosen factorization of the FFT length is given and can be used to provide an estimate of the run-time or numerical error. The wavetable structure is declared in the header file `gsl_fft_complex.h`.

type **gsl_fft_complex_wavetable**

This is a structure that holds the factorization and trigonometric lookup tables for the mixed radix fft algorithm. It has the following components:

`size_t n`	This is the number of complex data points
`size_t nf`	This is the number of factors that the length `n` was decomposed into.
`size_t factor[64]`	This is the array of factors. Only the first `nf` elements are used.
`gsl_complex * trig`	This is a pointer to a preallocated trigonometric lookup table of `n` complex elements.
`gsl_complex * twiddle[64]`	This is an array of pointers into `trig`, giving the twiddle factors for each pass.

type **`gsl_fft_complex_workspace`**

The mixed radix algorithms require additional working space to hold the intermediate steps of the transform.

gsl_fft_complex_workspace ***`gsl_fft_complex_workspace_alloc`**(size_t n)

This function allocates a workspace for a complex transform of length *`n`*.

void **`gsl_fft_complex_workspace_free`**(*gsl_fft_complex_workspace* *workspace)

This function frees the memory associated with the workspace *`workspace`*. The workspace can be freed if no further FFTs of the same length will be needed.

The following functions compute the transform,

int **`gsl_fft_complex_forward`**(gsl_complex_packed_array data, size_t stride, size_t n, const *gsl_fft_complex_wavetable* *wavetable, *gsl_fft_complex_workspace* *work)

int **`gsl_fft_complex_transform`**(gsl_complex_packed_array data, size_t stride, size_t n, const *gsl_fft_complex_wavetable* *wavetable, *gsl_fft_complex_workspace* *work, gsl_fft_direction sign)

int **`gsl_fft_complex_backward`**(gsl_complex_packed_array data, size_t stride, size_t n, const *gsl_fft_complex_wavetable* *wavetable, *gsl_fft_complex_workspace* *work)

int **`gsl_fft_complex_inverse`**(gsl_complex_packed_array data, size_t stride, size_t n, const *gsl_fft_complex_wavetable* *wavetable, *gsl_fft_complex_workspace* *work)

These functions compute forward, backward and inverse FFTs of length *`n`* with stride *`stride`*, on the packed complex array *`data`*, using a mixed radix decimation-in-frequency algorithm. There is no restriction on the length *`n`*. Efficient modules are provided for subtransforms of length 2, 3, 4, 5, 6 and 7. Any remaining factors are computed with a slow, $O(n^2)$, general-n module. The caller must supply a *`wavetable`* containing the trigonometric lookup tables and a workspace *`work`*. For the `transform` version of the function the `sign` argument can be either `forward` (-1) or `backward` $(+1)$.

The functions return a value of `0` if no errors were detected. The following `gsl_errno` conditions are defined for these functions:

GSL_EDOM	The length of the data *`n`* is not a positive integer (i.e. *`n`* is zero).
GSL_EINVAL	The length of the data *`n`* and the length used to compute the given *`wavetable`* do not match.

Here is an example program which computes the FFT of a short pulse in a sample of length 630 $(= 2 * 3 * 3 * 5 * 7)$ using the mixed-radix algorithm.

```
#include <stdio.h>
#include <math.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_fft_complex.h>

```

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```
#define REAL(z,i) ((z)[2*(i)])
#define IMAG(z,i) ((z)[2*(i)+1])

int
main (void)
{
  int i;
  const int n = 630;
  double data[2*n];

  gsl_fft_complex_wavetable * wavetable;
  gsl_fft_complex_workspace * workspace;

  for (i = 0; i < n; i++)
    {
      REAL(data,i) = 0.0;
      IMAG(data,i) = 0.0;
    }

  data[0] = 1.0;

  for (i = 1; i <= 10; i++)
    {
      REAL(data,i) = REAL(data,n-i) = 1.0;
    }

  for (i = 0; i < n; i++)
    {
      printf ("%d: %e %e\n", i, REAL(data,i),
                                IMAG(data,i));
    }
  printf ("\n");

  wavetable = gsl_fft_complex_wavetable_alloc (n);
  workspace = gsl_fft_complex_workspace_alloc (n);

  for (i = 0; i < (int) wavetable->nf; i++)
    {
       printf ("# factor %d: %zu\n", i,
               wavetable->factor[i]);
    }

  gsl_fft_complex_forward (data, 1, n,
                           wavetable, workspace);

  for (i = 0; i < n; i++)
    {
      printf ("%d: %e %e\n", i, REAL(data,i),
                                IMAG(data,i));
    }

  gsl_fft_complex_wavetable_free (wavetable);
```

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```
  gsl_fft_complex_workspace_free (workspace);
  return 0;
}
```

Note that we have assumed that the program is using the default `gsl` error handler (which calls `abort()` for any errors). If you are not using a safe error handler you would need to check the return status of all the `gsl` routines.

16.5 Overview of real data FFTs

The functions for real data are similar to those for complex data. However, there is an important difference between forward and inverse transforms. The Fourier transform of a real sequence is not real. It is a complex sequence with a special symmetry:

$$z_k = z_{n-k}^*$$

A sequence with this symmetry is called *conjugate-complex* or *half-complex*. This different structure requires different storage layouts for the forward transform (from real to half-complex) and inverse transform (from half-complex back to real). As a consequence the routines are divided into two sets: functions in `gsl_fft_real` which operate on real sequences and functions in `gsl_fft_halfcomplex` which operate on half-complex sequences.

Functions in `gsl_fft_real` compute the frequency coefficients of a real sequence. The half-complex coefficients c of a real sequence x are given by Fourier analysis,

$$c_k = \sum_{j=0}^{n-1} x_j \exp(-2\pi ijk/n)$$

Functions in `gsl_fft_halfcomplex` compute inverse or backwards transforms. They reconstruct real sequences by Fourier synthesis from their half-complex frequency coefficients, c,

$$x_j = \frac{1}{n} \sum_{k=0}^{n-1} c_k \exp(2\pi ijk/n)$$

The symmetry of the half-complex sequence implies that only half of the complex numbers in the output need to be stored. The remaining half can be reconstructed using the half-complex symmetry condition. This works for all lengths, even and odd—when the length is even the middle value where $k = n/2$ is also real. Thus only `n` real numbers are required to store the half-complex sequence, and the transform of a real sequence can be stored in the same size array as the original data.

The precise storage arrangements depend on the algorithm, and are different for radix-2 and mixed-radix routines. The radix-2 function operates in-place, which constrains the locations where each element can be stored. The restriction forces real and imaginary parts to be stored far apart. The mixed-radix algorithm does not have this restriction, and it stores the real and imaginary parts of a given term in neighboring locations (which is desirable for better locality of memory accesses).

16.6 Radix-2 FFT routines for real data

This section describes radix-2 FFT algorithms for real data. They use the Cooley-Tukey algorithm to compute in-place FFTs for lengths which are a power of 2.

The radix-2 FFT functions for real data are declared in the header files `gsl_fft_real.h`

int **gsl_fft_real_radix2_transform**(double data[], size_t stride, size_t n)

This function computes an in-place radix-2 FFT of length *n* and stride *stride* on the real array *data*. The output is a half-complex sequence, which is stored in-place. The arrangement of the half-complex terms uses the following scheme: for $k < n/2$ the real part of the k-th term is stored in location k, and the corresponding imaginary part is stored in location $n - k$. Terms with $k > n/2$ can be reconstructed using the symmetry $z_k = z^*_{n-k}$. The terms for $k = 0$ and $k = n/2$ are both purely real, and count as a special case. Their real parts are stored in locations 0 and $n/2$ respectively, while their imaginary parts which are zero are not stored.

The following table shows the correspondence between the output *data* and the equivalent results obtained by considering the input data as a complex sequence with zero imaginary part (assuming *stride* = 1}):

```
complex[0].real    =    data[0]
complex[0].imag    =    0
complex[1].real    =    data[1]
complex[1].imag    =    data[n-1]
...............         ................
complex[k].real    =    data[k]
complex[k].imag    =    data[n-k]
...............         ................
complex[n/2].real  =    data[n/2]
complex[n/2].imag  =    0
...............         ................
complex[k'].real   =    data[k]        k' = n - k
complex[k'].imag   =   -data[n-k]
...............         ................
complex[n-1].real  =    data[1]
complex[n-1].imag  =   -data[n-1]
```

Note that the output data can be converted into the full complex sequence using the function *gsl_fft_halfcomplex_radix2_unpack()* described below.

The radix-2 FFT functions for halfcomplex data are declared in the header file `gsl_fft_halfcomplex.h`.

int **gsl_fft_halfcomplex_radix2_inverse**(double data[], size_t stride, size_t n)

int **gsl_fft_halfcomplex_radix2_backward**(double data[], size_t stride, size_t n)

These functions compute the inverse or backwards in-place radix-2 FFT of length *n* and stride *stride* on the half-complex sequence *data* stored according the output scheme used by `gsl_fft_real_radix2()`. The result is a real array stored in natural order.

int **gsl_fft_halfcomplex_radix2_unpack**(const double halfcomplex_coefficient[], gsl_complex_packed_array complex_coefficient, size_t stride, size_t n)

This function converts *halfcomplex_coefficient*, an array of half-complex coefficients as returned by *gsl_fft_real_radix2_transform()*, into an ordinary complex array, *complex_coefficient*. It fills in the complex array using the symmetry $z_k = z^*_{n-k}$ to reconstruct the redundant elements. The algorithm for the conversion is:

```
complex_coefficient[0].real = halfcomplex_coefficient[0];
complex_coefficient[0].imag = 0.0;
```

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```
for (i = 1; i < n - i; i++)
  {
    double hc_real = halfcomplex_coefficient[i*stride];
    double hc_imag = halfcomplex_coefficient[(n-i)*stride];
    complex_coefficient[i*stride].real = hc_real;
    complex_coefficient[i*stride].imag = hc_imag;
    complex_coefficient[(n - i)*stride].real = hc_real;
    complex_coefficient[(n - i)*stride].imag = -hc_imag;
  }

if (i == n - i)
  {
    complex_coefficient[i*stride].real = halfcomplex_coefficient[(n - 1)*stride];
    complex_coefficient[i*stride].imag = 0.0;
  }
```

16.7 Mixed-radix FFT routines for real data

This section describes mixed-radix FFT algorithms for real data. The mixed-radix functions work for FFTs of any length. They are a reimplementation of the real-FFT routines in the Fortran FFTPACK library by Paul Swarztrauber. The theory behind the algorithm is explained in the article "Fast Mixed-Radix Real Fourier Transforms" by Clive Temperton. The routines here use the same indexing scheme and basic algorithms as FFTPACK.

The functions use the FFTPACK storage convention for half-complex sequences. In this convention the half-complex transform of a real sequence is stored with frequencies in increasing order, starting at zero, with the real and imaginary parts of each frequency in neighboring locations. When a value is known to be real the imaginary part is not stored. The imaginary part of the zero-frequency component is never stored. It is known to be zero (since the zero frequency component is simply the sum of the input data (all real)). For a sequence of even length the imaginary part of the frequency $n/2$ is not stored either, since the symmetry $z_k = z_{n-k}^*$ implies that this is purely real too.

The storage scheme is best shown by some examples. The table below shows the output for an odd-length sequence, $n = 5$. The two columns give the correspondence between the 5 values in the half-complex sequence returned by *gsl_fft_real_transform()*, `halfcomplex[]` and the values `complex[]` that would be returned if the same real input sequence were passed to *gsl_fft_complex_backward()* as a complex sequence (with imaginary parts set to `0`):

```
complex[0].real  =  halfcomplex[0]
complex[0].imag  =  0
complex[1].real  =  halfcomplex[1]
complex[1].imag  =  halfcomplex[2]
complex[2].real  =  halfcomplex[3]
complex[2].imag  =  halfcomplex[4]
complex[3].real  =  halfcomplex[3]
complex[3].imag  = -halfcomplex[4]
complex[4].real  =  halfcomplex[1]
complex[4].imag  = -halfcomplex[2]
```

The upper elements of the `complex` array, `complex[3]` and `complex[4]` are filled in using the symmetry condition. The imaginary part of the zero-frequency term `complex[0].imag` is known to be zero by the symmetry.

The next table shows the output for an even-length sequence, $n = 6$. In the even case there are two values which are purely real:

```
complex[0].real  =  halfcomplex[0]
complex[0].imag  =  0
complex[1].real  =  halfcomplex[1]
complex[1].imag  =  halfcomplex[2]
complex[2].real  =  halfcomplex[3]
complex[2].imag  =  halfcomplex[4]
complex[3].real  =  halfcomplex[5]
complex[3].imag  =  0
complex[4].real  =  halfcomplex[3]
complex[4].imag  = -halfcomplex[4]
complex[5].real  =  halfcomplex[1]
complex[5].imag  = -halfcomplex[2]
```

The upper elements of the `complex` array, `complex[4]` and `complex[5]` are filled in using the symmetry condition. Both `complex[0].imag` and `complex[3].imag` are known to be zero.

All these functions are declared in the header files `gsl_fft_real.h` and `gsl_fft_halfcomplex.h`.

type **`gsl_fft_real_wavetable`**

type **`gsl_fft_halfcomplex_wavetable`**

These data structures contain lookup tables for an FFT of a fixed size.

gsl_fft_real_wavetable ***`gsl_fft_real_wavetable_alloc`**(size_t n)

gsl_fft_halfcomplex_wavetable ***`gsl_fft_halfcomplex_wavetable_alloc`**(size_t n)

These functions prepare trigonometric lookup tables for an FFT of size n real elements. The functions return a pointer to the newly allocated struct if no errors were detected, and a null pointer in the case of error. The length `n` is factorized into a product of subtransforms, and the factors and their trigonometric coefficients are stored in the wavetable. The trigonometric coefficients are computed using direct calls to `sin` and `cos`, for accuracy. Recursion relations could be used to compute the lookup table faster, but if an application performs many FFTs of the same length then computing the wavetable is a one-off overhead which does not affect the final throughput.

The wavetable structure can be used repeatedly for any transform of the same length. The table is not modified by calls to any of the other FFT functions. The appropriate type of wavetable must be used for forward real or inverse half-complex transforms.

void **`gsl_fft_real_wavetable_free`**(*gsl_fft_real_wavetable* *wavetable)

void **`gsl_fft_halfcomplex_wavetable_free`**(*gsl_fft_halfcomplex_wavetable* *wavetable)

These functions free the memory associated with the wavetable `wavetable`. The wavetable can be freed if no further FFTs of the same length will be needed.

The mixed radix algorithms require additional working space to hold the intermediate steps of the transform,

type **`gsl_fft_real_workspace`**

This workspace contains parameters needed to compute a real FFT.

gsl_fft_real_workspace ***`gsl_fft_real_workspace_alloc`**(size_t n)

This function allocates a workspace for a real transform of length `n`. The same workspace can be used for both forward real and inverse halfcomplex transforms.

void **`gsl_fft_real_workspace_free`**(*gsl_fft_real_workspace* *workspace)

This function frees the memory associated with the workspace `workspace`. The workspace can be freed if no further FFTs of the same length will be needed.

The following functions compute the transforms of real and half-complex data, int **gsl_fft_real_transform**(double data[], size_t stride, size_t n, const *gsl_fft_real_wavetable* *wavetable, *gsl_fft_real_workspace* *work)

int **gsl_fft_halfcomplex_transform**(double data[], size_t stride, size_t n, const *gsl_fft_halfcomplex_wavetable* *wavetable, *gsl_fft_real_workspace* *work)

These functions compute the FFT of `data`, a real or half-complex array of length `n`, using a mixed radix decimation-in-frequency algorithm. For `gsl_fft_real_transform()` `data` is an array of time-ordered real data. For `gsl_fft_halfcomplex_transform()` `data` contains Fourier coefficients in the half-complex ordering described above. There is no restriction on the length `n`. Efficient modules are provided for subtransforms of length 2, 3, 4 and 5. Any remaining factors are computed with a slow, $O(n^2)$, general-n module. The caller must supply a `wavetable` containing trigonometric lookup tables and a workspace `work`.

int **gsl_fft_real_unpack**(const double real_coefficient[], gsl_complex_packed_array complex_coefficient, size_t stride, size_t n)

This function converts a single real array, `real_coefficient` into an equivalent complex array, `complex_coefficient`, (with imaginary part set to zero), suitable for `gsl_fft_complex` routines. The algorithm for the conversion is simply:

```
for (i = 0; i < n; i++)
  {
    complex_coefficient[i*stride].real = real_coefficient[i*stride];
    complex_coefficient[i*stride].imag = 0.0;
  }
```

int **gsl_fft_halfcomplex_unpack**(const double halfcomplex_coefficient[], gsl_complex_packed_array complex_coefficient, size_t stride, size_t n)

This function converts `halfcomplex_coefficient`, an array of half-complex coefficients as returned by `gsl_fft_real_transform()`, into an ordinary complex array, `complex_coefficient`. It fills in the complex array using the symmetry $z_k = z^*_{n-k}$ to reconstruct the redundant elements. The algorithm for the conversion is:

```
complex_coefficient[0].real = halfcomplex_coefficient[0];
complex_coefficient[0].imag = 0.0;

for (i = 1; i < n - i; i++)
  {
    double hc_real = halfcomplex_coefficient[(2 * i - 1)*stride];
    double hc_imag = halfcomplex_coefficient[(2 * i)*stride];
    complex_coefficient[i*stride].real = hc_real;
    complex_coefficient[i*stride].imag = hc_imag;
    complex_coefficient[(n - i)*stride].real = hc_real;
    complex_coefficient[(n - i)*stride].imag = -hc_imag;
  }

if (i == n - i)
  {
    complex_coefficient[i*stride].real = halfcomplex_coefficient[(n - 1)*stride];
    complex_coefficient[i*stride].imag = 0.0;
  }
```

Here is an example program using `gsl_fft_real_transform()` and `gsl_fft_halfcomplex_inverse()`. It generates a real signal in the shape of a square pulse. The pulse is Fourier transformed to frequency space, and all but the lowest ten frequency components are removed from the array of Fourier coefficients returned by `gsl_fft_real_transform()`.

The remaining Fourier coefficients are transformed back to the time-domain, to give a filtered version of the square pulse. Since Fourier coefficients are stored using the half-complex symmetry both positive and negative frequencies are removed and the final filtered signal is also real.

```
#include <stdio.h>
#include <math.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_fft_real.h>
#include <gsl/gsl_fft_halfcomplex.h>

int
main (void)
{
  int i, n = 100;
  double data[n];

  gsl_fft_real_wavetable * real;
  gsl_fft_halfcomplex_wavetable * hc;
  gsl_fft_real_workspace * work;

  for (i = 0; i < n; i++)
    {
      data[i] = 0.0;
    }

  for (i = n / 3; i < 2 * n / 3; i++)
    {
      data[i] = 1.0;
    }

  for (i = 0; i < n; i++)
    {
      printf ("%d: %e\n", i, data[i]);
    }
  printf ("\n");

  work = gsl_fft_real_workspace_alloc (n);
  real = gsl_fft_real_wavetable_alloc (n);

  gsl_fft_real_transform (data, 1, n,
                          real, work);

  gsl_fft_real_wavetable_free (real);

  for (i = 11; i < n; i++)
    {
      data[i] = 0;
    }

  hc = gsl_fft_halfcomplex_wavetable_alloc (n);

  gsl_fft_halfcomplex_inverse (data, 1, n,
                               hc, work);
```

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```
  gsl_fft_halfcomplex_wavetable_free (hc);

  for (i = 0; i < n; i++)
    {
      printf ("%d: %e\n", i, data[i]);
    }

  gsl_fft_real_workspace_free (work);
  return 0;
}
```

The program output is shown in Fig. 16.2.

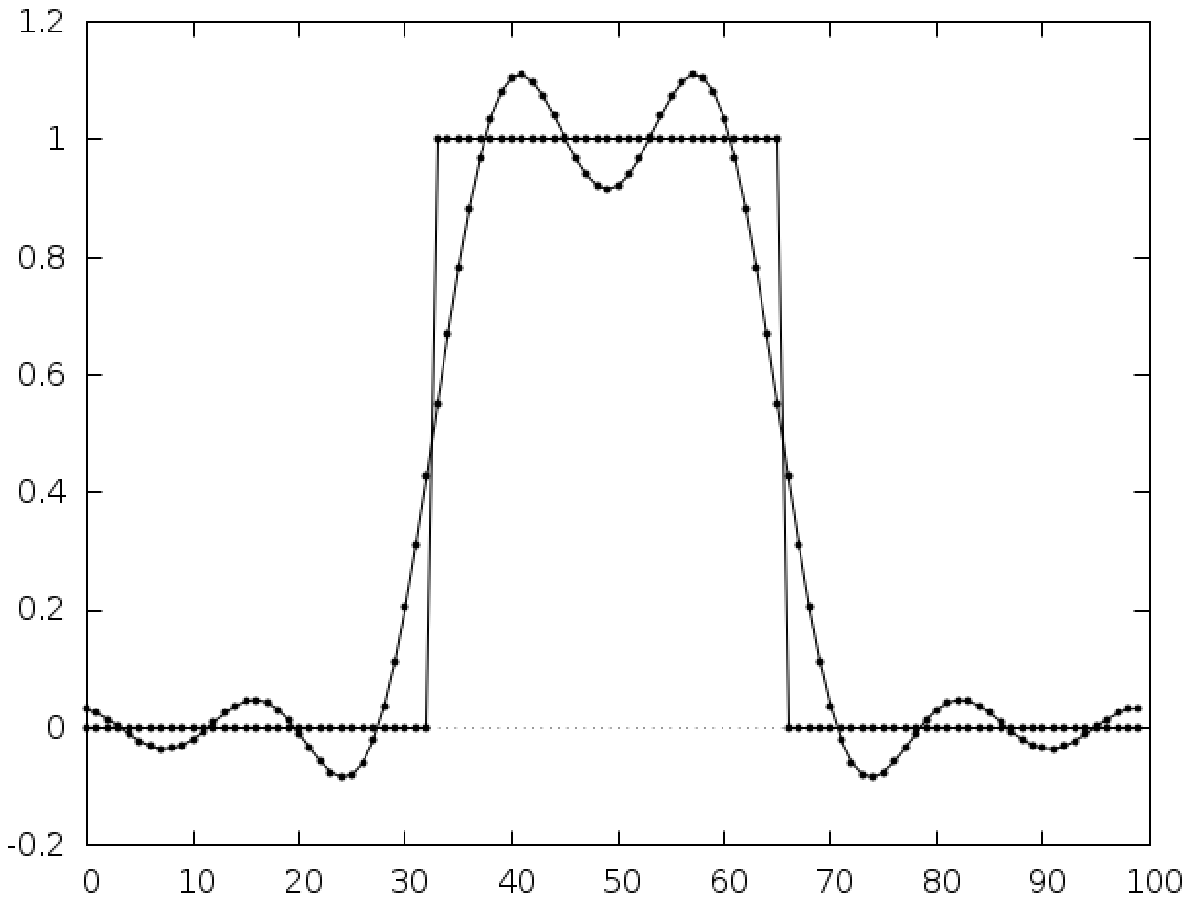

Fig. 16.2: Low-pass filtered version of a real pulse, output from the example program.

16.8 References and Further Reading

A good starting point for learning more about the FFT is the following review article,

- P. Duhamel and M. Vetterli. Fast Fourier transforms: A tutorial review and a state of the art. Signal Processing, 19:259–299, 1990.

To find out about the algorithms used in the GSL routines you may want to consult the document "GSL FFT Algorithms" (it is included in GSL, as `doc/fftalgorithms.tex`). This has general information on FFTs and explicit derivations of the implementation for each routine. There are also references to the relevant literature. For convenience some of the more important references are reproduced below.

There are several introductory books on the FFT with example programs, such as "The Fast Fourier Transform" by Brigham and "DFT/FFT and Convolution Algorithms" by Burrus and Parks,

- E. Oran Brigham. "The Fast Fourier Transform". Prentice Hall, 1974.
- C. S. Burrus and T. W. Parks. "DFT/FFT and Convolution Algorithms", Wiley, 1984.

Both these introductory books cover the radix-2 FFT in some detail. The mixed-radix algorithm at the heart of the FFTPACK routines is reviewed in Clive Temperton's paper,

- Clive Temperton, Self-sorting mixed-radix fast Fourier transforms, Journal of Computational Physics, 52(1):1–23, 1983.

The derivation of FFTs for real-valued data is explained in the following two articles,

- Henrik V. Sorenson, Douglas L. Jones, Michael T. Heideman, and C. Sidney Burrus. Real-valued fast Fourier transform algorithms. "IEEE Transactions on Acoustics, Speech, and Signal Processing", ASSP-35(6):849–863, 1987.
- Clive Temperton. Fast mixed-radix real Fourier transforms. "Journal of Computational Physics", 52:340–350, 1983.

In 1979 the IEEE published a compendium of carefully-reviewed Fortran FFT programs in "Programs for Digital Signal Processing". It is a useful reference for implementations of many different FFT algorithms,

- Digital Signal Processing Committee and IEEE Acoustics, Speech, and Signal Processing Committee, editors. Programs for Digital Signal Processing. IEEE Press, 1979.

For large-scale FFT work we recommend the use of the dedicated FFTW library by Frigo and Johnson. The FFTW library is self-optimizing—it automatically tunes itself for each hardware platform in order to achieve maximum performance. It is available under the GNU GPL.

- FFTW Website, http://www.fftw.org/

The source code for FFTPACK is available from http://www.netlib.org/fftpack/

CHAPTER

SEVENTEEN

NUMERICAL INTEGRATION

This chapter describes routines for performing numerical integration (quadrature) of a function in one dimension. There are routines for adaptive and non-adaptive integration of general functions, with specialised routines for specific cases. These include integration over infinite and semi-infinite ranges, singular integrals, including logarithmic singularities, computation of Cauchy principal values and oscillatory integrals. The library reimplements the algorithms used in QUADPACK, a numerical integration package written by Piessens, de Doncker-Kapenga, Ueberhuber and Kahaner. Fortran code for QUADPACK is available on Netlib. Also included are non-adaptive, fixed-order Gauss-Legendre integration routines with high precision coefficients, as well as fixed-order quadrature rules for a variety of weighting functions from IQPACK.

The functions described in this chapter are declared in the header file `gsl_integration.h`.

17.1 Introduction

Each algorithm computes an approximation to a definite integral of the form,

$$I = \int_a^b f(x)w(x)dx$$

where $w(x)$ is a weight function (for general integrands $w(x) = 1$). The user provides absolute and relative error bounds $(epsabs, epsrel)$ which specify the following accuracy requirement,

$$|RESULT - I| \leq \max(epsabs, epsrel|I|)$$

where $RESULT$ is the numerical approximation obtained by the algorithm. The algorithms attempt to estimate the absolute error $ABSERR = |RESULT - I|$ in such a way that the following inequality holds,

$$|RESULT - I| \leq ABSERR \leq \max(epsabs, epsrel|I|)$$

In short, the routines return the first approximation which has an absolute error smaller than $epsabs$ or a relative error smaller than $epsrel$.

Note that this is an *either-or* constraint, not simultaneous. To compute to a specified absolute error, set $epsrel$ to zero. To compute to a specified relative error, set $epsabs$ to zero. The routines will fail to converge if the error bounds are too stringent, but always return the best approximation obtained up to that stage.

The algorithms in QUADPACK use a naming convention based on the following letters:

```
Q - quadrature routine

N - non-adaptive integrator
A - adaptive integrator
```

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```
G - general integrand (user-defined)
W - weight function with integrand

S - singularities can be more readily integrated
P - points of special difficulty can be supplied
I - infinite range of integration
O - oscillatory weight function, cos or sin
F - Fourier integral
C - Cauchy principal value
```

The algorithms are built on pairs of quadrature rules, a higher order rule and a lower order rule. The higher order rule is used to compute the best approximation to an integral over a small range. The difference between the results of the higher order rule and the lower order rule gives an estimate of the error in the approximation.

17.1.1 Integrands without weight functions

The algorithms for general functions (without a weight function) are based on Gauss-Kronrod rules.

A Gauss-Kronrod rule begins with a classical Gaussian quadrature rule of order m. This is extended with additional points between each of the abscissae to give a higher order Kronrod rule of order $2m + 1$. The Kronrod rule is efficient because it reuses existing function evaluations from the Gaussian rule.

The higher order Kronrod rule is used as the best approximation to the integral, and the difference between the two rules is used as an estimate of the error in the approximation.

17.1.2 Integrands with weight functions

For integrands with weight functions the algorithms use Clenshaw-Curtis quadrature rules.

A Clenshaw-Curtis rule begins with an n-th order Chebyshev polynomial approximation to the integrand. This polynomial can be integrated exactly to give an approximation to the integral of the original function. The Chebyshev expansion can be extended to higher orders to improve the approximation and provide an estimate of the error.

17.1.3 Integrands with singular weight functions

The presence of singularities (or other behavior) in the integrand can cause slow convergence in the Chebyshev approximation. The modified Clenshaw-Curtis rules used in QUADPACK separate out several common weight functions which cause slow convergence.

These weight functions are integrated analytically against the Chebyshev polynomials to precompute *modified Chebyshev moments*. Combining the moments with the Chebyshev approximation to the function gives the desired integral. The use of analytic integration for the singular part of the function allows exact cancellations and substantially improves the overall convergence behavior of the integration.

17.2 QNG non-adaptive Gauss-Kronrod integration

The QNG algorithm is a non-adaptive procedure which uses fixed Gauss-Kronrod-Patterson abscissae to sample the integrand at a maximum of 87 points. It is provided for fast integration of smooth functions.

int **gsl_integration_qng**(const *gsl_function* *f, double a, double b, double epsabs, double epsrel, double *result, double *abserr, size_t *neval)

This function applies the Gauss-Kronrod 10-point, 21-point, 43-point and 87-point integration rules in succession until an estimate of the integral of f over (a, b) is achieved within the desired absolute and relative error limits, `epsabs` and `epsrel`. The function returns the final approximation, `result`, an estimate of the absolute error, `abserr` and the number of function evaluations used, `neval`. The Gauss-Kronrod rules are designed in such a way that each rule uses all the results of its predecessors, in order to minimize the total number of function evaluations.

17.3 QAG adaptive integration

The QAG algorithm is a simple adaptive integration procedure. The integration region is divided into subintervals, and on each iteration the subinterval with the largest estimated error is bisected. This reduces the overall error rapidly, as the subintervals become concentrated around local difficulties in the integrand. These subintervals are managed by the following struct,

type **gsl_integration_workspace**

This workspace handles the memory for the subinterval ranges, results and error estimates.

gsl_integration_workspace ***gsl_integration_workspace_alloc**(size_t n)

This function allocates a workspace sufficient to hold `n` double precision intervals, their integration results and error estimates. One workspace may be used multiple times as all necessary reinitialization is performed automatically by the integration routines.

void **gsl_integration_workspace_free**(*gsl_integration_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_integration_qag**(const *gsl_function* *f, double a, double b, double epsabs, double epsrel, size_t limit, int key, *gsl_integration_workspace* *workspace, double *result, double *abserr)

This function applies an integration rule adaptively until an estimate of the integral of f over (a, b) is achieved within the desired absolute and relative error limits, `epsabs` and `epsrel`. The function returns the final approximation, `result`, and an estimate of the absolute error, `abserr`. The integration rule is determined by the value of `key`, which should be chosen from the following symbolic names,

Symbolic Name	Key
GSL_INTEG_GAUSS15	1
GSL_INTEG_GAUSS21	2
GSL_INTEG_GAUSS31	3
GSL_INTEG_GAUSS41	4
GSL_INTEG_GAUSS51	5
GSL_INTEG_GAUSS61	6

corresponding to the 15, 21, 31, 41, 51 and 61 point Gauss-Kronrod rules. The higher-order rules give better accuracy for smooth functions, while lower-order rules save time when the function contains local difficulties, such as discontinuities.

On each iteration the adaptive integration strategy bisects the interval with the largest error estimate. The subintervals and their results are stored in the memory provided by `workspace`. The maximum number of subintervals is given by `limit`, which may not exceed the allocated size of the workspace.

17.4 QAGS adaptive integration with singularities

The presence of an integrable singularity in the integration region causes an adaptive routine to concentrate new subintervals around the singularity. As the subintervals decrease in size the successive approximations to the integral converge in a limiting fashion. This approach to the limit can be accelerated using an extrapolation procedure. The QAGS algorithm combines adaptive bisection with the Wynn epsilon-algorithm to speed up the integration of many types of integrable singularities.

int **gsl_integration_qags**(const *gsl_function* *f, double a, double b, double epsabs, double epsrel, size_t limit, *gsl_integration_workspace* *workspace, double *result, double *abserr)

This function applies the Gauss-Kronrod 21-point integration rule adaptively until an estimate of the integral of f over (a, b) is achieved within the desired absolute and relative error limits, `epsabs` and `epsrel`. The results are extrapolated using the epsilon-algorithm, which accelerates the convergence of the integral in the presence of discontinuities and integrable singularities. The function returns the final approximation from the extrapolation, `result`, and an estimate of the absolute error, `abserr`. The subintervals and their results are stored in the memory provided by `workspace`. The maximum number of subintervals is given by `limit`, which may not exceed the allocated size of the workspace.

17.5 QAGP adaptive integration with known singular points

int **gsl_integration_qagp**(const *gsl_function* *f, double *pts, size_t npts, double epsabs, double epsrel, size_t limit, *gsl_integration_workspace* *workspace, double *result, double *abserr)

This function applies the adaptive integration algorithm QAGS taking account of the user-supplied locations of singular points. The array `pts` of length `npts` should contain the endpoints of the integration ranges defined by the integration region and locations of the singularities. For example, to integrate over the region (a, b) with break-points at x_1, x_2, x_3 (where $a < x_1 < x_2 < x_3 < b$) the following `pts` array should be used:

```
pts[0] = a
pts[1] = x_1
pts[2] = x_2
pts[3] = x_3
pts[4] = b
```

with `npts` = 5.

If you know the locations of the singular points in the integration region then this routine will be faster than `gsl_integration_qags()`.

17.6 QAGI adaptive integration on infinite intervals

int **gsl_integration_qagi**(*gsl_function* *f, double epsabs, double epsrel, size_t limit, *gsl_integration_workspace* *workspace, double *result, double *abserr)

This function computes the integral of the function `f` over the infinite interval $(-\infty, +\infty)$. The integral is mapped onto the semi-open interval $(0, 1]$ using the transformation $x = (1 - t)/t$,

$$\int_{-\infty}^{+\infty} dx f(x) = \int_0^1 dt (f((1-t)/t) + f(-(1-t)/t))/t^2.$$

It is then integrated using the QAGS algorithm. The normal 21-point Gauss-Kronrod rule of QAGS is replaced by a 15-point rule, because the transformation can generate an integrable singularity at the origin. In this case a lower-order rule is more efficient.

int **gsl_integration_qagiu**(*gsl_function* *f, double a, double epsabs, double epsrel, size_t limit, *gsl_integration_workspace* *workspace, double *result, double *abserr)

This function computes the integral of the function `f` over the semi-infinite interval $(a, +\infty)$. The integral is mapped onto the semi-open interval $(0, 1]$ using the transformation $x = a + (1 - t)/t$,

$$\int_a^{+\infty} dx f(x) = \int_0^1 dt f(a + (1 - t)/t)/t^2$$

and then integrated using the QAGS algorithm.

int **gsl_integration_qagil**(*gsl_function* *f, double b, double epsabs, double epsrel, size_t limit, *gsl_integration_workspace* *workspace, double *result, double *abserr)

This function computes the integral of the function `f` over the semi-infinite interval $(-\infty, b)$. The integral is mapped onto the semi-open interval $(0, 1]$ using the transformation $x = b - (1 - t)/t$,

$$\int_{-\infty}^{b} dx f(x) = \int_0^1 dt f(b - (1 - t)/t)/t^2$$

and then integrated using the QAGS algorithm.

17.7 QAWC adaptive integration for Cauchy principal values

int **gsl_integration_qawc**(*gsl_function* *f, double a, double b, double c, double epsabs, double epsrel, size_t limit, *gsl_integration_workspace* *workspace, double *result, double *abserr)

This function computes the Cauchy principal value of the integral of f over (a, b), with a singularity at `c`,

$$I = \int_a^b dx \frac{f(x)}{x - c} = \lim_{\epsilon \to 0} \left\{ \int_a^{c-\epsilon} dx \frac{f(x)}{x - c} + \int_{c+\epsilon}^{b} dx \frac{f(x)}{x - c} \right\}$$

The adaptive bisection algorithm of QAG is used, with modifications to ensure that subdivisions do not occur at the singular point $x = c$. When a subinterval contains the point $x = c$ or is close to it then a special 25-point modified Clenshaw-Curtis rule is used to control the singularity. Further away from the singularity the algorithm uses an ordinary 15-point Gauss-Kronrod integration rule.

17.8 QAWS adaptive integration for singular functions

The QAWS algorithm is designed for integrands with algebraic-logarithmic singularities at the end-points of an integration region. In order to work efficiently the algorithm requires a precomputed table of Chebyshev moments.

type **gsl_integration_qaws_table**

This structure contains precomputed quantities for the QAWS algorithm.

gsl_integration_qaws_table ***gsl_integration_qaws_table_alloc**(double alpha, double beta, int mu, int nu)

This function allocates space for a `gsl_integration_qaws_table` struct describing a singular weight function $w(x)$ with the parameters $(\alpha, \beta, \mu, \nu)$,

$$w(x) = (x - a)^\alpha (b - x)^\beta \log^\mu (x - a) \log^\nu (b - x)$$

where $\alpha > -1$, $\beta > -1$, and $\mu = 0, 1$, $\nu = 0, 1$. The weight function can take four different forms depending on the values of μ and ν,

Weight function $w(x)$	(μ, ν)
$(x-a)^\alpha (b-x)^\beta$	$(0,0)$
$(x-a)^\alpha (b-x)^\beta \log(x-a)$	$(1,0)$
$(x-a)^\alpha (b-x)^\beta \log(b-x)$	$(0,1)$
$(x-a)^\alpha (b-x)^\beta \log(x-a) \log(b-x)$	$(1,1)$

The singular points (a, b) do not have to be specified until the integral is computed, where they are the endpoints of the integration range.

The function returns a pointer to the newly allocated table `gsl_integration_qaws_table` if no errors were detected, and 0 in the case of error.

int **gsl_integration_qaws_table_set**(*gsl_integration_qaws_table* *t, double alpha, double beta, int mu, int nu)

This function modifies the parameters $(\alpha, \beta, \mu, \nu)$ of an existing `gsl_integration_qaws_table` struct `t`.

void **gsl_integration_qaws_table_free**(*gsl_integration_qaws_table* *t)

This function frees all the memory associated with the `gsl_integration_qaws_table` struct `t`.

int **gsl_integration_qaws**(*gsl_function* *f, const double a, const double b, *gsl_integration_qaws_table* *t, const double epsabs, const double epsrel, const size_t limit, *gsl_integration_workspace* *workspace, double *result, double *abserr)

This function computes the integral of the function $f(x)$ over the interval (a, b) with the singular weight function $(x-a)^\alpha (b-x)^\beta \log^\mu(x-a) \log^\nu(b-x)$. The parameters of the weight function $(\alpha, \beta, \mu, \nu)$ are taken from the table `t`. The integral is,

$$I = \int_a^b dx f(x)(x-a)^\alpha (b-x)^\beta \log^\mu(x-a) \log^\nu(b-x).$$

The adaptive bisection algorithm of QAG is used. When a subinterval contains one of the endpoints then a special 25-point modified Clenshaw-Curtis rule is used to control the singularities. For subintervals which do not include the endpoints an ordinary 15-point Gauss-Kronrod integration rule is used.

17.9 QAWO adaptive integration for oscillatory functions

The QAWO algorithm is designed for integrands with an oscillatory factor, $\sin(\omega x)$ or $\cos(\omega x)$. In order to work efficiently the algorithm requires a table of Chebyshev moments which must be pre-computed with calls to the functions below.

gsl_integration_qawo_table ***gsl_integration_qawo_table_alloc**(double omega, double L, enum gsl_integration_qawo_enum sine, size_t n)

This function allocates space for a `gsl_integration_qawo_table` struct and its associated workspace describing a sine or cosine weight function $w(x)$ with the parameters (ω, L),

$$w(x) = \left\{ \begin{array}{c} \sin(\omega x) \\ \cos(\omega x) \end{array} \right\}$$

The parameter `L` must be the length of the interval over which the function will be integrated $L = b - a$. The choice of sine or cosine is made with the parameter `sine` which should be chosen from one of the two following symbolic values:

GSL_INTEG_COSINE

GSL_INTEG_SINE

The `gsl_integration_qawo_table` is a table of the trigonometric coefficients required in the integration process. The parameter `n` determines the number of levels of coefficients that are computed. Each level corresponds to one bisection of the interval L, so that `n` levels are sufficient for subintervals down to the length $L/2^n$. The integration routine `gsl_integration_qawo()` returns the error `GSL_ETABLE` if the number of levels is insufficient for the requested accuracy.

int **gsl_integration_qawo_table_set**(gsl_integration_qawo_table *t, double omega, double L, enum gsl_integration_qawo_enum sine)

This function changes the parameters `omega`, `L` and `sine` of the existing workspace `t`.

int **gsl_integration_qawo_table_set_length**(gsl_integration_qawo_table *t, double L)

This function allows the length parameter `L` of the workspace `t` to be changed.

void **gsl_integration_qawo_table_free**(gsl_integration_qawo_table *t)

This function frees all the memory associated with the workspace `t`.

int **gsl_integration_qawo**(*gsl_function* *f, const double a, const double epsabs, const double epsrel, const size_t limit, *gsl_integration_workspace* *workspace, gsl_integration_qawo_table *wf, double *result, double *abserr)

This function uses an adaptive algorithm to compute the integral of f over (a, b) with the weight function $\sin(\omega x)$ or $\cos(\omega x)$ defined by the table `wf`,

$$I = \int_a^b dx f(x) \left\{ \begin{array}{c} \sin(\omega x) \\ \cos(\omega x) \end{array} \right\}$$

The results are extrapolated using the epsilon-algorithm to accelerate the convergence of the integral. The function returns the final approximation from the extrapolation, `result`, and an estimate of the absolute error, `abserr`. The subintervals and their results are stored in the memory provided by `workspace`. The maximum number of subintervals is given by `limit`, which may not exceed the allocated size of the workspace.

Those subintervals with "large" widths d where $d\omega > 4$ are computed using a 25-point Clenshaw-Curtis integration rule, which handles the oscillatory behavior. Subintervals with a "small" widths where $d\omega < 4$ are computed using a 15-point Gauss-Kronrod integration.

17.10 QAWF adaptive integration for Fourier integrals

int **gsl_integration_qawf**(*gsl_function* *f, const double a, const double epsabs, const size_t limit, *gsl_integration_workspace* *workspace, *gsl_integration_workspace* *cycle_workspace, gsl_integration_qawo_table *wf, double *result, double *abserr)

This function attempts to compute a Fourier integral of the function `f` over the semi-infinite interval $[a, +\infty)$

$$I = \int_a^{+\infty} dx f(x) \left\{ \begin{array}{c} \sin(\omega x) \\ \cos(\omega x) \end{array} \right\}$$

The parameter ω and choice of $\sin$ or $\cos$ is taken from the table `wf` (the length `L` can take any value, since it is overridden by this function to a value appropriate for the Fourier integration). The integral is computed using the QAWO algorithm over each of the subintervals,

$$\begin{aligned} C_1 &= [a, a + c] \\ C_2 &= [a + c, a + 2c] \\ \ldots &= \ldots \\ C_k &= [a + (k - 1)c, a + kc] \end{aligned}$$

where $c = (2 floor(|\omega|) + 1)\pi/|\omega|$. The width c is chosen to cover an odd number of periods so that the contributions from the intervals alternate in sign and are monotonically decreasing when `f` is positive and monotonically decreasing. The sum of this sequence of contributions is accelerated using the epsilon-algorithm.

This function works to an overall absolute tolerance of *abserr*. The following strategy is used: on each interval C_k the algorithm tries to achieve the tolerance

$$TOL_k = u_k abserr$$

where $u_k = (1 - p)p^{k-1}$ and $p = 9/10$. The sum of the geometric series of contributions from each interval gives an overall tolerance of *abserr*.

If the integration of a subinterval leads to difficulties then the accuracy requirement for subsequent intervals is relaxed,

$$TOL_k = u_k \max\left(abserr, \max_{i<k}(E_i)\right)$$

where E_k is the estimated error on the interval C_k.

The subintervals and their results are stored in the memory provided by *workspace*. The maximum number of subintervals is given by *limit*, which may not exceed the allocated size of the workspace. The integration over each subinterval uses the memory provided by *cycle_workspace* as workspace for the QAWO algorithm.

17.11 CQUAD doubly-adaptive integration

CQUAD is a new doubly-adaptive general-purpose quadrature routine which can handle most types of singularities, non-numerical function values such as `Inf` or `NaN`, as well as some divergent integrals. It generally requires more function evaluations than the integration routines in QUADPACK, yet fails less often for difficult integrands.

The underlying algorithm uses a doubly-adaptive scheme in which Clenshaw-Curtis quadrature rules of increasing degree are used to compute the integral in each interval. The L_2-norm of the difference between the underlying interpolatory polynomials of two successive rules is used as an error estimate. The interval is subdivided if the difference between two successive rules is too large or a rule of maximum degree has been reached.

gsl_integration_cquad_workspace ***gsl_integration_cquad_workspace_alloc**(size_t n)

This function allocates a workspace sufficient to hold the data for *n* intervals. The number *n* is not the maximum number of intervals that will be evaluated. If the workspace is full, intervals with smaller error estimates will be discarded. A minimum of 3 intervals is required and for most functions, a workspace of size 100 is sufficient.

void **gsl_integration_cquad_workspace_free**(gsl_integration_cquad_workspace *w)

This function frees the memory associated with the workspace *w*.

int **gsl_integration_cquad**(const *gsl_function* *f, double a, double b, double epsabs, double epsrel, gsl_integration_cquad_workspace *workspace, double *result, double *abserr, size_t *nevals)

This function computes the integral of f over (a, b) within the desired absolute and relative error limits, *epsabs* and *epsrel* using the CQUAD algorithm. The function returns the final approximation, *result*, an estimate of the absolute error, *abserr*, and the number of function evaluations required, *nevals*.

The CQUAD algorithm divides the integration region into subintervals, and in each iteration, the subinterval with the largest estimated error is processed. The algorithm uses Clenshaw-Curtis quadrature rules of degree 4, 8, 16 and 32 over 5, 9, 17 and 33 nodes respectively. Each interval is initialized with the lowest-degree rule. When an interval is processed, the next-higher degree rule is evaluated and an error estimate is computed based on the L_2-norm of the difference between the underlying interpolating polynomials of both rules. If the highest-degree rule has already been used, or the interpolatory polynomials differ significantly, the interval is bisected.

The subintervals and their results are stored in the memory provided by *workspace*. If the error estimate or the number of function evaluations is not needed, the pointers *abserr* and *nevals* can be set to `NULL`.

17.12 Romberg integration

The Romberg integration method estimates the definite integral

$$I = \int_a^b f(x)dx$$

by applying Richardson extrapolation on the trapezoidal rule, using equally spaced points with spacing

$$h_k = (b-a)2^{-k}$$

for $k = 1, \ldots, n$. For each k, Richardson extrapolation is used $k-1$ times on previous approximations to improve the order of accuracy as much as possible. Romberg integration typically works well (and converges quickly) for smooth integrands with no singularities in the interval or at the end points.

gsl_integration_romberg_workspace ***gsl_integration_romberg_alloc**(const size_t n)

This function allocates a workspace for Romberg integration, specifying a maximum of n iterations, or divisions of the interval. Since the number of divisions is $2^n + 1$, n can be kept relatively small (i.e. 10 or 20). It is capped at a maximum value of 30 to prevent overflow. The size of the workspace is $O(2n)$.

void **gsl_integration_romberg_free**(gsl_integration_romberg_workspace *w)

This function frees the memory associated with the workspace `w`.

int **gsl_integration_romberg**(const *gsl_function* *f, const double a, const double b, const double epsabs, const double epsrel, double *result, size_t *neval, gsl_integration_romberg_workspace *w)

This function integrates $f(x)$, specified by `f`, from `a` to `b`, storing the answer in `result`. At each step in the iteration, convergence is tested by checking:

$$|I_k - I_{k-1}| \le \max\left(epsabs, epsrel \times |I_k|\right)$$

where I_k is the current approximation and I_{k-1} is the approximation of the previous iteration. If the method does not converge within the previously specified n iterations, the function stores the best current estimate in `result` and returns `GSL_EMAXITER`. If the method converges, the function returns `GSL_SUCCESS`. The total number of function evaluations is returned in `neval`.

17.13 Gauss-Legendre integration

The fixed-order Gauss-Legendre integration routines are provided for fast integration of smooth functions with known polynomial order. The n-point Gauss-Legendre rule is exact for polynomials of order $2n-1$ or less. For example, these rules are useful when integrating basis functions to form mass matrices for the Galerkin method. Unlike other numerical integration routines within the library, these routines do not accept absolute or relative error bounds.

gsl_integration_glfixed_table ***gsl_integration_glfixed_table_alloc**(size_t n)

This function determines the Gauss-Legendre abscissae and weights necessary for an n-point fixed order integration scheme. If possible, high precision precomputed coefficients are used. If precomputed weights are not available, lower precision coefficients are computed on the fly.

double **gsl_integration_glfixed**(const *gsl_function* *f, double a, double b, const gsl_integration_glfixed_table *t)

This function applies the Gauss-Legendre integration rule contained in table `t` and returns the result.

int **gsl_integration_glfixed_point**(double a, double b, size_t i, double *xi, double *wi, const gsl_integration_glfixed_table *t)

For `i` in $[0, \ldots, n-1]$, this function obtains the `i`-th Gauss-Legendre point `xi` and weight `wi` on the interval [`a`, `b`]. The points and weights are ordered by increasing point value. A function f may be integrated on [`a`, `b`] by summing $wi * f(xi)$ over `i`.

void **gsl_integration_glfixed_table_free**(gsl_integration_glfixed_table *t)

This function frees the memory associated with the table `t`.

17.14 Fixed point quadratures

The routines in this section approximate an integral by the sum

$$\int_a^b w(x)f(x)dx = \sum_{i=1}^n w_i f(x_i)$$

where $f(x)$ is the function to be integrated and $w(x)$ is a weighting function. The n weights w_i and nodes x_i are carefully chosen so that the result is exact when $f(x)$ is a polynomial of degree $2n - 1$ or less. Once the user chooses the order n and weighting function $w(x)$, the weights w_i and nodes x_i can be precomputed and used to efficiently evaluate integrals for any number of functions $f(x)$.

This method works best when $f(x)$ is well approximated by a polynomial on the interval (a, b), and so is not suitable for functions with singularities. Since the user specifies ahead of time how many quadrature nodes will be used, these routines do not accept absolute or relative error bounds. The table below lists the weighting functions currently supported.

Name	Interval	Weighting function $w(x)$	Constraints
Legendre	(a, b)	1	$b > a$
Chebyshev Type 1	(a, b)	$1/\sqrt{(b-x)(x-a)}$	$b > a$
Gegenbauer	(a, b)	$((b-x)(x-a))^\alpha$	$\alpha > -1, b > a$
Jacobi	(a, b)	$(b-x)^\alpha(x-a)^\beta$	$\alpha, \beta > -1, b > a$
Laguerre	(a, ∞)	$(x-a)^\alpha \exp(-b(x-a))$	$\alpha > -1, b > 0$
Hermite	$(-\infty, \infty)$	$\lvert x-a\rvert^\alpha \exp(-b(x-a)^2)$	$\alpha > -1, b > 0$
Exponential	(a, b)	$\lvert x-(a+b)/2\rvert^\alpha$	$\alpha > -1, b > a$
Rational	(a, ∞)	$(x-a)^\alpha(x+b)^\beta$	$\alpha > -1, \alpha+\beta+2n < 0, a+b > 0$
Chebyshev Type 2	(a, b)	$\sqrt{(b-x)(x-a)}$	$b > a$

The fixed point quadrature routines use the following workspace to store the nodes and weights, as well as additional variables for intermediate calculations:

type **gsl_integration_fixed_workspace**

This workspace is used for fixed point quadrature rules and looks like this:

```
typedef struct
{
  size_t n;        /* number of nodes/weights */
  double *weights; /* quadrature weights */
  double *x;       /* quadrature nodes */
  double *diag;    /* diagonal of Jacobi matrix */
  double *subdiag; /* subdiagonal of Jacobi matrix */
  const gsl_integration_fixed_type * type;
} gsl_integration_fixed_workspace;
```

gsl_integration_fixed_workspace ***gsl_integration_fixed_alloc**(const *gsl_integration_fixed_type* *T, const size_t n, const double a, const double b, const double alpha, const double beta)

This function allocates a workspace for computing integrals with interpolating quadratures using `n` quadrature nodes. The parameters `a`, `b`, `alpha`, and `beta` specify the integration interval and/or weighting function for the various quadrature types. See the *table* above for constraints on these parameters. The size of the workspace is $O(4n)$.

type **gsl_integration_fixed_type**

The type of quadrature used is specified by `T` which can be set to the following choices:

gsl_integration_fixed_type ***gsl_integration_fixed_legendre**

This specifies Legendre quadrature integration. The parameters `alpha` and `beta` are ignored for this type.

gsl_integration_fixed_type ***gsl_integration_fixed_chebyshev**

This specifies Chebyshev type 1 quadrature integration. The parameters `alpha` and `beta` are ignored for this type.

gsl_integration_fixed_type ***gsl_integration_fixed_gegenbauer**

This specifies Gegenbauer quadrature integration. The parameter `beta` is ignored for this type.

gsl_integration_fixed_type ***gsl_integration_fixed_jacobi**

This specifies Jacobi quadrature integration.

gsl_integration_fixed_type ***gsl_integration_fixed_laguerre**

This specifies Laguerre quadrature integration. The parameter `beta` is ignored for this type.

gsl_integration_fixed_type ***gsl_integration_fixed_hermite**

This specifies Hermite quadrature integration. The parameter `beta` is ignored for this type.

gsl_integration_fixed_type ***gsl_integration_fixed_exponential**

This specifies exponential quadrature integration. The parameter `beta` is ignored for this type.

gsl_integration_fixed_type ***gsl_integration_fixed_rational**

This specifies rational quadrature integration.

gsl_integration_fixed_type ***gsl_integration_fixed_chebyshev2**

This specifies Chebyshev type 2 quadrature integration. The parameters `alpha` and `beta` are ignored for this type.

void **gsl_integration_fixed_free**(*gsl_integration_fixed_workspace* *w)

This function frees the memory assocated with the workspace `w`

size_t **gsl_integration_fixed_n**(const *gsl_integration_fixed_workspace* *w)

This function returns the number of quadrature nodes and weights.

double ***gsl_integration_fixed_nodes**(const *gsl_integration_fixed_workspace* *w)

This function returns a pointer to an array of size `n` containing the quadrature nodes x_i.

double ***gsl_integration_fixed_weights**(const *gsl_integration_fixed_workspace* *w)

This function returns a pointer to an array of size `n` containing the quadrature weights w_i.

int **gsl_integration_fixed**(const *gsl_function* *func, double *result, const *gsl_integration_fixed_workspace* *w)

This function integrates the function $f(x)$ provided in `func` using previously computed fixed quadrature rules. The integral is approximated as

$$\sum_{i=1}^{n} w_i f(x_i)$$

where w_i are the quadrature weights and x_i are the quadrature nodes computed previously by `gsl_integration_fixed_alloc()`. The sum is stored in `result` on output.

17.15 Error codes

In addition to the standard error codes for invalid arguments the functions can return the following values,

GSL_EMAXITER	the maximum number of subdivisions was exceeded.
GSL_EROUND	cannot reach tolerance because of roundoff error, or roundoff error was detected in the extrapolation table.
GSL_ESING	a non-integrable singularity or other bad integrand behavior was found in the integration interval.
GSL_EDIVERGE	the integral is divergent, or too slowly convergent to be integrated numerically.
GSL_EDOM	error in the values of the input arguments

17.16 Examples

17.16.1 Adaptive integration example

The integrator QAGS will handle a large class of definite integrals. For example, consider the following integral, which has an algebraic-logarithmic singularity at the origin,

$$\int_0^1 x^{-1/2} \log(x) dx = -4$$

The program below computes this integral to a relative accuracy bound of 1e-7.

```
#include <stdio.h>
#include <math.h>
#include <gsl/gsl_integration.h>

double f (double x, void * params) {
  double alpha = *(double *) params;
  double f = log(alpha*x) / sqrt(x);
  return f;
}

int
main (void)
{
  gsl_integration_workspace * w
    = gsl_integration_workspace_alloc (1000);

  double result, error;
  double expected = -4.0;
  double alpha = 1.0;

  gsl_function F;
  F.function = &f;
  F.params = &alpha;

  gsl_integration_qags (&F, 0, 1, 0, 1e-7, 1000,
                        w, &result, &error);

  printf ("result          = % .18f\n", result);
```

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```
  printf ("exact result    = % .18f\n", expected);
  printf ("estimated error = % .18f\n", error);
  printf ("actual error    = % .18f\n", result - expected);
  printf ("intervals       = %zu\n", w->size);

  gsl_integration_workspace_free (w);

  return 0;
}
```

The results below show that the desired accuracy is achieved after 8 subdivisions.

```
result          = -4.000000000000085265
exact result    = -4.000000000000000000
estimated error =  0.000000000000135447
actual error    = -0.000000000000085265
intervals       = 8
```

In fact, the extrapolation procedure used by QAGS produces an accuracy of almost twice as many digits. The error estimate returned by the extrapolation procedure is larger than the actual error, giving a margin of safety of one order of magnitude.

17.16.2 Fixed-point quadrature example

In this example, we use a fixed-point quadrature rule to integrate the integral

$$\int_{-\infty}^{\infty} e^{-x^2} \left(x^m + 1 \right) dx = \begin{cases} \sqrt{\pi} + \Gamma\left(\frac{m+1}{2}\right), & m \text{ even} \\ \sqrt{\pi}, & m \text{ odd} \end{cases}$$

for integer m. Consulting our *table* of fixed point quadratures, we see that this integral can be evaluated with a Hermite quadrature rule, setting $\alpha = 0, a = 0, b = 1$. Since we are integrating a polynomial of degree m, we need to choose the number of nodes $n \geq (m+1)/2$ to achieve the best results.

First we will try integrating for $m = 10, n = 5$, which does not satisfy our criteria above:

```
$ ./integration2 10 5
```

The output is,

```
m               = 10
intervals       = 5
result          =  47.468529694563351029
exact result    =  54.115231635459025483
actual error    = -6.646701940895674454
```

So, we find a large error. Now we try integrating for $m = 10, n = 6$ which does satisfy the criteria above:

```
$ ./integration2 10 6
```

The output is,

```
m               = 10
intervals       = 6
```

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```
result          =  54.115231635459096537
exact result    =  54.115231635459025483
actual error    =  0.000000000000071054
```

The program is given below.

```
#include <stdio.h>
#include <math.h>
#include <gsl/gsl_integration.h>
#include <gsl/gsl_sf_gamma.h>

double
f(double x, void * params)
{
  int m = *(int *) params;
  double f = gsl_pow_int(x, m) + 1.0;
  return f;
}

int
main (int argc, char *argv[])
{
  gsl_integration_fixed_workspace * w;
  const gsl_integration_fixed_type * T = gsl_integration_fixed_hermite;
  int m = 10;
  int n = 6;
  double expected, result;
  gsl_function F;

  if (argc > 1)
    m = atoi(argv[1]);

  if (argc > 2)
    n = atoi(argv[2]);

  w = gsl_integration_fixed_alloc(T, n, 0.0, 1.0, 0.0, 0.0);

  F.function = &f;
  F.params = &m;

  gsl_integration_fixed(&F, &result, w);

  if (m % 2 == 0)
    expected = M_SQRTPI + gsl_sf_gamma(0.5*(1.0 + m));
  else
    expected = M_SQRTPI;

  printf ("m               = %d\n", m);
  printf ("intervals       = %zu\n", gsl_integration_fixed_n(w));
  printf ("result          = % .18f\n", result);
  printf ("exact result    = % .18f\n", expected);
  printf ("actual error    = % .18f\n", result - expected);
```

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```
  gsl_integration_fixed_free (w);

  return 0;
}
```

17.17 References and Further Reading

The following book is the definitive reference for QUADPACK, and was written by the original authors. It provides descriptions of the algorithms, program listings, test programs and examples. It also includes useful advice on numerical integration and many references to the numerical integration literature used in developing QUADPACK.

- R. Piessens, E. de Doncker-Kapenga, C.W. Ueberhuber, D.K. Kahaner. QUADPACK A subroutine package for automatic integration Springer Verlag, 1983.

The CQUAD integration algorithm is described in the following paper:

- P. Gonnet, "Increasing the Reliability of Adaptive Quadrature Using Explicit Interpolants", ACM Transactions on Mathematical Software, Volume 37 (2010), Issue 3, Article 26.

The fixed-point quadrature routines are based on IQPACK, described in the following papers:

- S. Elhay, J. Kautsky, Algorithm 655: IQPACK, FORTRAN Subroutines for the Weights of Interpolatory Quadrature, ACM Transactions on Mathematical Software, Volume 13, Number 4, December 1987, pages 399-415.
- J. Kautsky, S. Elhay, Calculation of the Weights of Interpolatory Quadratures, Numerische Mathematik, Volume 40, Number 3, October 1982, pages 407-422.

CHAPTER

EIGHTEEN

RANDOM NUMBER GENERATION

The library provides a large collection of random number generators which can be accessed through a uniform interface. Environment variables allow you to select different generators and seeds at runtime, so that you can easily switch between generators without needing to recompile your program. Each instance of a generator keeps track of its own state, allowing the generators to be used in multi-threaded programs. Additional functions are available for transforming uniform random numbers into samples from continuous or discrete probability distributions such as the Gaussian, log-normal or Poisson distributions.

These functions are declared in the header file `gsl_rng.h`.

18.1 General comments on random numbers

In 1988, Park and Miller wrote a paper entitled "Random number generators: good ones are hard to find." [Commun.: ACM, 31, 1192–1201]. Fortunately, some excellent random number generators are available, though poor ones are still in common use. You may be happy with the system-supplied random number generator on your computer, but you should be aware that as computers get faster, requirements on random number generators increase. Nowadays, a simulation that calls a random number generator millions of times can often finish before you can make it down the hall to the coffee machine and back.

A very nice review of random number generators was written by Pierre L'Ecuyer, as Chapter 4 of the book: Handbook on Simulation, Jerry Banks, ed. (Wiley, 1997). The chapter is available in postscript from L'Ecuyer's ftp site (see references). Knuth's volume on Seminumerical Algorithms (originally published in 1968) devotes 170 pages to random number generators, and has recently been updated in its 3rd edition (1997). It is brilliant, a classic. If you don't own it, you should stop reading right now, run to the nearest bookstore, and buy it.

A good random number generator will satisfy both theoretical and statistical properties. Theoretical properties are often hard to obtain (they require real math!), but one prefers a random number generator with a long period, low serial correlation, and a tendency **not** to "fall mainly on the planes." Statistical tests are performed with numerical simulations. Generally, a random number generator is used to estimate some quantity for which the theory of probability provides an exact answer. Comparison to this exact answer provides a measure of "randomness".

18.2 The Random Number Generator Interface

It is important to remember that a random number generator is not a "real" function like sine or cosine. Unlike real functions, successive calls to a random number generator yield different return values. Of course that is just what you want for a random number generator, but to achieve this effect, the generator must keep track of some kind of "state" variable. Sometimes this state is just an integer (sometimes just the value of the previously generated random number), but often it is more complicated than that and may involve a whole array of numbers, possibly with some indices thrown in. To use the random number generators, you do not need to know the details of what comprises the state, and besides that varies from algorithm to algorithm.

type **gsl_rng_type**

type **gsl_rng**

The random number generator library uses two special structs, *gsl_rng_type* which holds static information about each type of generator and *gsl_rng* which describes an instance of a generator created from a given *gsl_rng_type*.

The functions described in this section are declared in the header file gsl_rng.h.

18.3 Random number generator initialization

gsl_rng ***gsl_rng_alloc**(const *gsl_rng_type* *T)

This function returns a pointer to a newly-created instance of a random number generator of type *T*. For example, the following code creates an instance of the Tausworthe generator:

```
gsl_rng * r = gsl_rng_alloc (gsl_rng_taus);
```

If there is insufficient memory to create the generator then the function returns a null pointer and the error handler is invoked with an error code of *GSL_ENOMEM*.

The generator is automatically initialized with the default seed, *gsl_rng_default_seed*. This is zero by default but can be changed either directly or by using the environment variable *GSL_RNG_SEED*.

The details of the available generator types are described later in this chapter.

void **gsl_rng_set**(const *gsl_rng* *r, unsigned long int s)

This function initializes (or "seeds") the random number generator. If the generator is seeded with the same value of *s* on two different runs, the same stream of random numbers will be generated by successive calls to the routines below. If different values of $s \geq 1$ are supplied, then the generated streams of random numbers should be completely different. If the seed *s* is zero then the standard seed from the original implementation is used instead. For example, the original Fortran source code for the ranlux generator used a seed of 314159265, and so choosing *s* equal to zero reproduces this when using *gsl_rng_ranlux*.

When using multiple seeds with the same generator, choose seed values greater than zero to avoid collisions with the default setting.

Note that the most generators only accept 32-bit seeds, with higher values being reduced modulo 2^{32}. For generators with smaller ranges the maximum seed value will typically be lower.

void **gsl_rng_free**(*gsl_rng* *r)

This function frees all the memory associated with the generator *r*.

18.4 Sampling from a random number generator

The following functions return uniformly distributed random numbers, either as integers or double precision floating point numbers. Inline versions of these functions are used when HAVE_INLINE is defined. To obtain non-uniform distributions, see *Random Number Distributions*.

unsigned long int **gsl_rng_get**(const *gsl_rng* *r)

This function returns a random integer from the generator *r*. The minimum and maximum values depend on the algorithm used, but all integers in the range [min, max] are equally likely. The values of min and max can be determined using the auxiliary functions *gsl_rng_max()* and *gsl_rng_min()*.

double **gsl_rng_uniform**(const *gsl_rng* *r)

This function returns a double precision floating point number uniformly distributed in the range [0,1). The range includes 0.0 but excludes 1.0. The value is typically obtained by dividing the result of gsl_rng_get(r) by `gsl_rng_max(r) + 1.0` in double precision. Some generators compute this ratio internally so that they can provide floating point numbers with more than 32 bits of randomness (the maximum number of bits that can be portably represented in a single `unsigned long int`).

double **gsl_rng_uniform_pos**(const *gsl_rng* *r)

This function returns a positive double precision floating point number uniformly distributed in the range (0,1), excluding both 0.0 and 1.0. The number is obtained by sampling the generator with the algorithm of *gsl_rng_uniform()* until a non-zero value is obtained. You can use this function if you need to avoid a singularity at 0.0.

unsigned long int **gsl_rng_uniform_int**(const *gsl_rng* *r, unsigned long int n)

This function returns a random integer from 0 to $n-1$ inclusive by scaling down and/or discarding samples from the generator *r*. All integers in the range $[0, n-1]$ are produced with equal probability. For generators with a non-zero minimum value an offset is applied so that zero is returned with the correct probability.

Note that this function is designed for sampling from ranges smaller than the range of the underlying generator. The parameter *n* must be less than or equal to the range of the generator *r*. If *n* is larger than the range of the generator then the function calls the error handler with an error code of *GSL_EINVAL* and returns zero.

In particular, this function is not intended for generating the full range of unsigned integer values $[0, 2^{32}-1]$. Instead choose a generator with the maximal integer range and zero minimum value, such as *gsl_rng_ranlxd1*, *gsl_rng_mt19937* or *gsl_rng_taus*, and sample it directly using *gsl_rng_get()*. The range of each generator can be found using the auxiliary functions described in the next section.

18.5 Auxiliary random number generator functions

The following functions provide information about an existing generator. You should use them in preference to hard-coding the generator parameters into your own code.

const char ***gsl_rng_name**(const *gsl_rng* *r)

This function returns a pointer to the name of the generator. For example:

```
printf ("r is a '%s' generator\n", gsl_rng_name (r));
```

would print something like:

```
r is a 'taus' generator
```

unsigned long int **gsl_rng_max**(const *gsl_rng* *r)

This function returns the largest value that *gsl_rng_get()* can return.

unsigned long int **gsl_rng_min**(const *gsl_rng* *r)

This function returns the smallest value that *gsl_rng_get()* can return. Usually this value is zero. There are some generators with algorithms that cannot return zero, and for these generators the minimum value is 1.

void ***gsl_rng_state**(const *gsl_rng* *r)

size_t **gsl_rng_size**(const *gsl_rng* *r)

These functions return a pointer to the state of generator *r* and its size. You can use this information to access the state directly. For example, the following code will write the state of a generator to a stream:

```
void * state = gsl_rng_state (r);
size_t n = gsl_rng_size (r);
fwrite (state, n, 1, stream);
```

const *gsl_rng_type* ****gsl_rng_types_setup**(void)

This function returns a pointer to an array of all the available generator types, terminated by a null pointer. The function should be called once at the start of the program, if needed. The following code fragment shows how to iterate over the array of generator types to print the names of the available algorithms:

```
const gsl_rng_type **t, **t0;

t0 = gsl_rng_types_setup ();

printf ("Available generators:\n");

for (t = t0; *t != 0; t++)
  {
    printf ("%s\n", (*t)->name);
  }
```

18.6 Random number environment variables

The library allows you to choose a default generator and seed from the environment variables *GSL_RNG_TYPE* and *GSL_RNG_SEED* and the function *gsl_rng_env_setup()*. This makes it easy try out different generators and seeds without having to recompile your program.

GSL_RNG_TYPE

This environment variable specifies the default random number generator. It should be the name of a generator, such as `taus` or `mt19937`.

GSL_RNG_SEED

This environment variable specifies the default seed for the random number generator

gsl_rng_type ***gsl_rng_default**

This global library variable specifies the default random number generator, and can be initialized from *GSL_RNG_TYPE* using *gsl_rng_env_setup()*. It is defined as follows:

```
extern const gsl_rng_type *gsl_rng_default
```

unsigned long int **gsl_rng_default_seed**

This global library variable specifies the seed for the default random number generator, and can be initialized from *GSL_RNG_SEED* using *gsl_rng_env_setup()*. It is set to zero by default and is defined as follows:

```
extern unsigned long int gsl_rng_default_seed
```

const *gsl_rng_type* ***gsl_rng_env_setup**(void)

This function reads the environment variables *GSL_RNG_TYPE* and *GSL_RNG_SEED* and uses their values to set the corresponding library variables *gsl_rng_default* and *gsl_rng_default_seed*.

The value of *GSL_RNG_SEED* is converted to an `unsigned long int` using the C library function `strtoul()`.

If you don't specify a generator for *GSL_RNG_TYPE* then *gsl_rng_mt19937* is used as the default. The initial value of *gsl_rng_default_seed* is zero.

Here is a short program which shows how to create a global generator using the environment variables *GSL_RNG_TYPE* and *GSL_RNG_SEED*,

```
#include <stdio.h>
#include <gsl/gsl_rng.h>
```

(continues on next page)

(continued from previous page)

```
gsl_rng * r;  /* global generator */

int
main (void)
{
  const gsl_rng_type * T;

  gsl_rng_env_setup();

  T = gsl_rng_default;
  r = gsl_rng_alloc (T);

  printf ("generator type: %s\n", gsl_rng_name (r));
  printf ("seed = %lu\n", gsl_rng_default_seed);
  printf ("first value = %lu\n", gsl_rng_get (r));

  gsl_rng_free (r);
  return 0;
}
```

Running the program without any environment variables uses the initial defaults, an `mt19937` generator with a seed of 0,

```
generator type: mt19937
seed = 0
first value = 4293858116
```

By setting the two variables on the command line we can change the default generator and the seed:

```
$ GSL_RNG_TYPE="taus" GSL_RNG_SEED=123 ./a.out
GSL_RNG_TYPE=taus
GSL_RNG_SEED=123
generator type: taus
seed = 123
first value = 2720986350
```

18.7 Copying random number generator state

The above methods do not expose the random number state which changes from call to call. It is often useful to be able to save and restore the state. To permit these practices, a few somewhat more advanced functions are supplied. These include:

int **gsl_rng_memcpy**(*gsl_rng* *dest, const *gsl_rng* *src)

This function copies the random number generator `src` into the pre-existing generator `dest`, making `dest` into an exact copy of `src`. The two generators must be of the same type.

gsl_rng ***gsl_rng_clone**(const *gsl_rng* *r)

This function returns a pointer to a newly created generator which is an exact copy of the generator `r`.

18.8 Reading and writing random number generator state

The library provides functions for reading and writing the random number state to a file as binary data.

int **gsl_rng_fwrite**(FILE *stream, const *gsl_rng* *r)

This function writes the random number state of the random number generator `r` to the stream `stream` in binary format. The return value is 0 for success and `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

int **gsl_rng_fread**(FILE *stream, *gsl_rng* *r)

This function reads the random number state into the random number generator `r` from the open stream `stream` in binary format. The random number generator `r` must be preinitialized with the correct random number generator type since type information is not saved. The return value is 0 for success and `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

18.9 Random number generator algorithms

The functions described above make no reference to the actual algorithm used. This is deliberate so that you can switch algorithms without having to change any of your application source code. The library provides a large number of generators of different types, including simulation quality generators, generators provided for compatibility with other libraries and historical generators from the past.

The following generators are recommended for use in simulation. They have extremely long periods, low correlation and pass most statistical tests. For the most reliable source of uncorrelated numbers, the second-generation RANLUX generators have the strongest proof of randomness.

gsl_rng_type ***gsl_rng_mt19937**

The MT19937 generator of Makoto Matsumoto and Takuji Nishimura is a variant of the twisted generalized feedback shift-register algorithm, and is known as the "Mersenne Twister" generator. It has a Mersenne prime period of $2^{19937} - 1$ (about 10^{6000}) and is equi-distributed in 623 dimensions. It has passed the DIEHARD statistical tests. It uses 624 words of state per generator and is comparable in speed to the other generators. The original generator used a default seed of 4357 and choosing `s` equal to zero in `gsl_rng_set()` reproduces this. Later versions switched to 5489 as the default seed, you can choose this explicitly via `gsl_rng_set()` instead if you require it.

For more information see,

- Makoto Matsumoto and Takuji Nishimura, "Mersenne Twister: A 623-dimensionally equidistributed uniform pseudorandom number generator". ACM Transactions on Modeling and Computer Simulation, Vol.: 8, No.: 1 (Jan. 1998), Pages 3–30

The generator `gsl_rng_mt19937` uses the second revision of the seeding procedure published by the two authors above in 2002. The original seeding procedures could cause spurious artifacts for some seed values. They are still available through the alternative generators `gsl_rng_mt19937_1999` and `gsl_rng_mt19937_1998`.

gsl_rng_type ***gsl_rng_ranlxs0**

gsl_rng_type ***gsl_rng_ranlxs1**

gsl_rng_type ***gsl_rng_ranlxs2**

The generator `ranlxs0` is a second-generation version of the RANLUX algorithm of Luscher, which produces "luxury random numbers". This generator provides single precision output (24 bits) at three luxury levels `ranlxs0`, `ranlxs1` and `ranlxs2`, in increasing order of strength. It uses double-precision floating point arithmetic internally and can be significantly faster than the integer version of `ranlux`, particularly on 64-bit architectures. The period of the generator is about 10^{171}. The algorithm has mathematically proven properties and can provide truly decorrelated numbers at a known level of randomness. The higher luxury levels provide increased decorrelation between samples as an additional safety margin.

Note that the range of allowed seeds for this generator is $[0, 2^{31} - 1]$. Higher seed values are wrapped modulo 2^{31}.

gsl_rng_type ***gsl_rng_ranlxd1**

gsl_rng_type ***gsl_rng_ranlxd2**

These generators produce double precision output (48 bits) from the RANLXS generator. The library provides two luxury levels `ranlxd1` and `ranlxd2`, in increasing order of strength.

gsl_rng_type ***gsl_rng_ranlux**

gsl_rng_type ***gsl_rng_ranlux389**

The `ranlux` generator is an implementation of the original algorithm developed by Luscher. It uses a lagged-fibonacci-with-skipping algorithm to produce "luxury random numbers". It is a 24-bit generator, originally designed for single-precision IEEE floating point numbers. This implementation is based on integer arithmetic, while the second-generation versions RANLXS and RANLXD described above provide floating-point implementations which will be faster on many platforms. The period of the generator is about 10^{171}. The algorithm has mathematically proven properties and it can provide truly decorrelated numbers at a known level of randomness. The default level of decorrelation recommended by Luscher is provided by `gsl_rng_ranlux`, while `gsl_rng_ranlux389` gives the highest level of randomness, with all 24 bits decorrelated. Both types of generator use 24 words of state per generator.

For more information see,

- M. Luscher, "A portable high-quality random number generator for lattice field theory calculations", Computer Physics Communications, 79 (1994) 100–110.
- F. James, "RANLUX: A Fortran implementation of the high-quality pseudo-random number generator of Luscher", Computer Physics Communications, 79 (1994) 111–114

gsl_rng_type ***gsl_rng_cmrg**

This is a combined multiple recursive generator by L'Ecuyer. Its sequence is,

$$z_n = (x_n - y_n) \mod m_1$$

where the two underlying generators x_n and y_n are,

$$\begin{aligned} x_n &= (a_1 x_{n-1} + a_2 x_{n-2} + a_3 x_{n-3}) \mod m_1 \\ y_n &= (b_1 y_{n-1} + b_2 y_{n-2} + b_3 y_{n-3}) \mod m_2 \end{aligned}$$

with coefficients $a_1 = 0$, $a_2 = 63308$, $a_3 = -183326$, $b_1 = 86098$, $b_2 = 0$, $b_3 = -539608$, and moduli $m_1 = 2^{31} - 1 = 2147483647$ and $m_2 = 2145483479$.

The period of this generator is $\operatorname{lcm}(m_1^3 - 1, m_2^3 - 1)$, which is approximately 2^{185} (about 10^{56}). It uses 6 words of state per generator. For more information see,

- P. L'Ecuyer, "Combined Multiple Recursive Random Number Generators", Operations Research, 44, 5 (1996), 816–822.

gsl_rng_type ***gsl_rng_mrg**

This is a fifth-order multiple recursive generator by L'Ecuyer, Blouin and Coutre. Its sequence is,

$$x_n = (a_1 x_{n-1} + a_5 x_{n-5}) \mod m$$

with $a_1 = 107374182$, $a_2 = a_3 = a_4 = 0$, $a_5 = 104480$ and $m = 2^{31} - 1$.

The period of this generator is about 10^{46}. It uses 5 words of state per generator. More information can be found in the following paper,

- P. L'Ecuyer, F. Blouin, and R. Coutre, "A search for good multiple recursive random number generators", ACM Transactions on Modeling and Computer Simulation 3, 87–98 (1993).

gsl_rng_type ***gsl_rng_taus**

gsl_rng_type ***gsl_rng_taus2**

This is a maximally equidistributed combined Tausworthe generator by L'Ecuyer. The sequence is,

$$x_n = (s^1_n \oplus s^2_n \oplus s^3_n)$$

where,

$$\begin{aligned} s^1_{n+1} &= (((s^1_n \& 4294967294) \ll 12) \oplus (((s^1_n \ll 13) \oplus s^1_n) \gg 19)) \\ s^2_{n+1} &= (((s^2_n \& 4294967288) \ll 4) \oplus (((s^2_n \ll 2) \oplus s^2_n) \gg 25)) \\ s^3_{n+1} &= (((s^3_n \& 4294967280) \ll 17) \oplus (((s^3_n \ll 3) \oplus s^3_n) \gg 11)) \end{aligned}$$

computed modulo 2^{32}. In the formulas above $\oplus$ denotes *exclusive-or*. Note that the algorithm relies on the properties of 32-bit unsigned integers and has been implemented using a bitmask of `0xFFFFFFFF` to make it work on 64 bit machines.

The period of this generator is 2^{88} (about 10^{26}). It uses 3 words of state per generator. For more information see,

- P. L'Ecuyer, "Maximally Equidistributed Combined Tausworthe Generators", Mathematics of Computation, 65, 213 (1996), 203–213.

The generator `gsl_rng_taus2` uses the same algorithm as `gsl_rng_taus` but with an improved seeding procedure described in the paper,

- P. L'Ecuyer, "Tables of Maximally Equidistributed Combined LFSR Generators", Mathematics of Computation, 68, 225 (1999), 261–269

The generator `gsl_rng_taus2` should now be used in preference to `gsl_rng_taus`.

gsl_rng_type ***gsl_rng_gfsr4**

The `gfsr4` generator is like a lagged-fibonacci generator, and produces each number as an `xor`'d sum of four previous values.

$$r_n = r_{n-A} \oplus r_{n-B} \oplus r_{n-C} \oplus r_{n-D}$$

Ziff (ref below) notes that "it is now widely known" that two-tap registers (such as R250, which is described below) have serious flaws, the most obvious one being the three-point correlation that comes from the definition of the generator. Nice mathematical properties can be derived for GFSR's, and numerics bears out the claim that 4-tap GFSR's with appropriately chosen offsets are as random as can be measured, using the author's test.

This implementation uses the values suggested the example on p392 of Ziff's article: $A = 471$, $B = 1586$, $C = 6988$, $D = 9689$.

If the offsets are appropriately chosen (such as the one ones in this implementation), then the sequence is said to be maximal; that means that the period is $2^D - 1$, where D is the longest lag. (It is one less than 2^D because it is not permitted to have all zeros in the `ra[]` array.) For this implementation with $D = 9689$ that works out to about 10^{2917}.

Note that the implementation of this generator using a 32-bit integer amounts to 32 parallel implementations of one-bit generators. One consequence of this is that the period of this 32-bit generator is the same as for the one-bit generator. Moreover, this independence means that all 32-bit patterns are equally likely, and in particular that 0 is an allowed random value. (We are grateful to Heiko Bauke for clarifying for us these properties of GFSR random number generators.)

For more information see,

- Robert M. Ziff, "Four-tap shift-register-sequence random-number generators", Computers in Physics, 12(4), Jul/Aug 1998, pp 385–392.

18.10 Unix random number generators

The standard Unix random number generators `rand`, `random` and `rand48` are provided as part of GSL. Although these generators are widely available individually often they aren't all available on the same platform. This makes it difficult to write portable code using them and so we have included the complete set of Unix generators in GSL for convenience. Note that these generators don't produce high-quality randomness and aren't suitable for work requiring accurate statistics. However, if you won't be measuring statistical quantities and just want to introduce some variation into your program then these generators are quite acceptable.

gsl_rng_type ***gsl_rng_rand**

This is the BSD `rand` generator. Its sequence is

$$x_{n+1} = (ax_n + c) \mod m$$

with $a = 1103515245$, $c = 12345$ and $m = 2^{31}$. The seed specifies the initial value, x_1. The period of this generator is 2^{31}, and it uses 1 word of storage per generator.

gsl_rng_type ***gsl_rng_random_bsd**

gsl_rng_type ***gsl_rng_random_libc5**

gsl_rng_type ***gsl_rng_random_glibc2**

These generators implement the `random` family of functions, a set of linear feedback shift register generators originally used in BSD Unix. There are several versions of `random` in use today: the original BSD version (e.g. on SunOS4), a libc5 version (found on older GNU/Linux systems) and a glibc2 version. Each version uses a different seeding procedure, and thus produces different sequences.

The original BSD routines accepted a variable length buffer for the generator state, with longer buffers providing higher-quality randomness. The `random` function implemented algorithms for buffer lengths of 8, 32, 64, 128 and 256 bytes, and the algorithm with the largest length that would fit into the user-supplied buffer was used. To support these algorithms additional generators are available with the following names:

```
gsl_rng_random8_bsd
gsl_rng_random32_bsd
gsl_rng_random64_bsd
gsl_rng_random128_bsd
gsl_rng_random256_bsd
```

where the numeric suffix indicates the buffer length. The original BSD `random` function used a 128-byte default buffer and so *`gsl_rng_random_bsd`* has been made equivalent to `gsl_rng_random128_bsd`. Corresponding versions of the `libc5` and `glibc2` generators are also available, with the names `gsl_rng_random8_libc5`, `gsl_rng_random8_glibc2`, etc.

gsl_rng_type ***gsl_rng_rand48**

This is the Unix `rand48` generator. Its sequence is

$$x_{n+1} = (ax_n + c) \mod m$$

defined on 48-bit unsigned integers with $a = 25214903917$, $c = 11$ and $m = 2^{48}$. The seed specifies the upper 32 bits of the initial value, x_1, with the lower 16 bits set to `0x330E`. The function *`gsl_rng_get()`* returns the upper 32 bits from each term of the sequence. This does not have a direct parallel in the original `rand48` functions, but forcing the result to type `long int` reproduces the output of `mrand48`. The function *`gsl_rng_uniform()`* uses the full 48 bits of internal state to return the double precision number x_n/m, which is equivalent to the function `drand48`. Note that some versions of the GNU C Library contained a bug in `mrand48` function which caused it to produce different results (only the lower 16-bits of the return value were set).

18.11 Other random number generators

The generators in this section are provided for compatibility with existing libraries. If you are converting an existing program to use GSL then you can select these generators to check your new implementation against the original one, using the same random number generator. After verifying that your new program reproduces the original results you can then switch to a higher-quality generator.

Note that most of the generators in this section are based on single linear congruence relations, which are the least sophisticated type of generator. In particular, linear congruences have poor properties when used with a non-prime modulus, as several of these routines do (e.g. with a power of two modulus, 2^{31} or 2^{32}). This leads to periodicity in the least significant bits of each number, with only the higher bits having any randomness. Thus if you want to produce a random bitstream it is best to avoid using the least significant bits.

gsl_rng_type ***gsl_rng_ranf**

This is the CRAY random number generator `RANF`. Its sequence is

$$x_{n+1} = (a x_n) \mod m$$

defined on 48-bit unsigned integers with $a = 44485709377909$ and $m = 2^{48}$. The seed specifies the lower 32 bits of the initial value, x_1, with the lowest bit set to prevent the seed taking an even value. The upper 16 bits of x_1 are set to 0. A consequence of this procedure is that the pairs of seeds 2 and 3, 4 and 5, etc.: produce the same sequences.

The generator compatible with the CRAY MATHLIB routine RANF. It produces double precision floating point numbers which should be identical to those from the original RANF.

There is a subtlety in the implementation of the seeding. The initial state is reversed through one step, by multiplying by the modular inverse of a mod m. This is done for compatibility with the original CRAY implementation.

Note that you can only seed the generator with integers up to 2^{32}, while the original CRAY implementation uses non-portable wide integers which can cover all 2^{48} states of the generator.

The function `gsl_rng_get()` returns the upper 32 bits from each term of the sequence. The function `gsl_rng_uniform()` uses the full 48 bits to return the double precision number x_n/m.

The period of this generator is 2^{46}.

gsl_rng_type ***gsl_rng_ranmar**

This is the RANMAR lagged-fibonacci generator of Marsaglia, Zaman and Tsang. It is a 24-bit generator, originally designed for single-precision IEEE floating point numbers. It was included in the CERNLIB high-energy physics library.

gsl_rng_type ***gsl_rng_r250**

This is the shift-register generator of Kirkpatrick and Stoll. The sequence is based on the recurrence

$$x_n = x_{n-103} \oplus x_{n-250}$$

where $\oplus$ denotes *exclusive-or*, defined on 32-bit words. The period of this generator is about 2^{250} and it uses 250 words of state per generator.

For more information see,

- S. Kirkpatrick and E. Stoll, "A very fast shift-register sequence random number generator", Journal of Computational Physics, 40, 517–526 (1981)

gsl_rng_type ***gsl_rng_tt800**

This is an earlier version of the twisted generalized feedback shift-register generator, and has been superseded by the development of MT19937. However, it is still an acceptable generator in its own right. It has a period of 2^{800} and uses 33 words of storage per generator.

For more information see,

- Makoto Matsumoto and Yoshiharu Kurita, "Twisted GFSR Generators II", ACM Transactions on Modelling and Computer Simulation, Vol.: 4, No.: 3, 1994, pages 254–266.

gsl_rng_type ***gsl_rng_vax***

This is the VAX generator `MTH$RANDOM`. Its sequence is,

$$x_{n+1} = (ax_n + c) \mod m$$

with $a = 69069$, $c = 1$ and $m = 2^{32}$. The seed specifies the initial value, x_1. The period of this generator is 2^{32} and it uses 1 word of storage per generator.

gsl_rng_type ***gsl_rng_transputer***

This is the random number generator from the INMOS Transputer Development system. Its sequence is,

$$x_{n+1} = (ax_n) \mod m$$

with $a = 1664525$ and $m = 2^{32}$. The seed specifies the initial value, x_1.

gsl_rng_type ***gsl_rng_randu***

This is the IBM `RANDU` generator. Its sequence is

$$x_{n+1} = (ax_n) \mod m$$

with $a = 65539$ and $m = 2^{31}$. The seed specifies the initial value, x_1. The period of this generator was only 2^{29}. It has become a textbook example of a poor generator.

gsl_rng_type ***gsl_rng_minstd***

This is Park and Miller's "minimal standard" MINSTD generator, a simple linear congruence which takes care to avoid the major pitfalls of such algorithms. Its sequence is,

$$x_{n+1} = (ax_n) \mod m$$

with $a = 16807$ and $m = 2^{31} - 1 = 2147483647$. The seed specifies the initial value, x_1. The period of this generator is about 2^{31}.

This generator was used in the IMSL Library (subroutine RNUN) and in MATLAB (the RAND function) in the past. It is also sometimes known by the acronym "GGL" (I'm not sure what that stands for).

For more information see,

- Park and Miller, "Random Number Generators: Good ones are hard to find", Communications of the ACM, October 1988, Volume 31, No 10, pages 1192–1201.

gsl_rng_type ***gsl_rng_uni***

gsl_rng_type ***gsl_rng_uni32***

This is a reimplementation of the 16-bit SLATEC random number generator RUNIF. A generalization of the generator to 32 bits is provided by *`gsl_rng_uni32`*. The original source code is available from NETLIB.

gsl_rng_type ***gsl_rng_slatec***

This is the SLATEC random number generator RAND. It is ancient. The original source code is available from NETLIB.

gsl_rng_type ***gsl_rng_zuf***

This is the ZUFALL lagged Fibonacci series generator of Peterson. Its sequence is,

$$t = u_{n-273} + u_{n-607}$$
$$u_n = t - \text{floor}(t)$$

The original source code is available from NETLIB. For more information see,

- W. Petersen, "Lagged Fibonacci Random Number Generators for the NEC SX-3", International Journal of High Speed Computing (1994).

gsl_rng_type ***gsl_rng_knuthran2**

This is a second-order multiple recursive generator described by Knuth in Seminumerical Algorithms, 3rd Ed., page 108. Its sequence is,

$$x_n = (a_1 x_{n-1} + a_2 x_{n-2}) \mod m$$

with $a_1 = 271828183$, $a_2 = 314159269$, and $m = 2^{31} - 1$.

gsl_rng_type ***gsl_rng_knuthran2002**

gsl_rng_type ***gsl_rng_knuthran**

This is a second-order multiple recursive generator described by Knuth in Seminumerical Algorithms, 3rd Ed., Section 3.6. Knuth provides its C code. The updated routine `gsl_rng_knuthran2002` is from the revised 9th printing and corrects some weaknesses in the earlier version, which is implemented as `gsl_rng_knuthran`.

gsl_rng_type ***gsl_rng_borosh13**

gsl_rng_type ***gsl_rng_fishman18**

gsl_rng_type ***gsl_rng_fishman20**

gsl_rng_type ***gsl_rng_lecuyer21**

gsl_rng_type ***gsl_rng_waterman14**

These multiplicative generators are taken from Knuth's Seminumerical Algorithms, 3rd Ed., pages 106–108. Their sequence is,

$$x_{n+1} = (a x_n) \mod m$$

where the seed specifies the initial value, x_1. The parameters a and m are as follows, Borosh-Niederreiter: $a = 1812433253$, $m = 2^{32}$, Fishman18: $a = 62089911$, $m = 2^{31} - 1$, Fishman20: $a = 48271$, $m = 2^{31} - 1$, L'Ecuyer: $a = 40692$, $m = 2^{31} - 249$, Waterman: $a = 1566083941$, $m = 2^{32}$.

gsl_rng_type ***gsl_rng_fishman2x**

This is the L'Ecuyer–Fishman random number generator. It is taken from Knuth's Seminumerical Algorithms, 3rd Ed., page 108. Its sequence is,

$$z_{n+1} = (x_n - y_n) \mod m$$

with $m = 2^{31} - 1$. x_n and y_n are given by the `fishman20` and `lecuyer21` algorithms. The seed specifies the initial value, x_1.

gsl_rng_type ***gsl_rng_coveyou**

This is the Coveyou random number generator. It is taken from Knuth's Seminumerical Algorithms, 3rd Ed., Section 3.2.2. Its sequence is,

$$x_{n+1} = (x_n(x_n + 1)) \mod m$$

with $m = 2^{32}$. The seed specifies the initial value, x_1.

18.12 Performance

The following table shows the relative performance of a selection the available random number generators. The fastest simulation quality generators are `taus`, `gfsr4` and `mt19937`. The generators which offer the best mathematically-proven quality are those based on the RANLUX algorithm:

```
1754 k ints/sec,    870 k doubles/sec, taus
1613 k ints/sec,    855 k doubles/sec, gfsr4
1370 k ints/sec,    769 k doubles/sec, mt19937
 565 k ints/sec,    571 k doubles/sec, ranlxs0
 400 k ints/sec,    405 k doubles/sec, ranlxs1
 490 k ints/sec,    389 k doubles/sec, mrg
 407 k ints/sec,    297 k doubles/sec, ranlux
 243 k ints/sec,    254 k doubles/sec, ranlxd1
 251 k ints/sec,    253 k doubles/sec, ranlxs2
 238 k ints/sec,    215 k doubles/sec, cmrg
 247 k ints/sec,    198 k doubles/sec, ranlux389
 141 k ints/sec,    140 k doubles/sec, ranlxd2
```

18.13 Examples

The following program demonstrates the use of a random number generator to produce uniform random numbers in the range [0.0, 1.0),

```
#include <stdio.h>
#include <gsl/gsl_rng.h>

int
main (void)
{
  const gsl_rng_type * T;
  gsl_rng * r;

  int i, n = 10;

  gsl_rng_env_setup();

  T = gsl_rng_default;
  r = gsl_rng_alloc (T);

  for (i = 0; i < n; i++)
    {
      double u = gsl_rng_uniform (r);
      printf ("%.5f\n", u);
    }

  gsl_rng_free (r);

  return 0;
}
```

Here is the output of the program,

```
0.99974
0.16291
0.28262
0.94720
```

(continues on next page)

(continued from previous page)

```
0.23166
0.48497
0.95748
0.74431
0.54004
0.73995
```

The numbers depend on the seed used by the generator. The default seed can be changed with the *GSL_RNG_SEED* environment variable to produce a different stream of numbers. The generator itself can be changed using the environment variable *GSL_RNG_TYPE*. Here is the output of the program using a seed value of 123 and the multiple-recursive generator `mrg`:

```
$ GSL_RNG_SEED=123 GSL_RNG_TYPE=mrg ./a.out
```

```
0.33050
0.86631
0.32982
0.67620
0.53391
0.06457
0.16847
0.70229
0.04371
0.86374
```

18.14 References and Further Reading

The subject of random number generation and testing is reviewed extensively in Knuth's *Seminumerical Algorithms*.

- Donald E. Knuth, The Art of Computer Programming: Seminumerical Algorithms (Vol 2, 3rd Ed, 1997), Addison-Wesley, ISBN 0201896842.

Further information is available in the review paper written by Pierre L'Ecuyer,

- P. L'Ecuyer, "Random Number Generation", Chapter 4 of the Handbook on Simulation, Jerry Banks Ed., Wiley, 1998, 93–137.
- http://www.iro.umontreal.ca/~lecuyer/papers.html in the file `handsim.ps`.

The source code for the DIEHARD random number generator tests is also available online,

- DIEHARD source code, G. Marsaglia, http://stat.fsu.edu/pub/diehard/

A comprehensive set of random number generator tests is available from NIST,

- NIST Special Publication 800-22, "A Statistical Test Suite for the Validation of Random Number Generators and Pseudo Random Number Generators for Cryptographic Applications".
- http://csrc.nist.gov/rng/

18.15 Acknowledgements

Thanks to Makoto Matsumoto, Takuji Nishimura and Yoshiharu Kurita for making the source code to their generators (MT19937, MM&TN; TT800, MM&YK) available under the GNU General Public License. Thanks to Martin Luscher for providing notes and source code for the RANLXS and RANLXD generators.

CHAPTER

NINETEEN

QUASI-RANDOM SEQUENCES

This chapter describes functions for generating quasi-random sequences in arbitrary dimensions. A quasi-random sequence progressively covers a d-dimensional space with a set of points that are uniformly distributed. Quasi-random sequences are also known as low-discrepancy sequences. The quasi-random sequence generators use an interface that is similar to the interface for random number generators, except that seeding is not required—each generator produces a single sequence.

The functions described in this section are declared in the header file `gsl_qrng.h`.

19.1 Quasi-random number generator initialization

type **`gsl_qrng`**

This is a workspace for computing quasi-random sequences.

gsl_qrng ***`gsl_qrng_alloc`**(const *gsl_qrng_type* *T, unsigned int d)

This function returns a pointer to a newly-created instance of a quasi-random sequence generator of type *`T`* and dimension *`d`*. If there is insufficient memory to create the generator then the function returns a null pointer and the error handler is invoked with an error code of *`GSL_ENOMEM`*.

void **`gsl_qrng_free`**(*gsl_qrng* *q)

This function frees all the memory associated with the generator *`q`*.

void **`gsl_qrng_init`**(*gsl_qrng* *q)

This function reinitializes the generator *`q`* to its starting point. Note that quasi-random sequences do not use a seed and always produce the same set of values.

19.2 Sampling from a quasi-random number generator

int **`gsl_qrng_get`**(const *gsl_qrng* *q, double x[])

This function stores the next point from the sequence generator *`q`* in the array *`x`*. The space available for *`x`* must match the dimension of the generator. The point *`x`* will lie in the range $0 < x_i < 1$ for each x_i. An inline version of this function is used when `HAVE_INLINE` is defined.

19.3 Auxiliary quasi-random number generator functions

const char ***gsl_qrng_name**(const *gsl_qrng* *q)

This function returns a pointer to the name of the generator.

size_t **gsl_qrng_size**(const *gsl_qrng* *q)

void ***gsl_qrng_state**(const *gsl_qrng* *q)

These functions return a pointer to the state of generator `r` and its size. You can use this information to access the state directly. For example, the following code will write the state of a generator to a stream:

```
void * state = gsl_qrng_state (q);
size_t n = gsl_qrng_size (q);
fwrite (state, n, 1, stream);
```

19.4 Saving and restoring quasi-random number generator state

int **gsl_qrng_memcpy**(*gsl_qrng* *dest, const *gsl_qrng* *src)

This function copies the quasi-random sequence generator `src` into the pre-existing generator `dest`, making `dest` into an exact copy of `src`. The two generators must be of the same type.

gsl_qrng ***gsl_qrng_clone**(const *gsl_qrng* *q)

This function returns a pointer to a newly created generator which is an exact copy of the generator `q`.

19.5 Quasi-random number generator algorithms

The following quasi-random sequence algorithms are available,

type **gsl_qrng_type**

gsl_qrng_type ***gsl_qrng_niederreiter_2**

This generator uses the algorithm described in Bratley, Fox, Niederreiter, ACM Trans. Model. Comp. Sim. 2, 195 (1992). It is valid up to 12 dimensions.

gsl_qrng_type ***gsl_qrng_sobol**

This generator uses the Sobol sequence described in Antonov, Saleev, USSR Comput. Maths. Math. Phys. 19, 252 (1980). It is valid up to 40 dimensions.

gsl_qrng_type ***gsl_qrng_halton**

gsl_qrng_type ***gsl_qrng_reversehalton**

These generators use the Halton and reverse Halton sequences described in J.H. Halton, Numerische Mathematik, 2, 84-90 (1960) and B. Vandewoestyne and R. Cools Computational and Applied Mathematics, 189, 1&2, 341-361 (2006). They are valid up to 1229 dimensions.

19.6 Examples

The following program prints the first 1024 points of the 2-dimensional Sobol sequence.

```
#include <stdio.h>
#include <gsl/gsl_qrng.h>

int
main (void)
{
  int i;
  gsl_qrng * q = gsl_qrng_alloc (gsl_qrng_sobol, 2);

  for (i = 0; i < 1024; i++)
    {
      double v[2];
      gsl_qrng_get (q, v);
      printf ("%.5f %.5f\n", v[0], v[1]);
    }

  gsl_qrng_free (q);
  return 0;
}
```

Here is the output from the program:

```
$ ./a.out
0.50000 0.50000
0.75000 0.25000
0.25000 0.75000
0.37500 0.37500
0.87500 0.87500
0.62500 0.12500
0.12500 0.62500
....
```

It can be seen that successive points progressively fill-in the spaces between previous points.

Fig. 19.1 shows the distribution in the x-y plane of the first 1024 points from the Sobol sequence,

19.7 References

The implementations of the quasi-random sequence routines are based on the algorithms described in the following paper,

- P. Bratley and B.L. Fox and H. Niederreiter, "Algorithm 738: Programs to Generate Niederreiter's Low-discrepancy Sequences", ACM Transactions on Mathematical Software, Vol.: 20, No.: 4, December, 1994, p.: 494–495.

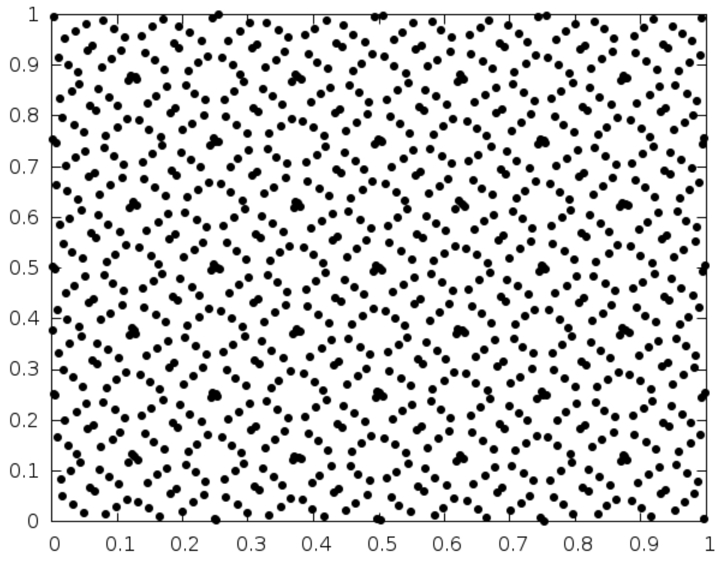


Fig. 19.1: Distribution of the first 1024 points from the quasi-random Sobol sequence

CHAPTER

TWENTY

RANDOM NUMBER DISTRIBUTIONS

This chapter describes functions for generating random variates and computing their probability distributions. Samples from the distributions described in this chapter can be obtained using any of the random number generators in the library as an underlying source of randomness.

In the simplest cases a non-uniform distribution can be obtained analytically from the uniform distribution of a random number generator by applying an appropriate transformation. This method uses one call to the random number generator. More complicated distributions are created by the *acceptance-rejection* method, which compares the desired distribution against a distribution which is similar and known analytically. This usually requires several samples from the generator.

The library also provides cumulative distribution functions and inverse cumulative distribution functions, sometimes referred to as quantile functions. The cumulative distribution functions and their inverses are computed separately for the upper and lower tails of the distribution, allowing full accuracy to be retained for small results.

The functions for random variates and probability density functions described in this section are declared in `gsl_randist.h`. The corresponding cumulative distribution functions are declared in `gsl_cdf.h`.

Note that the discrete random variate functions always return a value of type `unsigned int`, and on most platforms this has a maximum value of

$$2^{32} - 1 \approx 4.29 \times 10^9$$

They should only be called with a safe range of parameters (where there is a negligible probability of a variate exceeding this limit) to prevent incorrect results due to overflow.

20.1 Introduction

Continuous random number distributions are defined by a probability density function, $p(x)$, such that the probability of x occurring in the infinitesimal range x to $x + dx$ is $p(x)dx$.

The cumulative distribution function for the lower tail $P(x)$ is defined by the integral,

$$P(x) = \int_{-\infty}^{x} dx' p(x')$$

and gives the probability of a variate taking a value less than x.

The cumulative distribution function for the upper tail $Q(x)$ is defined by the integral,

$$Q(x) = \int_{x}^{+\infty} dx' p(x')$$

and gives the probability of a variate taking a value greater than x.

The upper and lower cumulative distribution functions are related by $P(x) + Q(x) = 1$ and satisfy $0 \leq P(x) \leq 1$, $0 \leq Q(x) \leq 1$.

The inverse cumulative distributions, $x = P^{-1}(P)$ and $x = Q^{-1}(Q)$ give the values of x which correspond to a specific value of P or Q. They can be used to find confidence limits from probability values.

For discrete distributions the probability of sampling the integer value k is given by $p(k)$, where $\sum_k p(k) = 1$. The cumulative distribution for the lower tail $P(k)$ of a discrete distribution is defined as,

$$P(k) = \sum_{i \leq k} p(i)$$

where the sum is over the allowed range of the distribution less than or equal to k.

The cumulative distribution for the upper tail of a discrete distribution $Q(k)$ is defined as

$$Q(k) = \sum_{i > k} p(i)$$

giving the sum of probabilities for all values greater than k. These two definitions satisfy the identity $P(k)+Q(k) = 1$.

If the range of the distribution is 1 to n inclusive then $P(n) = 1$, $Q(n) = 0$ while $P(1) = p(1)$, $Q(1) = 1 - p(1)$.

20.2 The Gaussian Distribution

double **gsl_ran_gaussian**(const *gsl_rng* *r, double sigma)

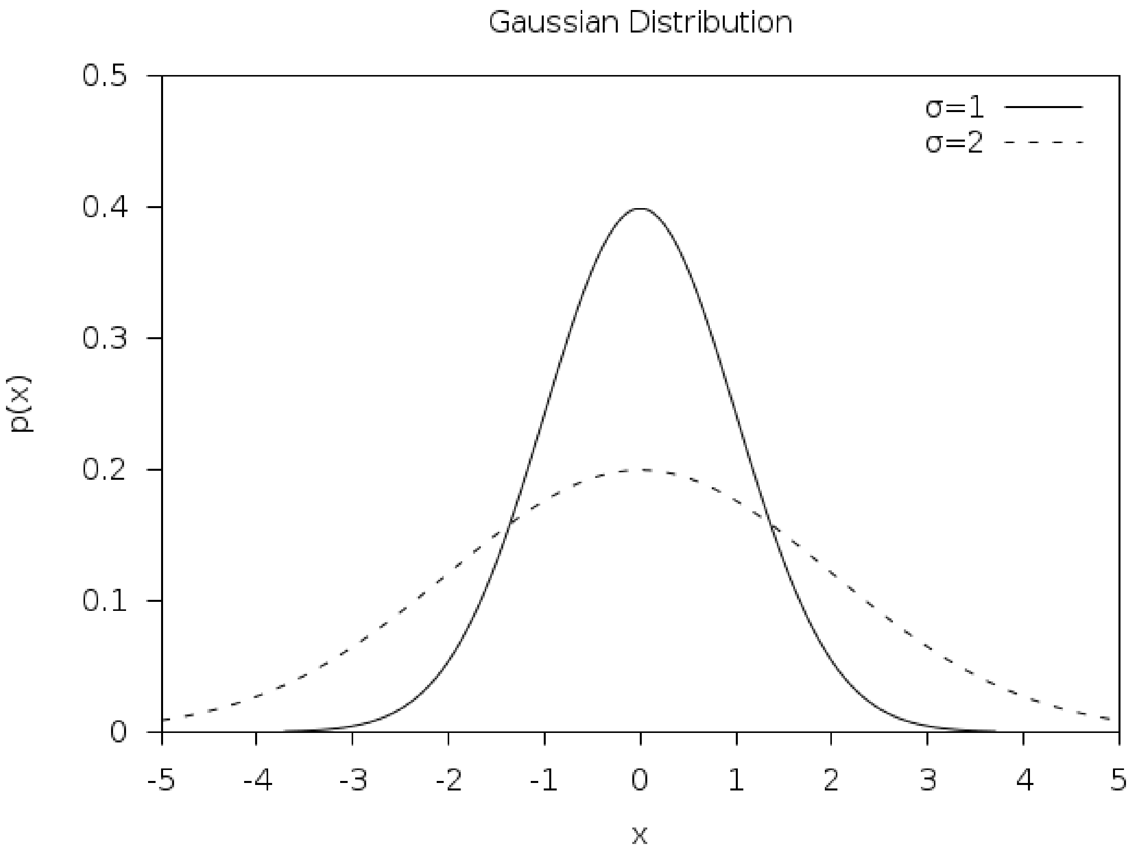
This function returns a Gaussian random variate, with mean zero and standard deviation `sigma`. The probability distribution for Gaussian random variates is,

$$p(x)dx = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-x^2/2\sigma^2)dx$$

for x in the range $-\infty$ to $+\infty$. Use the transformation $z = \mu + x$ on the numbers returned by `gsl_ran_gaussian()` to obtain a Gaussian distribution with mean μ. This function uses the Box-Muller algorithm which requires two calls to the random number generator `r`.

double **gsl_ran_gaussian_pdf**(double x, double sigma)

This function computes the probability density $p(x)$ at `x` for a Gaussian distribution with standard deviation `sigma`, using the formula given above.



double **gsl_ran_gaussian_ziggurat**(const *gsl_rng* *r, double sigma)

double **gsl_ran_gaussian_ratio_method**(const *gsl_rng* *r, double sigma)

This function computes a Gaussian random variate using the alternative Marsaglia-Tsang ziggurat and Kinderman-Monahan-Leva ratio methods. The Ziggurat algorithm is the fastest available algorithm in most cases.

double **gsl_ran_ugaussian**(const *gsl_rng* *r) double **gsl_ran_ugaussian_pdf**(double x)

double **gsl_ran_ugaussian_ratio_method**(const *gsl_rng* *r)

These functions compute results for the unit Gaussian distribution. They are equivalent to the functions above with a standard deviation of one, `sigma` = 1.

double **gsl_cdf_gaussian_P**(double x, double sigma)

double **gsl_cdf_gaussian_Q**(double x, double sigma)

double **gsl_cdf_gaussian_Pinv**(double P, double sigma)

double **gsl_cdf_gaussian_Qinv**(double Q, double sigma)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the Gaussian distribution with standard deviation *sigma*.

double **gsl_cdf_ugaussian_P**(double x)

double **gsl_cdf_ugaussian_Q**(double x)

double **gsl_cdf_ugaussian_Pinv**(double P)

double **gsl_cdf_ugaussian_Qinv**(double Q)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the unit Gaussian distribution.

20.3 The Gaussian Tail Distribution

double **gsl_ran_gaussian_tail**(const *gsl_rng* *r, double a, double sigma)

This function provides random variates from the upper tail of a Gaussian distribution with standard deviation `sigma`. The values returned are larger than the lower limit `a`, which must be positive. The method is based on Marsaglia's famous rectangle-wedge-tail algorithm (Ann. Math. Stat. 32, 894–899 (1961)), with this aspect explained in Knuth, v2, 3rd ed, p139,586 (exercise 11).

The probability distribution for Gaussian tail random variates is,

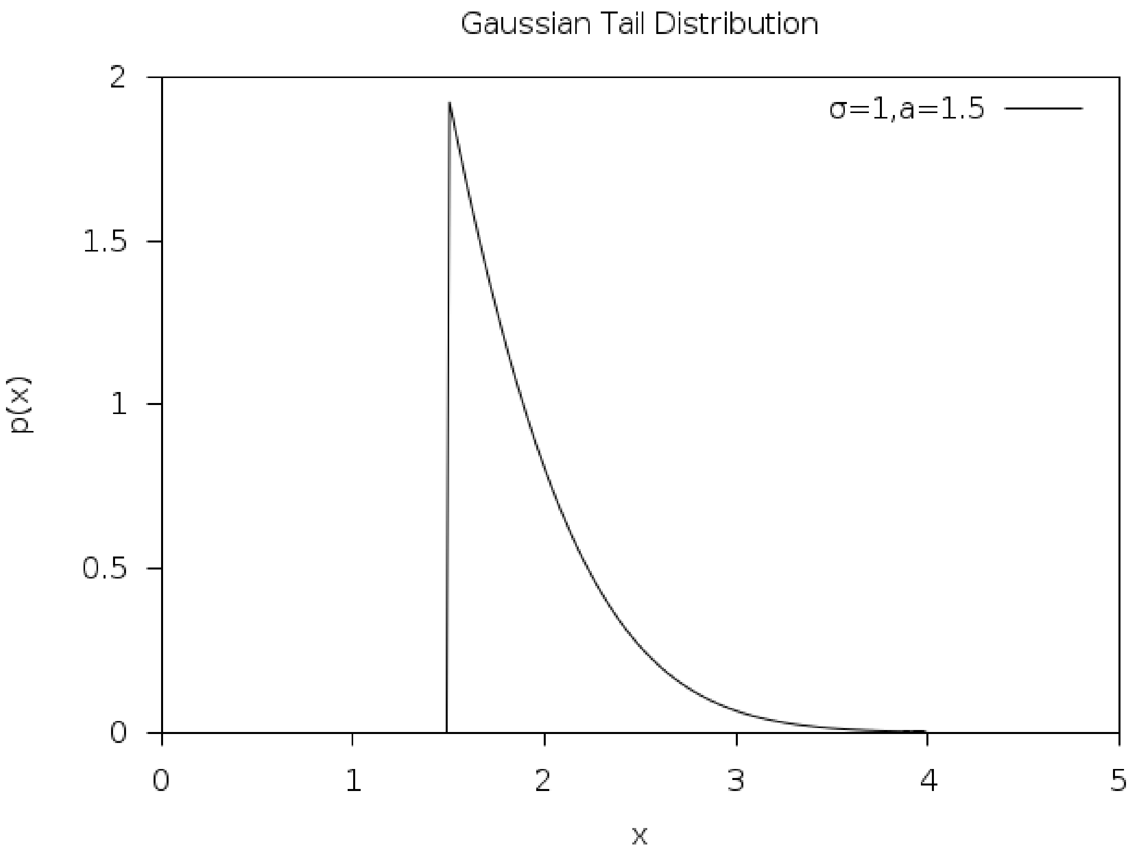
$$p(x)dx = \frac{1}{N(a;\sigma)\sqrt{2\pi\sigma^2}} \exp(-x^2/2\sigma^2)dx$$

for $x > a$ where $N(a;\sigma)$ is the normalization constant,

$$N(a;\sigma) = \frac{1}{2}\mathrm{erfc}\left(\frac{a}{\sqrt{2\sigma^2}}\right).$$

double **gsl_ran_gaussian_tail_pdf**(double x, double a, double sigma)

This function computes the probability density $p(x)$ at `x` for a Gaussian tail distribution with standard deviation `sigma` and lower limit `a`, using the formula given above.



double **gsl_ran_ugaussian_tail**(const *gsl_rng* *r, double a)

double **gsl_ran_ugaussian_tail_pdf**(double x, double a)

These functions compute results for the tail of a unit Gaussian distribution. They are equivalent to the functions above with a standard deviation of one, `sigma` = 1.

20.4 The Bivariate Gaussian Distribution

void **gsl_ran_bivariate_gaussian**(const *gsl_rng* *r, double sigma_x, double sigma_y, double rho, double *x, double *y)

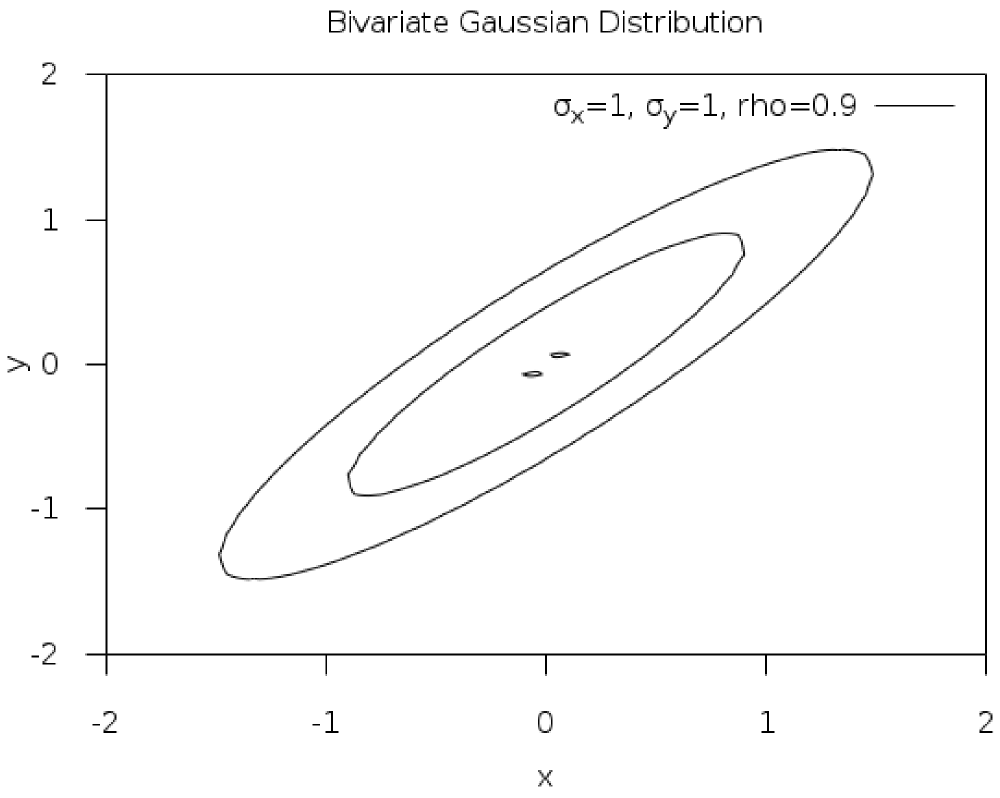
This function generates a pair of correlated Gaussian variates, with mean zero, correlation coefficient `rho` and standard deviations `sigma_x` and `sigma_y` in the x and y directions. The probability distribution for bivariate Gaussian random variates is,

$$p(x,y)dxdy = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}} \exp\left(-\frac{(x^2/\sigma_x^2 + y^2/\sigma_y^2 - 2\rho xy/(\sigma_x\sigma_y))}{2(1-\rho^2)}\right) dxdy$$

for x, y in the range $-\infty$ to $+\infty$. The correlation coefficient `rho` should lie between 1 and -1.

double **gsl_ran_bivariate_gaussian_pdf**(double x, double y, double sigma_x, double sigma_y, double rho)

This function computes the probability density $p(x, y)$ at (`x`, `y`) for a bivariate Gaussian distribution with standard deviations `sigma_x`, `sigma_y` and correlation coefficient `rho`, using the formula given above.



20.5 The Multivariate Gaussian Distribution

int **gsl_ran_multivariate_gaussian**(const *gsl_rng* *r, const *gsl_vector* *mu, const *gsl_matrix* *L, *gsl_vector* *result)

This function generates a random vector satisfying the k-dimensional multivariate Gaussian distribution with mean μ and variance-covariance matrix Σ. On input, the k-vector μ is given in `mu`, and the Cholesky factor of the k-by-k matrix $\Sigma = LL^T$ is given in the lower triangle of `L`, as output from `gsl_linalg_cholesky_decomp()`. The random vector is stored in `result` on output. The probability distribution for multivariate Gaussian random variates is

$$p(x_1,\dots,x_k)dx_1\dots dx_k = \frac{1}{\sqrt{(2\pi)^k|\Sigma|}}\exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)dx_1\dots dx_k$$

int **gsl_ran_multivariate_gaussian_pdf**(const *gsl_vector* *x, const *gsl_vector* *mu, const *gsl_matrix* *L, double *result, *gsl_vector* *work)

int **gsl_ran_multivariate_gaussian_log_pdf**(const *gsl_vector* *x, const *gsl_vector* *mu, const *gsl_matrix* *L, double *result, *gsl_vector* *work)

These functions compute $p(x)$ or $\log p(x)$ at the point `x`, using mean vector `mu` and variance-covariance matrix specified by its Cholesky factor `L` using the formula above. Additional workspace of length k is required in `work`.

int **gsl_ran_multivariate_gaussian_mean**(const *gsl_matrix* *X, *gsl_vector* *mu_hat)

Given a set of n samples X_j from a k-dimensional multivariate Gaussian distribution, this function computes the maximum likelihood estimate of the mean of the distribution, given by

$$\hat{\mu} = \frac{1}{n}\sum_{j=1}^{n} X_j$$

The samples $X_1, X_2, \dots, X_n$ are given in the n-by-k matrix `X`, and the maximum likelihood estimate of the mean is stored in `mu_hat` on output.

int **gsl_ran_multivariate_gaussian_vcov**(const *gsl_matrix* *X, *gsl_matrix* *sigma_hat)

Given a set of n samples X_j from a k-dimensional multivariate Gaussian distribution, this function computes the maximum likelihood estimate of the variance-covariance matrix of the distribution, given by

$$\hat{\Sigma} = \frac{1}{n}\sum_{j=1}^{n}\left(X_j - \hat{\mu}\right)\left(X_j - \hat{\mu}\right)^T$$

The samples $X_1, X_2, \dots, X_n$ are given in the n-by-k matrix `X` and the maximum likelihood estimate of the variance-covariance matrix is stored in `sigma_hat` on output.

20.6 The Exponential Distribution

double **gsl_ran_exponential**(const *gsl_rng* *r, double mu)

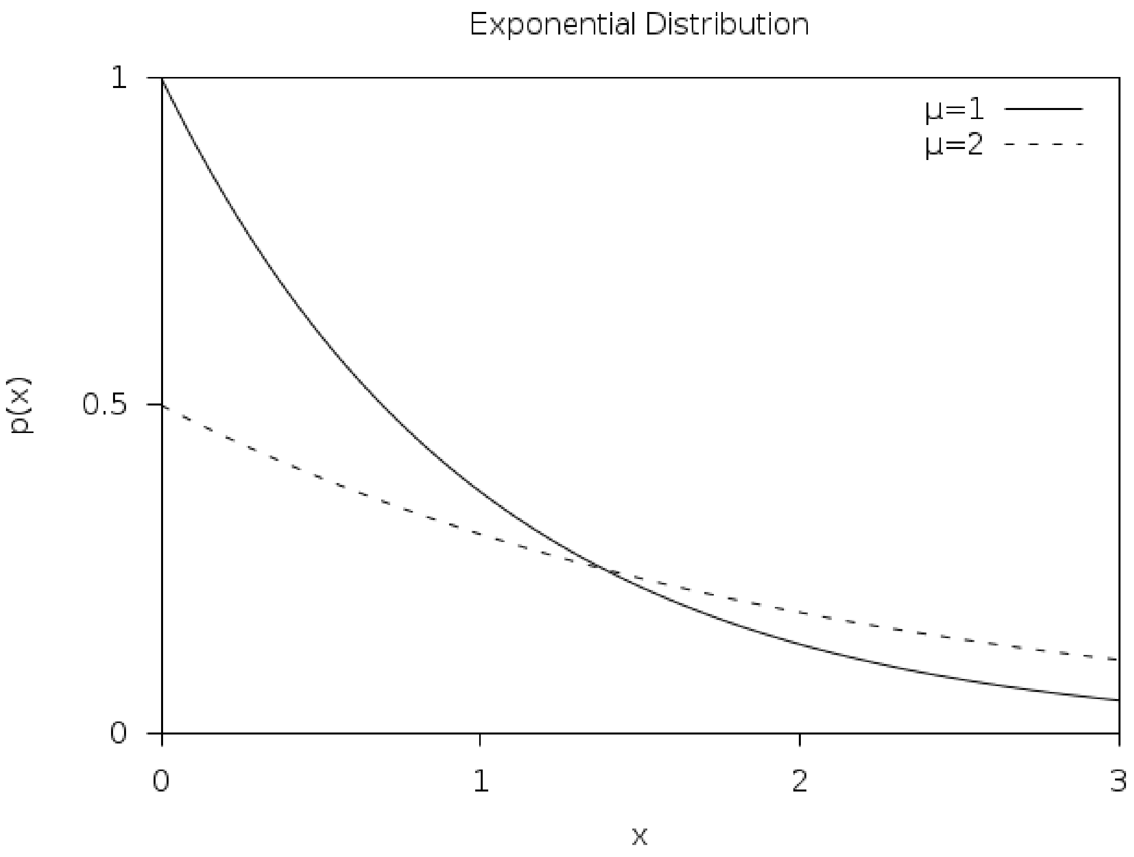
This function returns a random variate from the exponential distribution with mean *mu*. The distribution is,

$$p(x)dx = \frac{1}{\mu}\exp(-x/\mu)dx$$

for $x \geq 0$.

double **gsl_ran_exponential_pdf**(double x, double mu)

This function computes the probability density $p(x)$ at *x* for an exponential distribution with mean *mu*, using the formula given above.



double **gsl_cdf_exponential_P**(double x, double mu)

double **gsl_cdf_exponential_Q**(double x, double mu)

double **gsl_cdf_exponential_Pinv**(double P, double mu)

double **gsl_cdf_exponential_Qinv**(double Q, double mu)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the exponential distribution with mean *mu*.

20.7 The Laplace Distribution

double **gsl_ran_laplace**(const *gsl_rng* *r, double a)

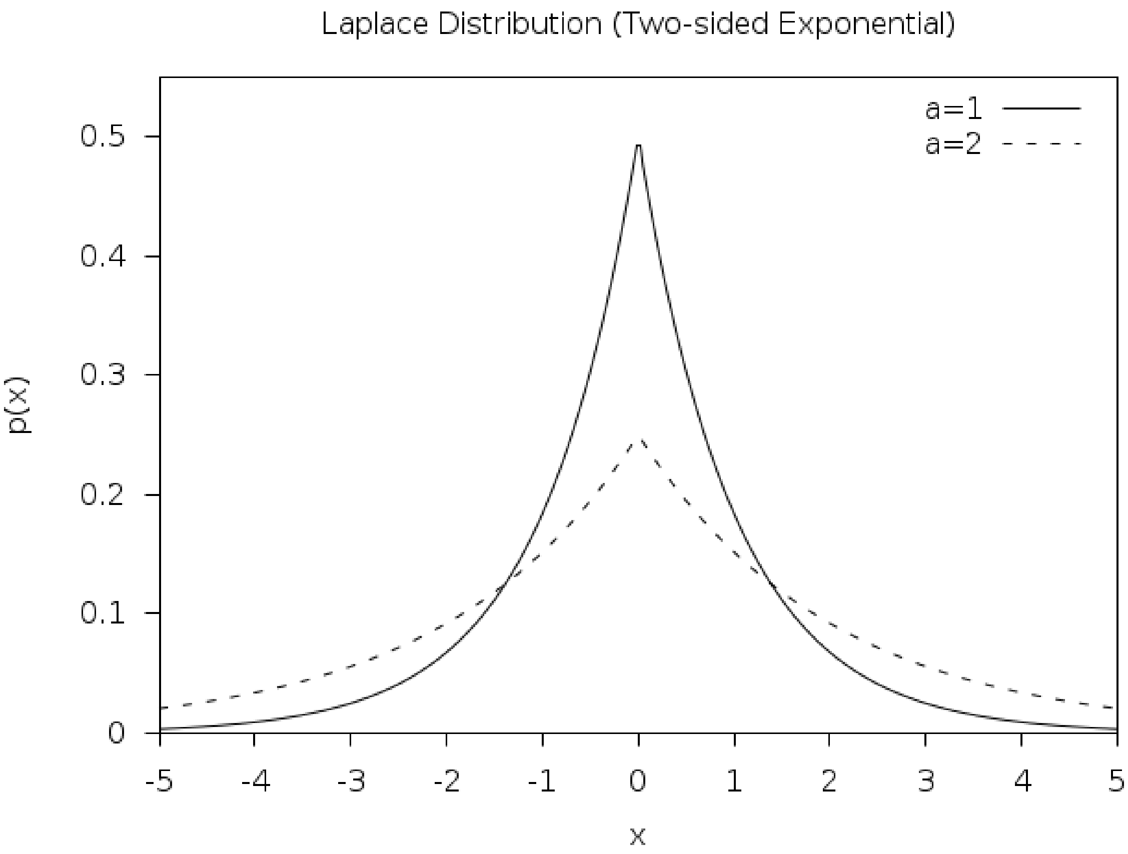
This function returns a random variate from the Laplace distribution with width a. The distribution is,

$$p(x)dx = \frac{1}{2a}\exp(-|x/a|)dx$$

for $-\infty < x < \infty$.

double **gsl_ran_laplace_pdf**(double x, double a)

This function computes the probability density $p(x)$ at x for a Laplace distribution with width a, using the formula given above.



double **gsl_cdf_laplace_P**(double x, double a)

double **gsl_cdf_laplace_Q**(double x, double a)

double **gsl_cdf_laplace_Pinv**(double P, double a)

double **gsl_cdf_laplace_Qinv**(double Q, double a)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the Laplace distribution with width a.

20.8 The Exponential Power Distribution

double **gsl_ran_exppow**(const *gsl_rng* *r, double a, double b)

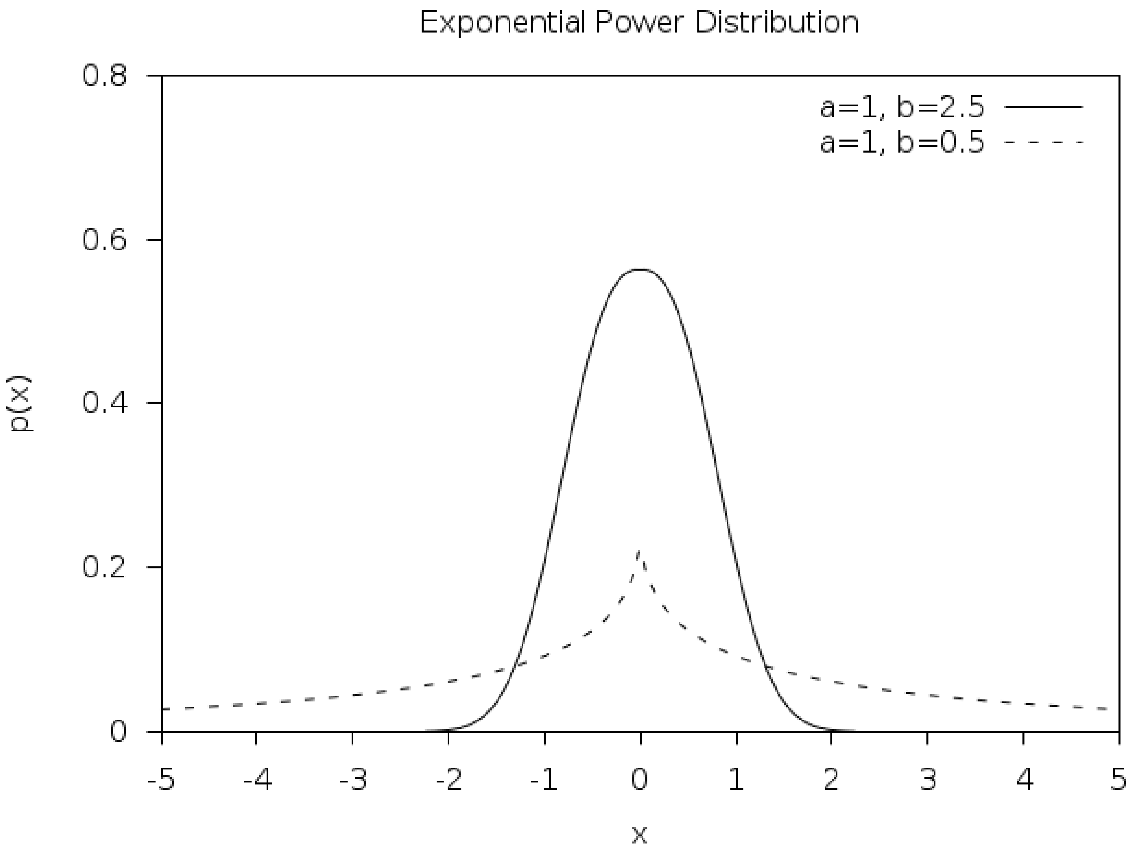
This function returns a random variate from the exponential power distribution with scale parameter *a* and exponent *b*. The distribution is,

$$p(x)dx = \frac{1}{2a\Gamma(1+1/b)} \exp(-|x/a|^b)dx$$

for $x \geq 0$. For $b = 1$ this reduces to the Laplace distribution. For $b = 2$ it has the same form as a Gaussian distribution, but with $a = \sqrt{2}\sigma$.

double **gsl_ran_exppow_pdf**(double x, double a, double b)

This function computes the probability density $p(x)$ at *x* for an exponential power distribution with scale parameter *a* and exponent *b*, using the formula given above.



double **gsl_cdf_exppow_P**(double x, double a, double b)

double **gsl_cdf_exppow_Q**(double x, double a, double b)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ for the exponential power distribution with parameters *a* and *b*.

20.9 The Cauchy Distribution

double **gsl_ran_cauchy**(const *gsl_rng* *r, double a)

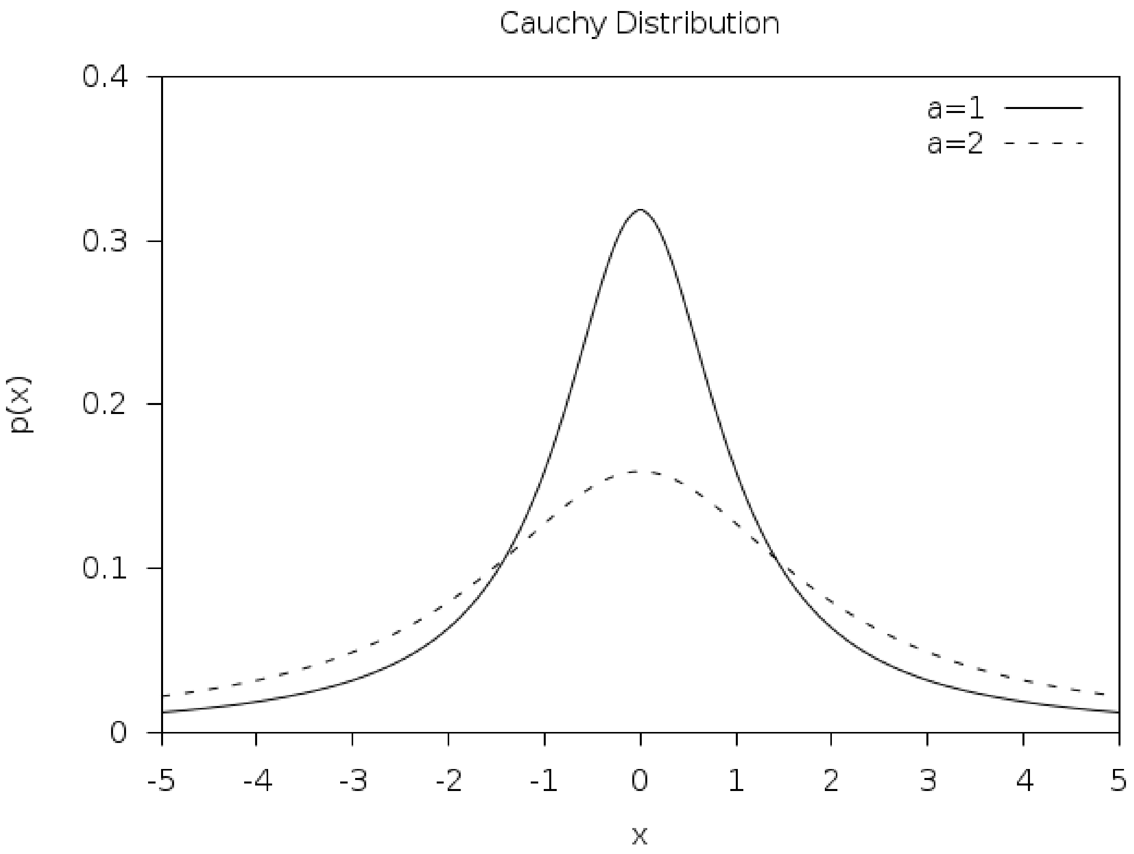
This function returns a random variate from the Cauchy distribution with scale parameter a. The probability distribution for Cauchy random variates is,

$$p(x)dx = \frac{1}{a\pi(1+(x/a)^2)}dx$$

for x in the range $-\infty$ to $+\infty$. The Cauchy distribution is also known as the Lorentz distribution.

double **gsl_ran_cauchy_pdf**(double x, double a)

This function computes the probability density $p(x)$ at x for a Cauchy distribution with scale parameter a, using the formula given above.



double **gsl_cdf_cauchy_P**(double x, double a)

double **gsl_cdf_cauchy_Q**(double x, double a)

double **gsl_cdf_cauchy_Pinv**(double P, double a)

double **gsl_cdf_cauchy_Qinv**(double Q, double a)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the Cauchy distribution with scale parameter a.

20.10 The Rayleigh Distribution

double **gsl_ran_rayleigh**(const *gsl_rng* *r, double sigma)

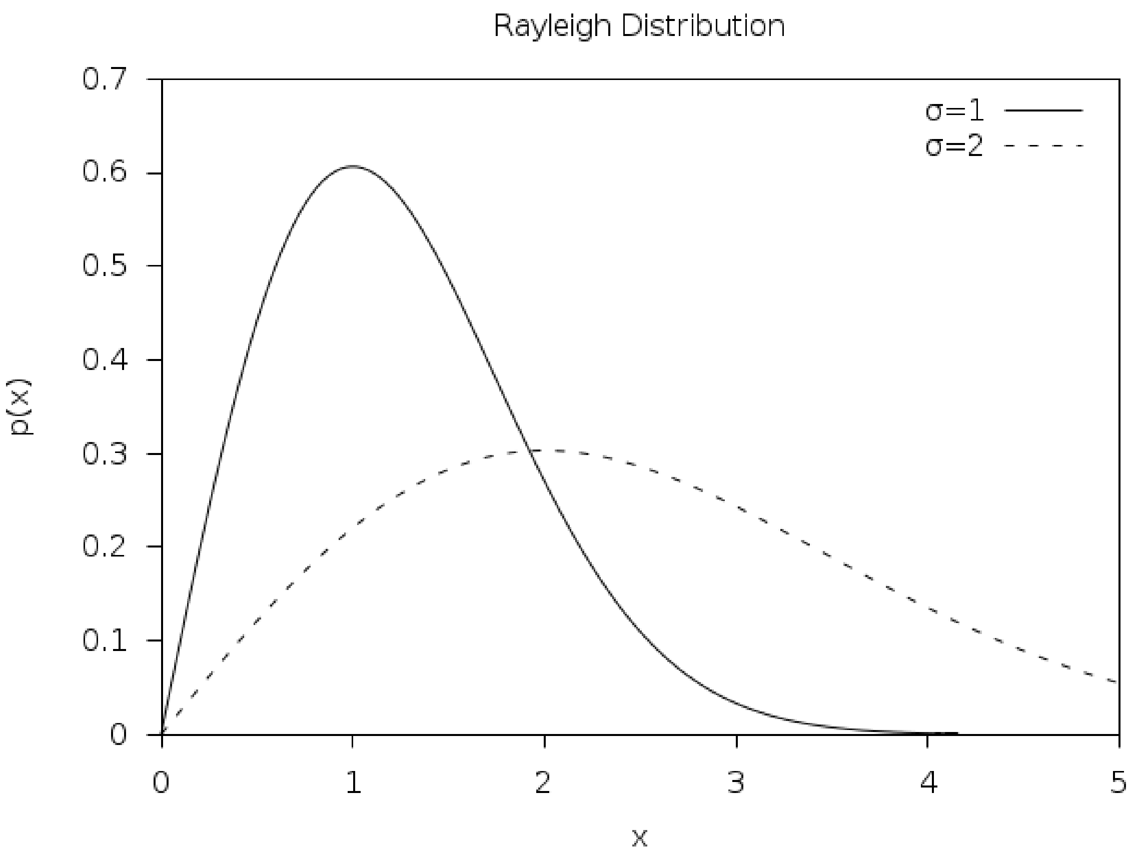
This function returns a random variate from the Rayleigh distribution with scale parameter *sigma*. The distribution is,

$$p(x)dx = \frac{x}{\sigma^2} \exp(-x^2/(2\sigma^2))dx$$

for $x > 0$.

double **gsl_ran_rayleigh_pdf**(double x, double sigma)

This function computes the probability density $p(x)$ at *x* for a Rayleigh distribution with scale parameter *sigma*, using the formula given above.



double **gsl_cdf_rayleigh_P**(double x, double sigma)

double **gsl_cdf_rayleigh_Q**(double x, double sigma)

double **gsl_cdf_rayleigh_Pinv**(double P, double sigma)

double **gsl_cdf_rayleigh_Qinv**(double Q, double sigma)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the Rayleigh distribution with scale parameter *sigma*.

20.11 The Rayleigh Tail Distribution

double **gsl_ran_rayleigh_tail**(const *gsl_rng* *r, double a, double sigma)

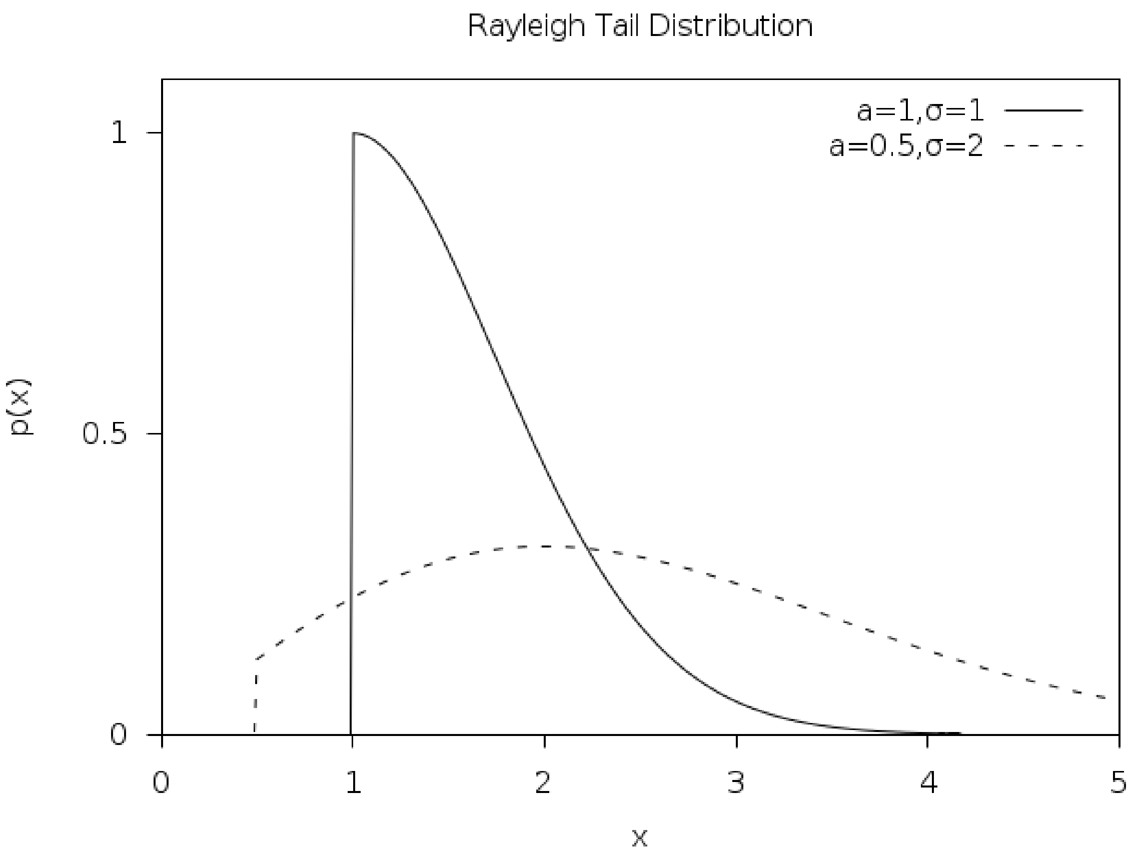
This function returns a random variate from the tail of the Rayleigh distribution with scale parameter `sigma` and a lower limit of `a`. The distribution is,

$$p(x)dx = \frac{x}{\sigma^2} \exp((a^2 - x^2)/(2\sigma^2))dx$$

for $x > a$.

double **gsl_ran_rayleigh_tail_pdf**(double x, double a, double sigma)

This function computes the probability density $p(x)$ at `x` for a Rayleigh tail distribution with scale parameter `sigma` and lower limit `a`, using the formula given above.



20.12 The Landau Distribution

double **gsl_ran_landau**(const *gsl_rng* *r)

This function returns a random variate from the Landau distribution. The probability distribution for Landau random variates is defined analytically by the complex integral,

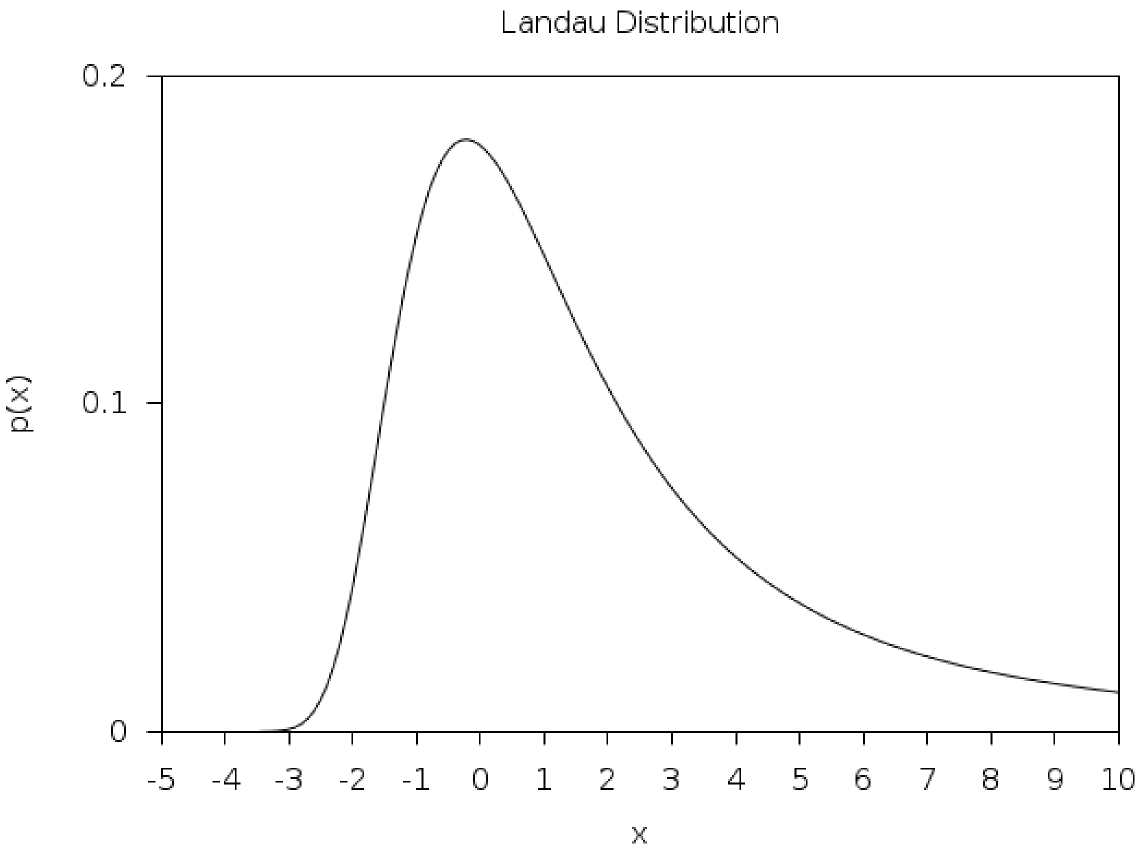
$$p(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \, \exp(s\log(s) + xs)$$

For numerical purposes it is more convenient to use the following equivalent form of the integral,

$$p(x) = (1/\pi) \int_0^\infty dt \exp(-t\log(t) - xt)\sin(\pi t).$$

double **gsl_ran_landau_pdf**(double x)

This function computes the probability density $p(x)$ at *x* for the Landau distribution using an approximation to the formula given above.



20.13 The Levy alpha-Stable Distributions

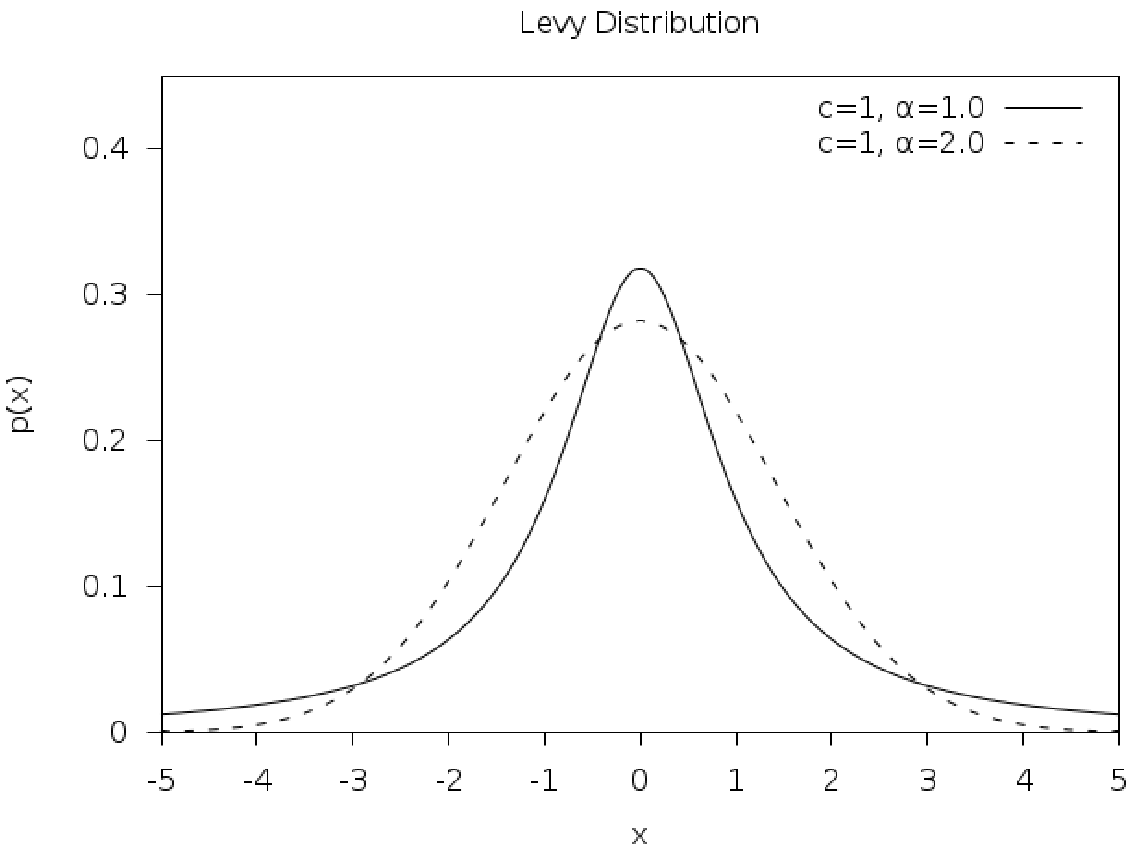
double **gsl_ran_levy**(const *gsl_rng* *r, double c, double alpha)

This function returns a random variate from the Levy symmetric stable distribution with scale `c` and exponent `alpha`. The symmetric stable probability distribution is defined by a Fourier transform,

$$p(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \exp(-itx - |ct|^{\alpha})$$

There is no explicit solution for the form of $p(x)$ and the library does not define a corresponding `pdf` function. For $\alpha = 1$ the distribution reduces to the Cauchy distribution. For $\alpha = 2$ it is a Gaussian distribution with $\sigma = \sqrt{2}c$. For $\alpha < 1$ the tails of the distribution become extremely wide.

The algorithm only works for $0 < \alpha \leq 2$.



20.14 The Levy skew alpha-Stable Distribution

double **gsl_ran_levy_skew**(const *gsl_rng* *r, double c, double alpha, double beta)

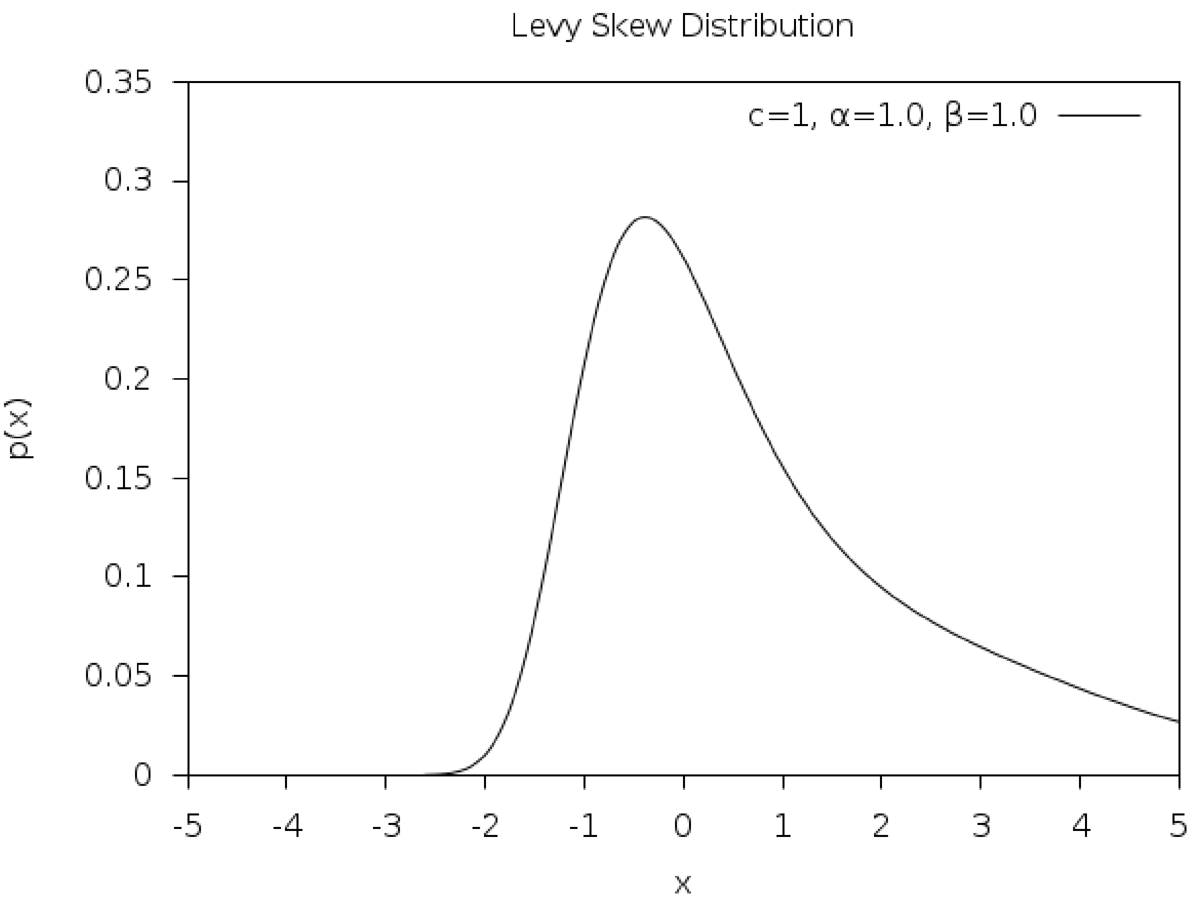
This function returns a random variate from the Levy skew stable distribution with scale `c`, exponent `alpha` and skewness parameter `beta`. The skewness parameter must lie in the range $[-1, 1]$. The Levy skew stable probability distribution is defined by a Fourier transform,

$$p(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \exp(-itx - |ct|^\alpha (1 - i\beta \operatorname{sgn}(t) \tan(\pi\alpha/2)))$$

When $\alpha = 1$ the term $\tan(\pi\alpha/2)$ is replaced by $-(2/\pi)\log|t|$. There is no explicit solution for the form of $p(x)$ and the library does not define a corresponding `pdf` function. For $\alpha = 2$ the distribution reduces to a Gaussian distribution with $\sigma = \sqrt{2}c$ and the skewness parameter has no effect. For $\alpha < 1$ the tails of the distribution become extremely wide. The symmetric distribution corresponds to $\beta = 0$.

The algorithm only works for $0 < \alpha \le 2$.

The Levy alpha-stable distributions have the property that if N alpha-stable variates are drawn from the distribution $p(c, \alpha, \beta)$ then the sum $Y = X_1 + X_2 + \cdots + X_N$ will also be distributed as an alpha-stable variate, $p(N^{1/\alpha}c, \alpha, \beta)$.



20.15 The Gamma Distribution

double **gsl_ran_gamma**(const *gsl_rng* *r, double a, double b)

This function returns a random variate from the gamma distribution. The distribution function is,

$$p(x)dx = \frac{1}{\Gamma(a)b^a} x^{a-1} e^{-x/b} dx$$

for $x > 0$.

The gamma distribution with an integer parameter *a* is known as the Erlang distribution.

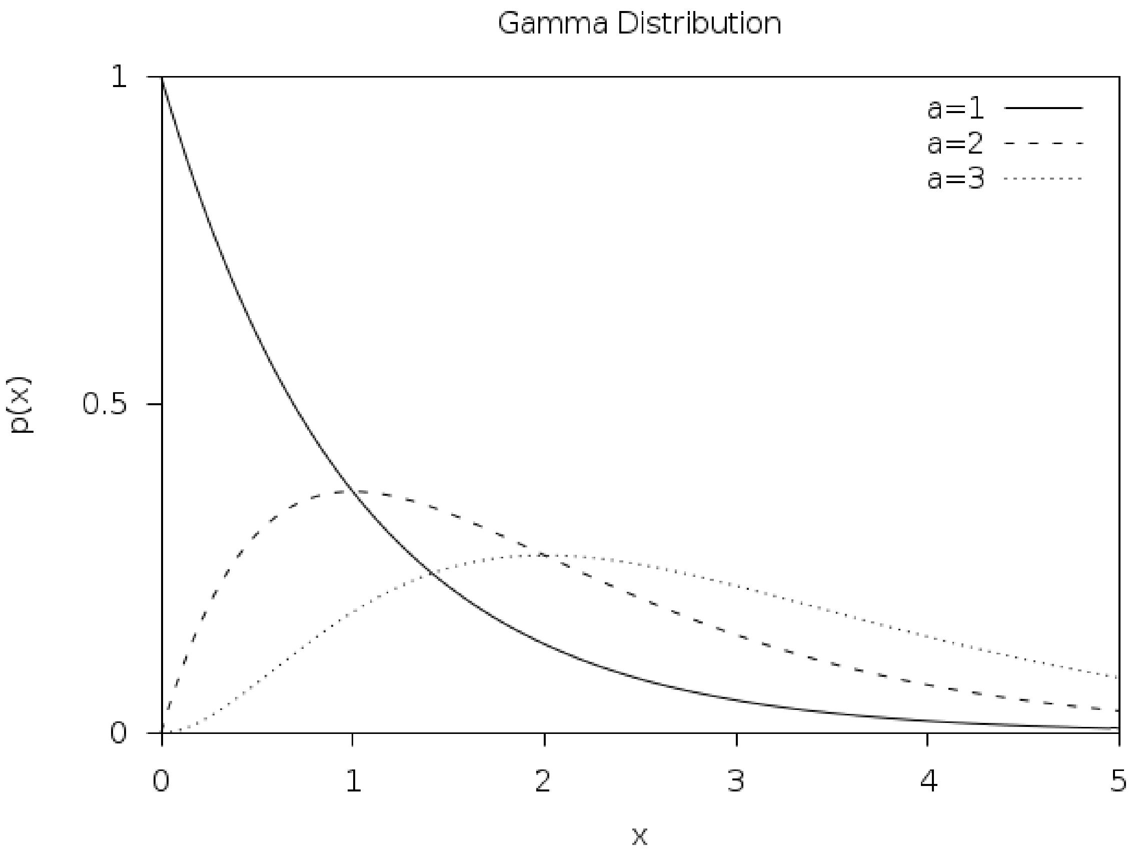
The variates are computed using the Marsaglia-Tsang fast gamma method. This function for this method was previously called `gsl_ran_gamma_mt()` and can still be accessed using this name.

double **gsl_ran_gamma_knuth**(const *gsl_rng* *r, double a, double b)

This function returns a gamma variate using the algorithms from Knuth (vol 2).

double **gsl_ran_gamma_pdf**(double x, double a, double b)

This function computes the probability density $p(x)$ at *x* for a gamma distribution with parameters *a* and *b*, using the formula given above.



double **gsl_cdf_gamma_P**(double x, double a, double b)

double **gsl_cdf_gamma_Q**(double x, double a, double b)

double **gsl_cdf_gamma_Pinv**(double P, double a, double b) double **`gsl_cdf_gamma_Qinv`**(double Q, double a, double b)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the gamma distribution with parameters *a* and *b*.

20.16 The Flat (Uniform) Distribution

double **gsl_ran_flat**(const *gsl_rng* *r, double a, double b)

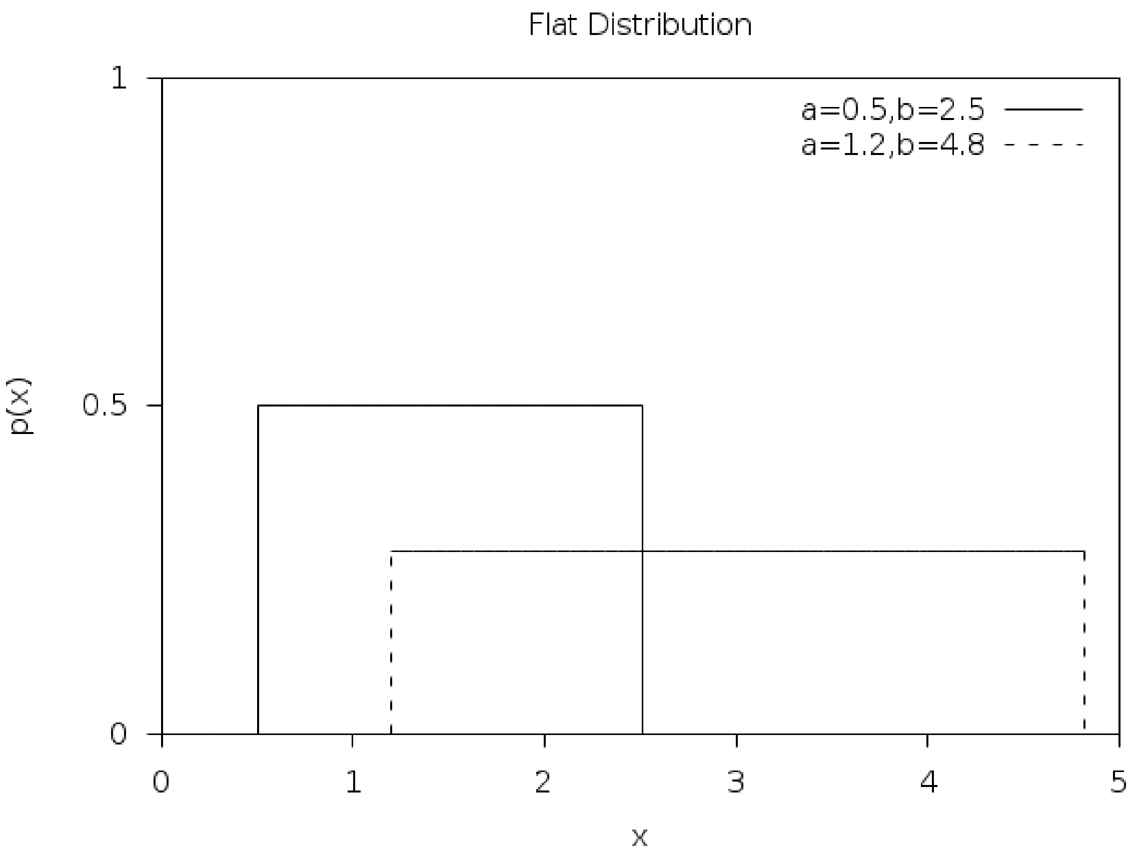
This function returns a random variate from the flat (uniform) distribution from *a* to *b*. The distribution is,

$$p(x)dx = \frac{1}{(b-a)}dx$$

if $a \leq x < b$ and 0 otherwise.

double **gsl_ran_flat_pdf**(double x, double a, double b)

This function computes the probability density $p(x)$ at *x* for a uniform distribution from *a* to *b*, using the formula given above.



double **gsl_cdf_flat_P**(double x, double a, double b)

double **gsl_cdf_flat_Q**(double x, double a, double b)

double **gsl_cdf_flat_Pinv**(double P, double a, double b)

double **gsl_cdf_flat_Qinv**(double Q, double a, double b)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for a uniform distribution from *a* to *b*.

20.17 The Lognormal Distribution

double **gsl_ran_lognormal**(const *gsl_rng* *r, double zeta, double sigma)

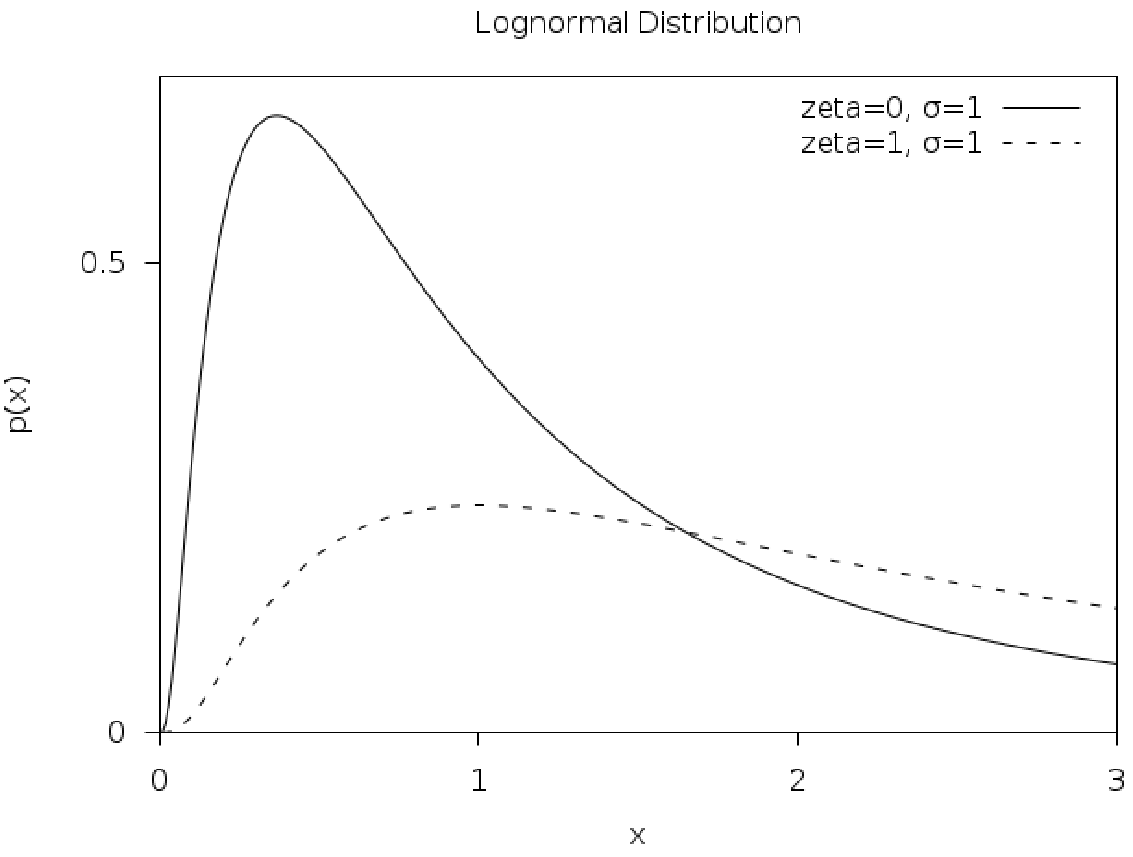
This function returns a random variate from the lognormal distribution. The distribution function is,

$$p(x)dx = \frac{1}{x\sqrt{2\pi\sigma^2}} \exp(-(\ln(x) - \zeta)^2/2\sigma^2)dx$$

for $x > 0$.

double **gsl_ran_lognormal_pdf**(double x, double zeta, double sigma)

This function computes the probability density $p(x)$ at `x` for a lognormal distribution with parameters `zeta` and `sigma`, using the formula given above.



double **gsl_cdf_lognormal_P**(double x, double zeta, double sigma)

double **gsl_cdf_lognormal_Q**(double x, double zeta, double sigma)

double **gsl_cdf_lognormal_Pinv**(double P, double zeta, double sigma)

double **gsl_cdf_lognormal_Qinv**(double Q, double zeta, double sigma)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the lognormal distribution with parameters `zeta` and `sigma`.

20.18 The Chi-squared Distribution

The chi-squared distribution arises in statistics. If Y_i are n independent Gaussian random variates with unit variance then the sum-of-squares,

$$X_i = \sum_i Y_i^2$$

has a chi-squared distribution with n degrees of freedom.

double **gsl_ran_chisq**(const *gsl_rng* *r, double nu)

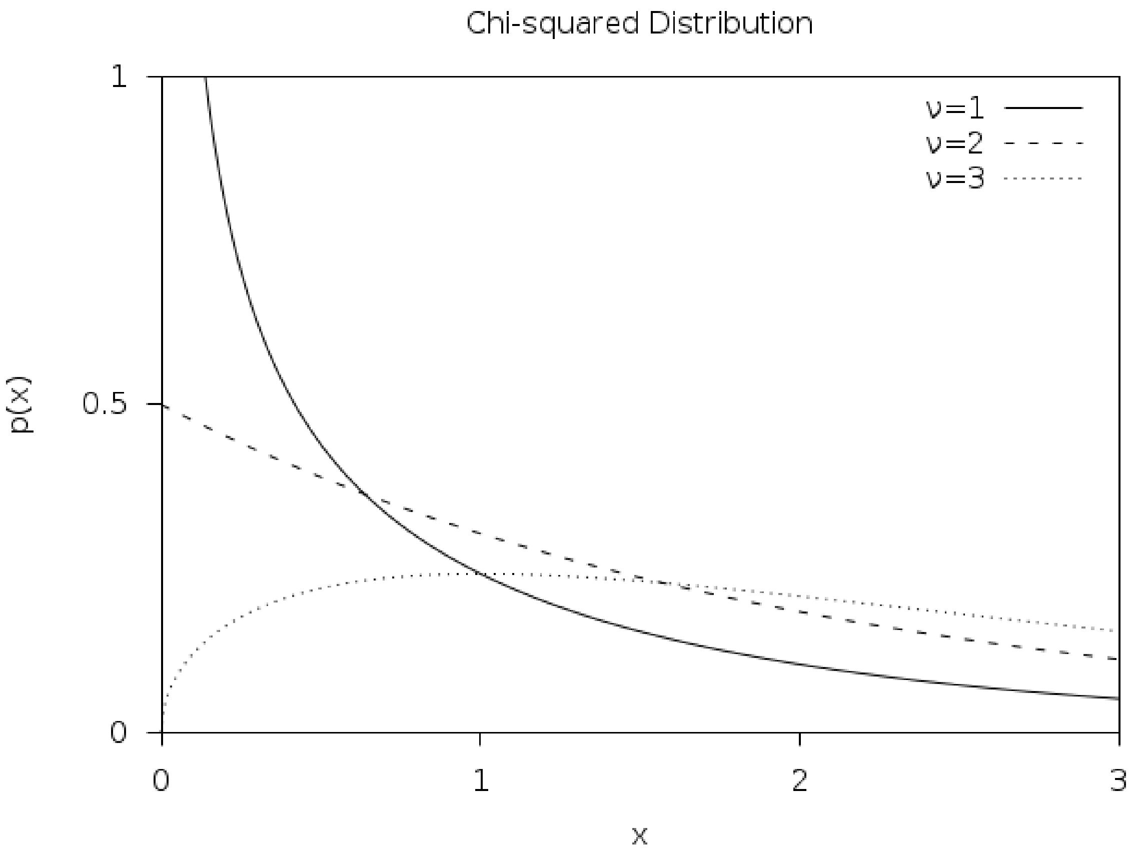
This function returns a random variate from the chi-squared distribution with *nu* degrees of freedom. The distribution function is,

$$p(x)dx = \frac{1}{2\Gamma(\nu/2)}(x/2)^{\nu/2-1}\exp(-x/2)dx$$

for $x \geq 0$.

double **gsl_ran_chisq_pdf**(double x, double nu)

This function computes the probability density $p(x)$ at *x* for a chi-squared distribution with *nu* degrees of freedom, using the formula given above.



double **gsl_cdf_chisq_P**(double x, double nu)

double **gsl_cdf_chisq_Q**(double x, double nu) double **gsl_cdf_chisq_Pinv**(double P, double nu)

double **gsl_cdf_chisq_Qinv**(double Q, double nu)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the chi-squared distribution with *nu* degrees of freedom.

20.19 The F-distribution

The F-distribution arises in statistics. If Y_1 and Y_2 are chi-squared deviates with ν_1 and ν_2 degrees of freedom then the ratio,

$$X = \frac{(Y_1/\nu_1)}{(Y_2/\nu_2)}$$

has an F-distribution $F(x;\nu_1,\nu_2)$.

double **gsl_ran_fdist**(const *gsl_rng* *r, double nu1, double nu2)

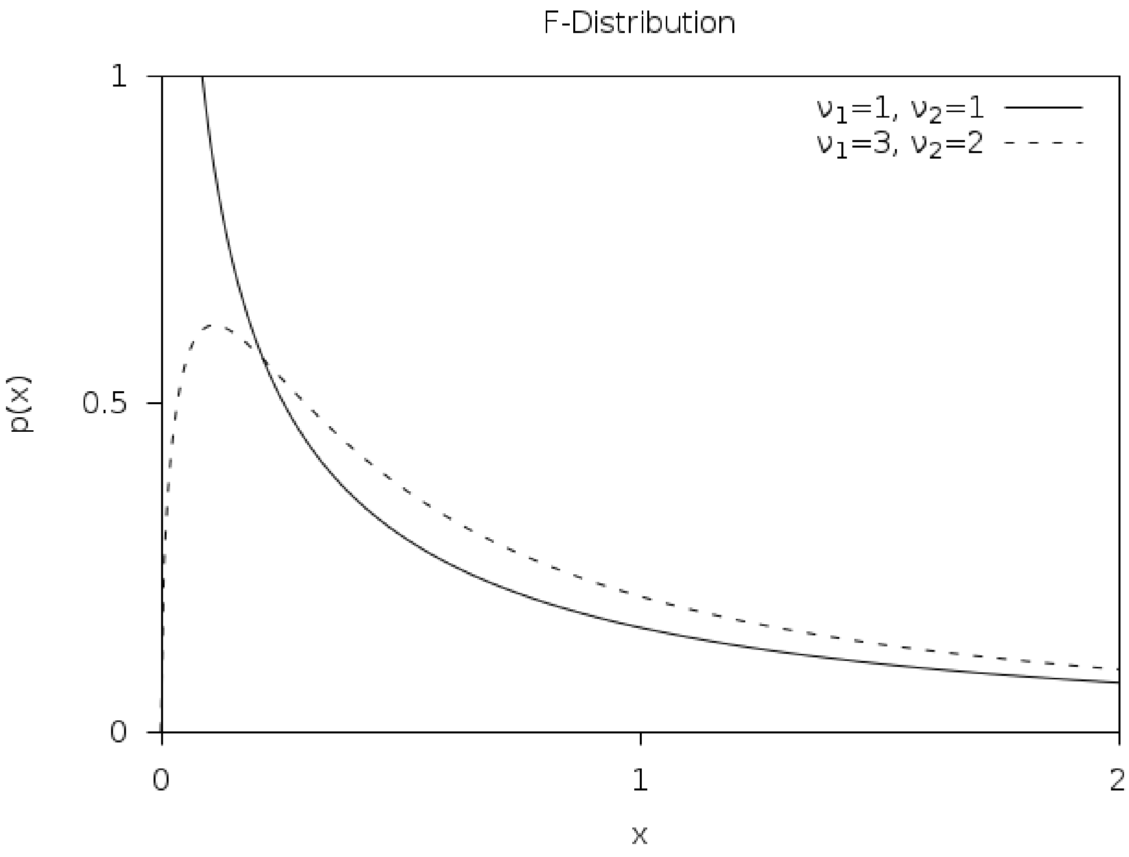
This function returns a random variate from the F-distribution with degrees of freedom *nu1* and *nu2*. The distribution function is,

$$p(x)dx = \frac{\Gamma((\nu_1+\nu_2)/2)}{\Gamma(\nu_1/2)\Gamma(\nu_2/2)} \nu_1^{\nu_1/2} \nu_2^{\nu_2/2} x^{\nu_1/2-1} (\nu_2+\nu_1 x)^{-\nu_1/2-\nu_2/2}$$

for $x \geq 0$.

double **gsl_ran_fdist_pdf**(double x, double nu1, double nu2)

This function computes the probability density $p(x)$ at *x* for an F-distribution with *nu1* and *nu2* degrees of freedom, using the formula given above.



double **gsl_cdf_fdist_P**(double x, double nu1, double nu2)

double **gsl_cdf_fdist_Q**(double x, double nu1, double nu2) double **gsl_cdf_fdist_Pinv**(double P, double nu1, double nu2)

double **gsl_cdf_fdist_Qinv**(double Q, double nu1, double nu2)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the F-distribution with *nu1* and *nu2* degrees of freedom.

20.20 The t-distribution

The t-distribution arises in statistics. If Y_1 has a normal distribution and Y_2 has a chi-squared distribution with ν degrees of freedom then the ratio,

$$X = \frac{Y_1}{\sqrt{Y_2/\nu}}$$

has a t-distribution $t(x;\nu)$ with ν degrees of freedom.

double **gsl_ran_tdist**(const *gsl_rng* *r, double nu)

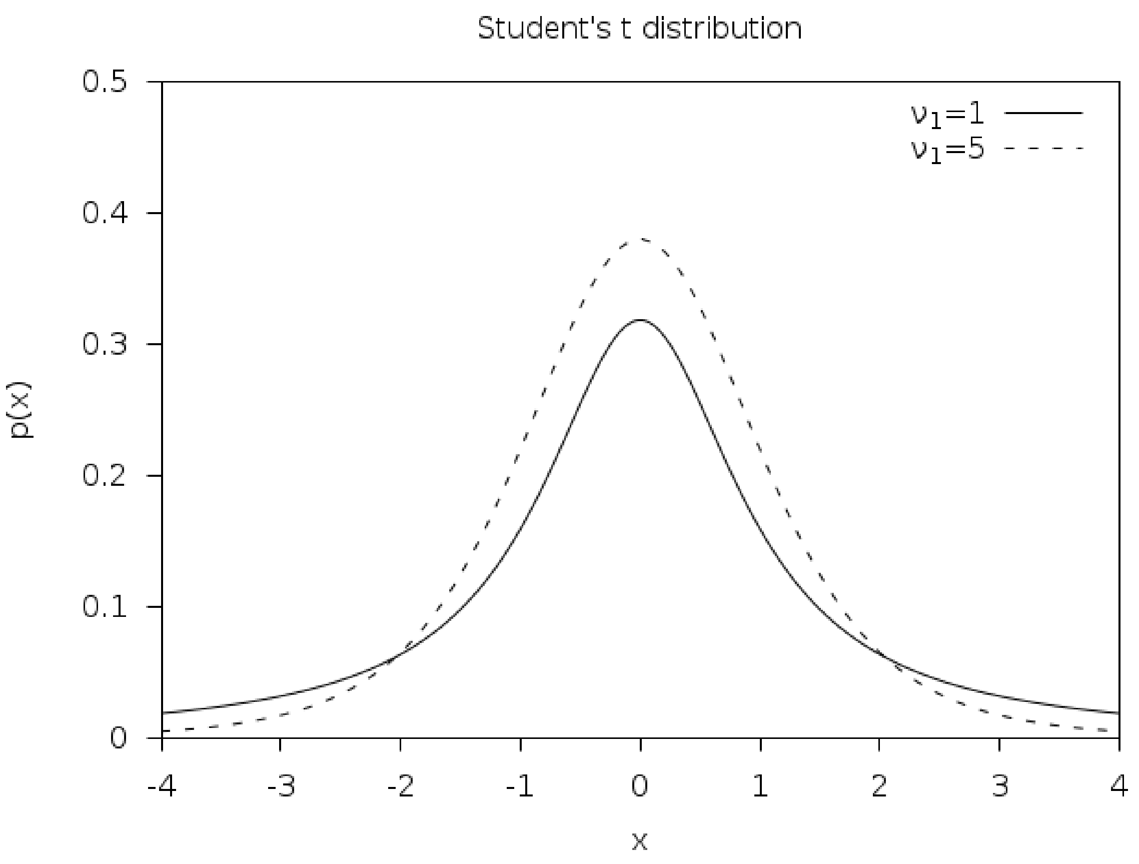
This function returns a random variate from the t-distribution. The distribution function is,

$$p(x)dx = \frac{\Gamma((\nu+1)/2)}{\sqrt{\pi\nu}\Gamma(\nu/2)}(1+x^2/\nu)^{-(\nu+1)/2}dx$$

for $-\infty < x < +\infty$.

double **gsl_ran_tdist_pdf**(double x, double nu)

This function computes the probability density $p(x)$ at *x* for a t-distribution with *nu* degrees of freedom, using the formula given above.



double **gsl_cdf_tdist_P**(double x, double nu)

double **gsl_cdf_tdist_Q**(double x, double nu)

double **gsl_cdf_tdist_Pinv**(double P, double nu) double **gsl_cdf_tdist_Qinv**(double Q, double nu)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the t-distribution with *nu* degrees of freedom.

20.21 The Beta Distribution

double **gsl_ran_beta**(const *gsl_rng* *r, double a, double b)

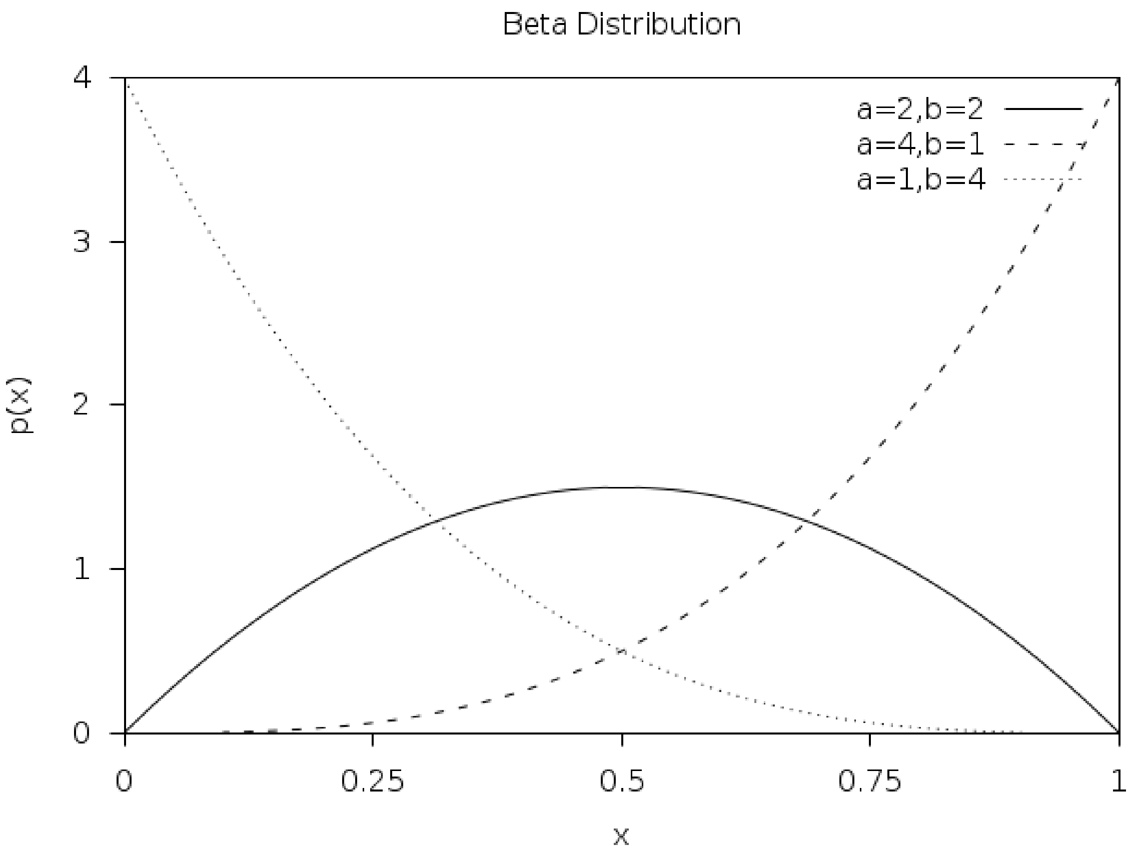
This function returns a random variate from the beta distribution. The distribution function is,

$$p(x)dx = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} x^{a-1}(1-x)^{b-1}dx$$

for $0 \leq x \leq 1$.

double **gsl_ran_beta_pdf**(double x, double a, double b)

This function computes the probability density $p(x)$ at *x* for a beta distribution with parameters *a* and *b*, using the formula given above.



double **gsl_cdf_beta_P**(double x, double a, double b)

double **gsl_cdf_beta_Q**(double x, double a, double b)

double **gsl_cdf_beta_Pinv**(double P, double a, double b)

double **gsl_cdf_beta_Qinv**(double Q, double a, double b)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the beta distribution with parameters *a* and *b*.

20.22 The Logistic Distribution

double **gsl_ran_logistic**(const *gsl_rng* *r, double a)

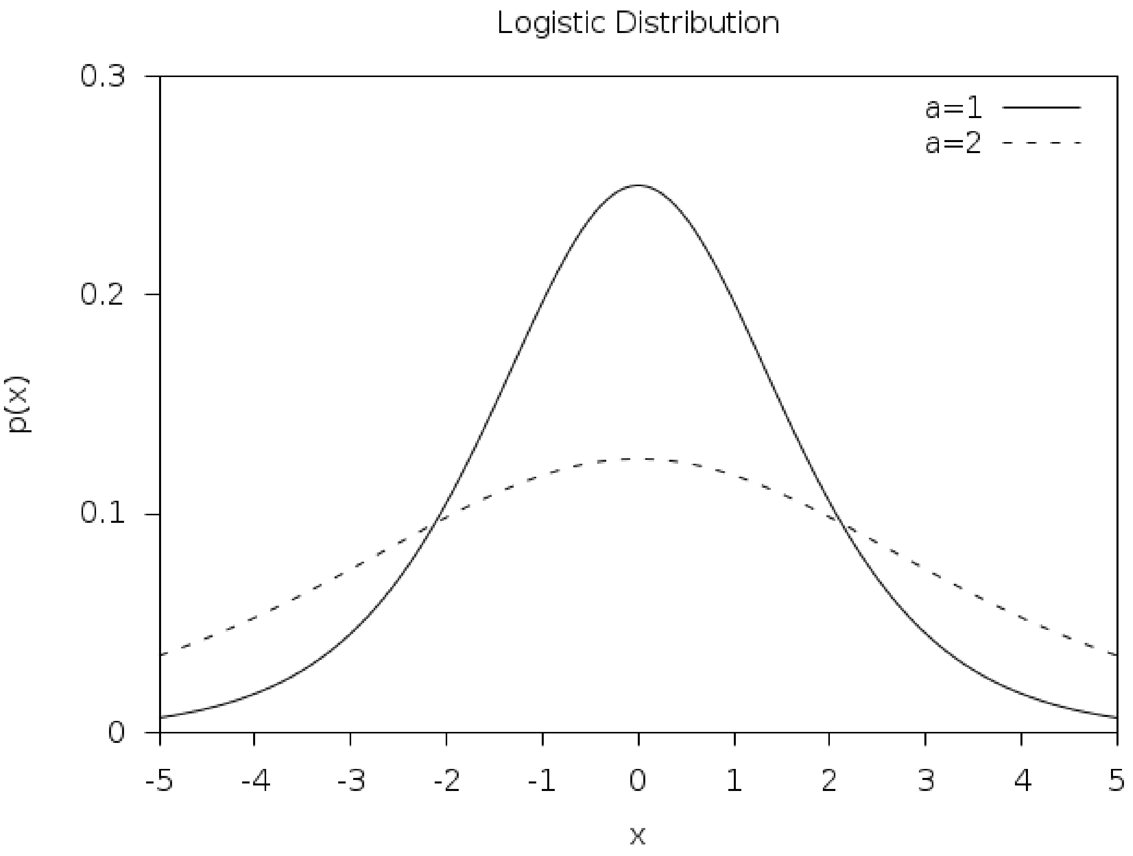
This function returns a random variate from the logistic distribution. The distribution function is,

$$p(x)dx = \frac{\exp(-x/a)}{a(1+\exp(-x/a))^2}dx$$

for $-\infty < x < +\infty$.

double **gsl_ran_logistic_pdf**(double x, double a)

This function computes the probability density $p(x)$ at `x` for a logistic distribution with scale parameter `a`, using the formula given above.



double **gsl_cdf_logistic_P**(double x, double a)

double **gsl_cdf_logistic_Q**(double x, double a)

double **gsl_cdf_logistic_Pinv**(double P, double a)

double **gsl_cdf_logistic_Qinv**(double Q, double a)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the logistic distribution with scale parameter `a`.

20.23 The Pareto Distribution

double **gsl_ran_pareto**(const *gsl_rng* *r, double a, double b)

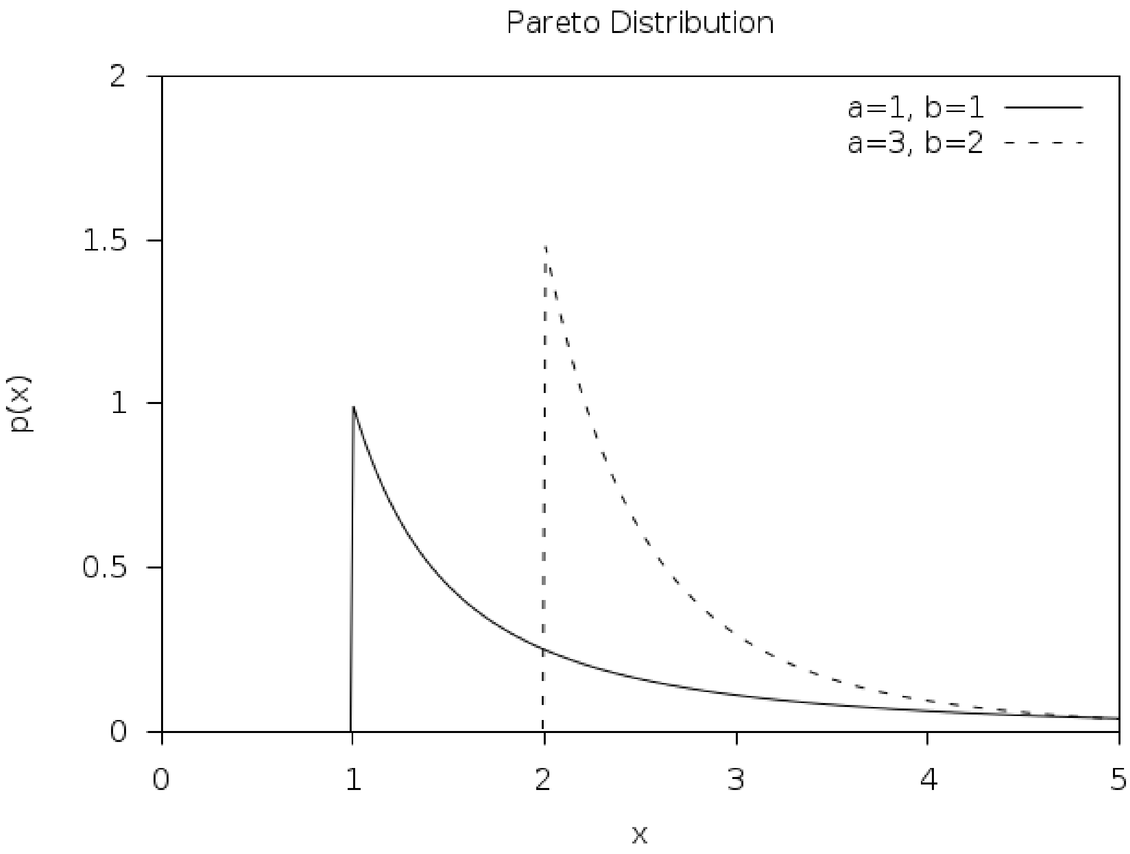
This function returns a random variate from the Pareto distribution of order a. The distribution function is,

$$p(x)dx = (a/b)/(x/b)^{a+1}dx$$

for $x \geq b$.

double **gsl_ran_pareto_pdf**(double x, double a, double b)

This function computes the probability density $p(x)$ at x for a Pareto distribution with exponent a and scale b, using the formula given above.



double **gsl_cdf_pareto_P**(double x, double a, double b)

double **gsl_cdf_pareto_Q**(double x, double a, double b)

double **gsl_cdf_pareto_Pinv**(double P, double a, double b)

double **gsl_cdf_pareto_Qinv**(double Q, double a, double b)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the Pareto distribution with exponent a and scale b.

20.24 Spherical Vector Distributions

The spherical distributions generate random vectors, located on a spherical surface. They can be used as random directions, for example in the steps of a random walk.

void **gsl_ran_dir_2d**(const *gsl_rng* *r, double *x, double *y)

void **gsl_ran_dir_2d_trig_method**(const *gsl_rng* *r, double *x, double *y)

This function returns a random direction vector v = (`x`, `y`) in two dimensions. The vector is normalized such that $|v|^2 = x^2 + y^2 = 1$. The obvious way to do this is to take a uniform random number between 0 and 2π and let `x` and `y` be the sine and cosine respectively. Two trig functions would have been expensive in the old days, but with modern hardware implementations, this is sometimes the fastest way to go. This is the case for the Pentium (but not the case for the Sun Sparcstation). One can avoid the trig evaluations by choosing `x` and `y` in the interior of a unit circle (choose them at random from the interior of the enclosing square, and then reject those that are outside the unit circle), and then dividing by $\sqrt{x^2 + y^2}$. A much cleverer approach, attributed to von Neumann (See Knuth, v2, 3rd ed, p140, exercise 23), requires neither trig nor a square root. In this approach, u and v are chosen at random from the interior of a unit circle, and then $x = (u^2 - v^2)/(u^2 + v^2)$ and $y = 2uv/(u^2 + v^2)$.

void **gsl_ran_dir_3d**(const *gsl_rng* *r, double *x, double *y, double *z)

This function returns a random direction vector v = (`x`, `y`, `z`) in three dimensions. The vector is normalized such that $|v|^2 = x^2 + y^2 + z^2 = 1$. The method employed is due to Robert E. Knop (CACM 13, 326 (1970)), and explained in Knuth, v2, 3rd ed, p136. It uses the surprising fact that the distribution projected along any axis is actually uniform (this is only true for 3 dimensions).

void **gsl_ran_dir_nd**(const *gsl_rng* *r, size_t n, double *x)

This function returns a random direction vector $v = (x_1, x_2, \ldots, x_n)$ in `n` dimensions. The vector is normalized such that $|v|^2 = x_1^2 + x_2^2 + \cdots + x_n^2 = 1$. The method uses the fact that a multivariate Gaussian distribution is spherically symmetric. Each component is generated to have a Gaussian distribution, and then the components are normalized. The method is described by Knuth, v2, 3rd ed, p135–136, and attributed to G. W. Brown, Modern Mathematics for the Engineer (1956).

20.25 The Weibull Distribution

double **gsl_ran_weibull**(const *gsl_rng* *r, double a, double b)

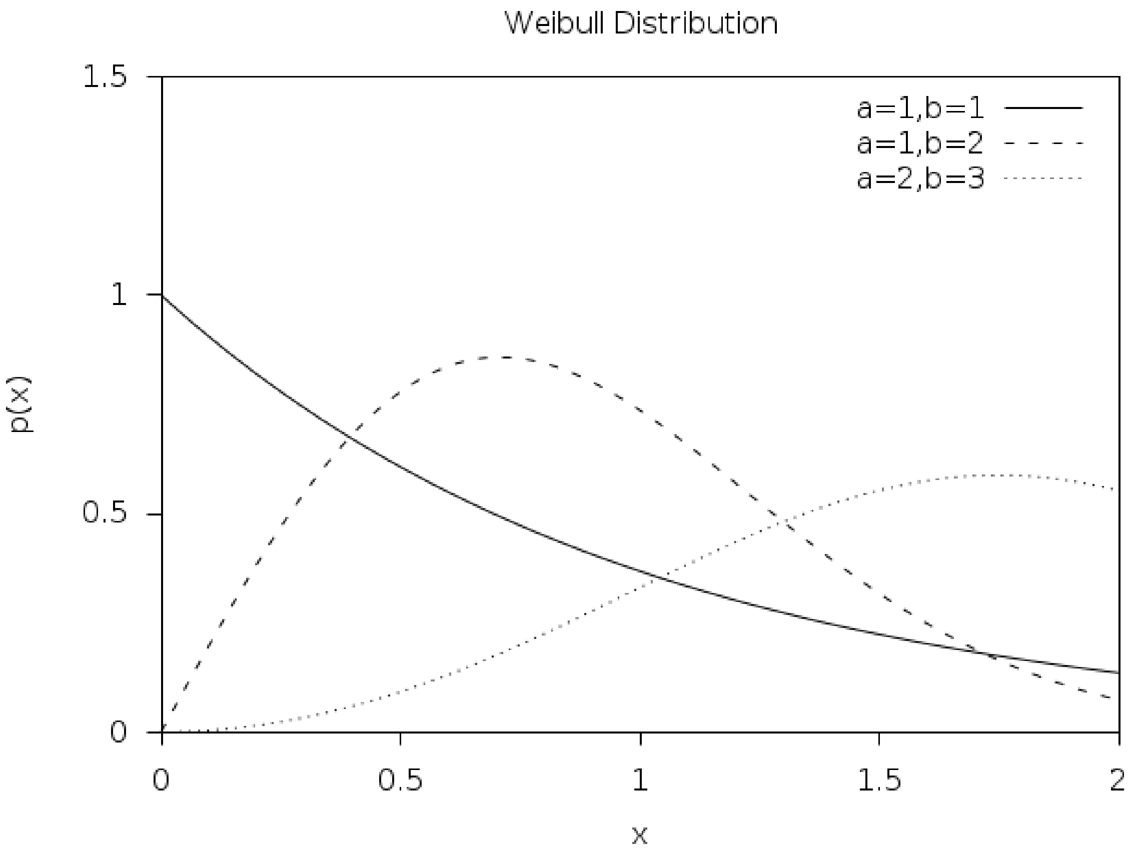
This function returns a random variate from the Weibull distribution. The distribution function is,

$$p(x)dx = \frac{b}{a^b} x^{b-1} \exp(-(x/a)^b) dx$$

for $x \geq 0$.

double **gsl_ran_weibull_pdf**(double x, double a, double b)

This function computes the probability density $p(x)$ at `x` for a Weibull distribution with scale `a` and exponent `b`, using the formula given above.



double **gsl_cdf_weibull_P**(double x, double a, double b)

double **gsl_cdf_weibull_Q**(double x, double a, double b)

double **gsl_cdf_weibull_Pinv**(double P, double a, double b)

double **gsl_cdf_weibull_Qinv**(double Q, double a, double b)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the Weibull distribution with scale `a` and exponent `b`.

20.26 The Type-1 Gumbel Distribution

double **gsl_ran_gumbel1**(const *gsl_rng* *r, double a, double b)

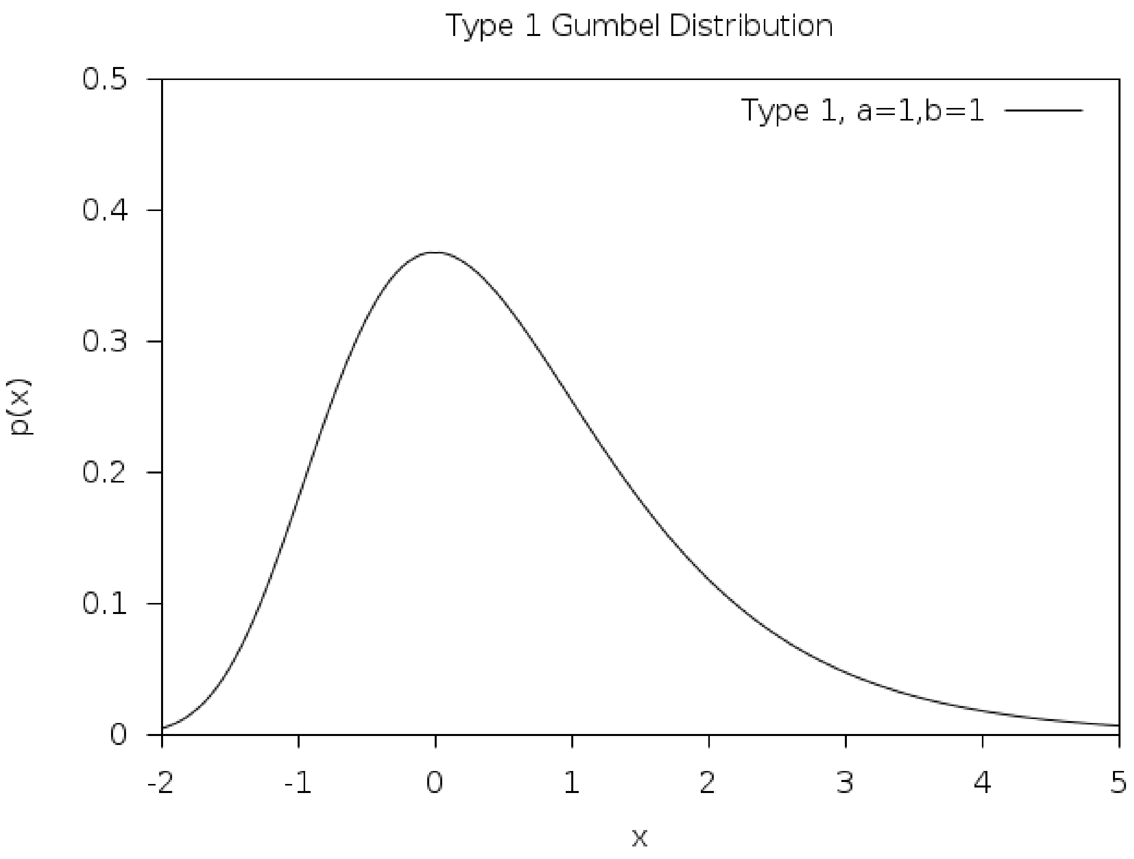
This function returns a random variate from the Type-1 Gumbel distribution. The Type-1 Gumbel distribution function is,

$$p(x)dx = ab \exp(-(b \exp(-ax) + ax))dx$$

for $-\infty < x < \infty$.

double **gsl_ran_gumbel1_pdf**(double x, double a, double b)

This function computes the probability density $p(x)$ at *x* for a Type-1 Gumbel distribution with parameters *a* and *b*, using the formula given above.



double **gsl_cdf_gumbel1_P**(double x, double a, double b)

double **gsl_cdf_gumbel1_Q**(double x, double a, double b)

double **gsl_cdf_gumbel1_Pinv**(double P, double a, double b)

double **gsl_cdf_gumbel1_Qinv**(double Q, double a, double b)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the Type-1 Gumbel distribution with parameters *a* and *b*.

20.27 The Type-2 Gumbel Distribution

double **gsl_ran_gumbel2**(const *gsl_rng* *r, double a, double b)

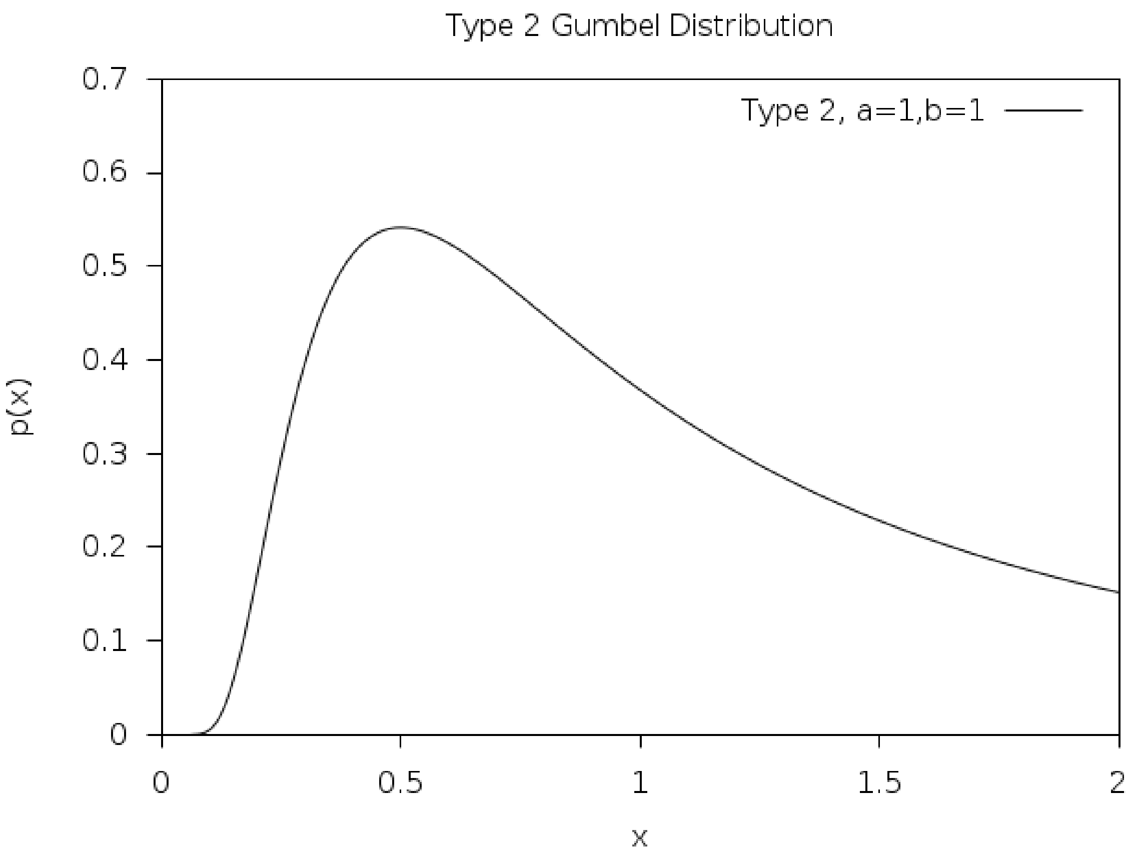
This function returns a random variate from the Type-2 Gumbel distribution. The Type-2 Gumbel distribution function is,

$$p(x)dx = abx^{-a-1}\exp(-bx^{-a})dx$$

for $0 < x < \infty$.

double **gsl_ran_gumbel2_pdf**(double x, double a, double b)

This function computes the probability density $p(x)$ at *x* for a Type-2 Gumbel distribution with parameters *a* and *b*, using the formula given above.



double **gsl_cdf_gumbel2_P**(double x, double a, double b)

double **gsl_cdf_gumbel2_Q**(double x, double a, double b)

double **gsl_cdf_gumbel2_Pinv**(double P, double a, double b)

double **gsl_cdf_gumbel2_Qinv**(double Q, double a, double b)

These functions compute the cumulative distribution functions $P(x)$, $Q(x)$ and their inverses for the Type-2 Gumbel distribution with parameters *a* and *b*.

20.28 The Dirichlet Distribution

void **gsl_ran_dirichlet**(const *gsl_rng* *r, size_t K, const double alpha[], double theta[])

This function returns an array of *K* random variates from a Dirichlet distribution of order *K*-1. The distribution function is

$$p(\theta_1, \ldots, \theta_K)\, d\theta_1 \cdots d\theta_K = \frac{1}{Z} \prod_{i=1}^{K} \theta_i^{\alpha_i - 1}\; \delta(1 - \sum_{i=1}^{K} \theta_i) d\theta_1 \cdots d\theta_K$$

for $\theta_i \geq 0$ and $\alpha_i > 0$. The delta function ensures that $\sum \theta_i = 1$. The normalization factor Z is

$$Z = \frac{\prod_{i=1}^{K} \Gamma(\alpha_i)}{\Gamma(\sum_{i=1}^{K} \alpha_i)}$$

The random variates are generated by sampling *K* values from gamma distributions with parameters $a = \alpha_i$, $b = 1$, and renormalizing. See A.M. Law, W.D. Kelton, *Simulation Modeling and Analysis* (1991).

double **gsl_ran_dirichlet_pdf**(size_t K, const double alpha[], const double theta[])

This function computes the probability density $p(\theta_1, \ldots, \theta_K)$ at `theta[K]` for a Dirichlet distribution with parameters `alpha[K]`, using the formula given above.

double **gsl_ran_dirichlet_lnpdf**(size_t K, const double alpha[], const double theta[])

This function computes the logarithm of the probability density $p(\theta_1, \ldots, \theta_K)$ for a Dirichlet distribution with parameters `alpha[K]`.

20.29 General Discrete Distributions

Given K discrete events with different probabilities $P[k]$, produce a random value k consistent with its probability.

The obvious way to do this is to preprocess the probability list by generating a cumulative probability array with $K+1$ elements:

$$C[0] = 0$$
$$C[k+1] = C[k] + P[k]$$

Note that this construction produces $C[K] = 1$. Now choose a uniform deviate u between 0 and 1, and find the value of k such that $C[k] \leq u < C[k+1]$. Although this in principle requires of order $\log K$ steps per random number generation, they are fast steps, and if you use something like $\lfloor uK \rfloor$ as a starting point, you can often do pretty well.

But faster methods have been devised. Again, the idea is to preprocess the probability list, and save the result in some form of lookup table; then the individual calls for a random discrete event can go rapidly. An approach invented by G. Marsaglia (Generating discrete random variables in a computer, Comm ACM 6, 37–38 (1963)) is very clever, and readers interested in examples of good algorithm design are directed to this short and well-written paper. Unfortunately, for large K, Marsaglia's lookup table can be quite large.

A much better approach is due to Alastair J. Walker (An efficient method for generating discrete random variables with general distributions, ACM Trans on Mathematical Software 3, 253–256 (1977); see also Knuth, v2, 3rd ed, p120–121,139). This requires two lookup tables, one floating point and one integer, but both only of size K. After preprocessing, the random numbers are generated in O(1) time, even for large K. The preprocessing suggested by Walker requires $O(K^2)$ effort, but that is not actually necessary, and the implementation provided here only takes $O(K)$ effort. In general, more preprocessing leads to faster generation of the individual random numbers, but a diminishing return is reached pretty early. Knuth points out that the optimal preprocessing is combinatorially difficult for large K.

This method can be used to speed up some of the discrete random number generators below, such as the binomial distribution. To use it for something like the Poisson Distribution, a modification would have to be made, since it only takes a finite set of K outcomes.

type **`gsl_ran_discrete_t`**

This structure contains the lookup table for the discrete random number generator.

gsl_ran_discrete_t ***`gsl_ran_discrete_preproc`**(size_t K, const double *P)

This function returns a pointer to a structure that contains the lookup table for the discrete random number generator. The array `P` contains the probabilities of the discrete events; these array elements must all be positive, but they needn't add up to one (so you can think of them more generally as "weights")—the preprocessor will normalize appropriately. This return value is used as an argument for the `gsl_ran_discrete()` function below.

size_t **`gsl_ran_discrete`**(const *gsl_rng* *r, const *gsl_ran_discrete_t* *g)

After the preprocessor, above, has been called, you use this function to get the discrete random numbers.

double **`gsl_ran_discrete_pdf`**(size_t k, const *gsl_ran_discrete_t* *g)

Returns the probability $P[k]$ of observing the variable `k`. Since $P[k]$ is not stored as part of the lookup table, it must be recomputed; this computation takes $O(K)$, so if `K` is large and you care about the original array $P[k]$ used to create the lookup table, then you should just keep this original array $P[k]$ around.

void **`gsl_ran_discrete_free`**(*gsl_ran_discrete_t* *g)

De-allocates the lookup table pointed to by `g`.

20.30 The Poisson Distribution

unsigned int **gsl_ran_poisson**(const *gsl_rng* *r, double mu)

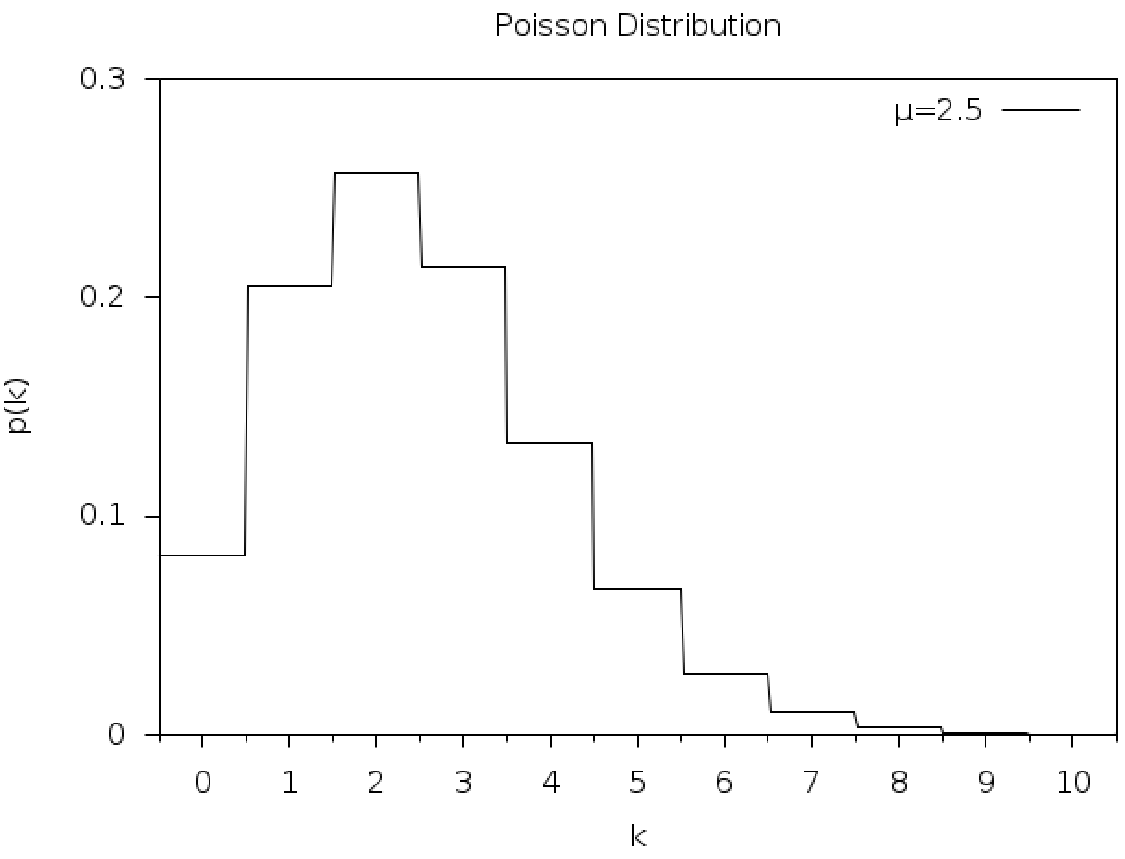
This function returns a random integer from the Poisson distribution with mean *mu*. The probability distribution for Poisson variates is,

$$p(k) = \frac{\mu^k}{k!} \exp(-\mu)$$

for $k \geq 0$.

double **gsl_ran_poisson_pdf**(unsigned int k, double mu)

This function computes the probability $p(k)$ of obtaining *k* from a Poisson distribution with mean *mu*, using the formula given above.



double **gsl_cdf_poisson_P**(unsigned int k, double mu)

double **gsl_cdf_poisson_Q**(unsigned int k, double mu)

These functions compute the cumulative distribution functions $P(k)$, $Q(k)$ for the Poisson distribution with parameter *mu*.

20.31 The Bernoulli Distribution

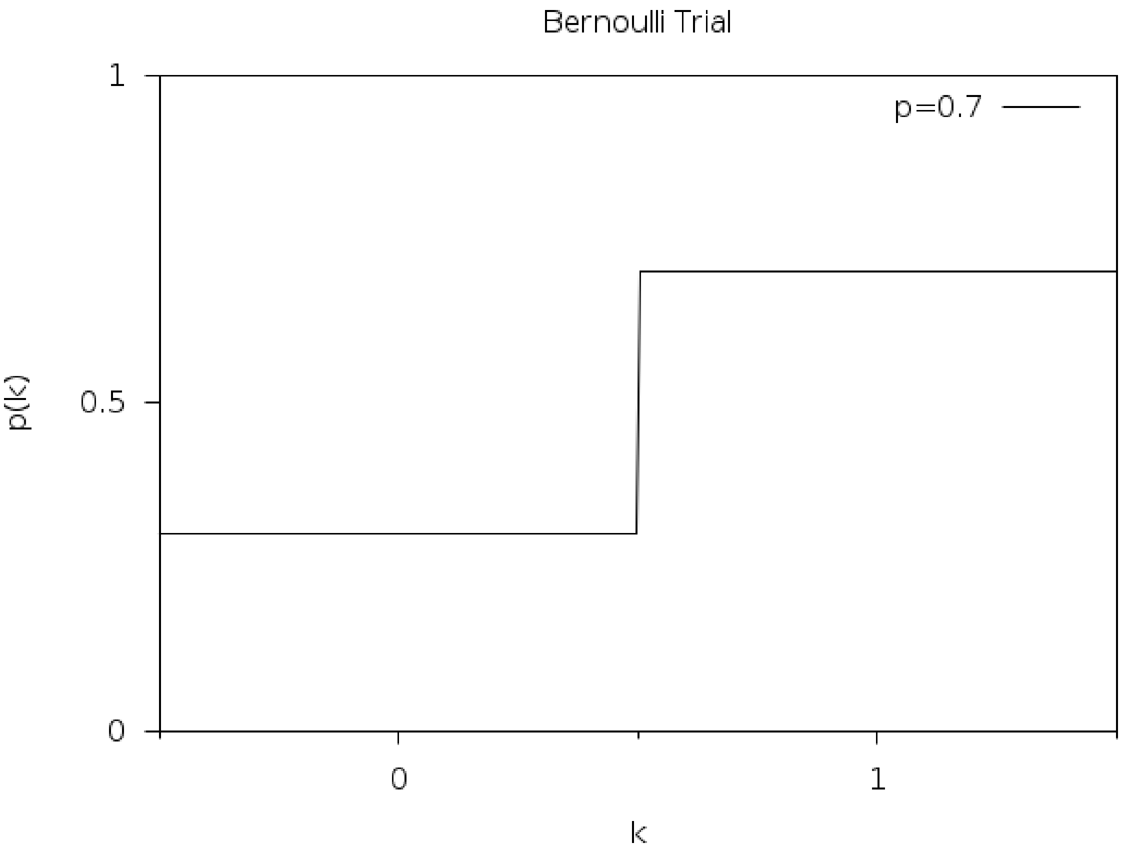
unsigned int **gsl_ran_bernoulli**(const *gsl_rng* *r, double p)

This function returns either 0 or 1, the result of a Bernoulli trial with probability p. The probability distribution for a Bernoulli trial is,

$$p(0) = 1 - p$$
$$p(1) = p$$

double **gsl_ran_bernoulli_pdf**(unsigned int k, double p)

This function computes the probability $p(k)$ of obtaining k from a Bernoulli distribution with probability parameter p, using the formula given above.



20.32 The Binomial Distribution

unsigned int **gsl_ran_binomial**(const *gsl_rng* *r, double p, unsigned int n)

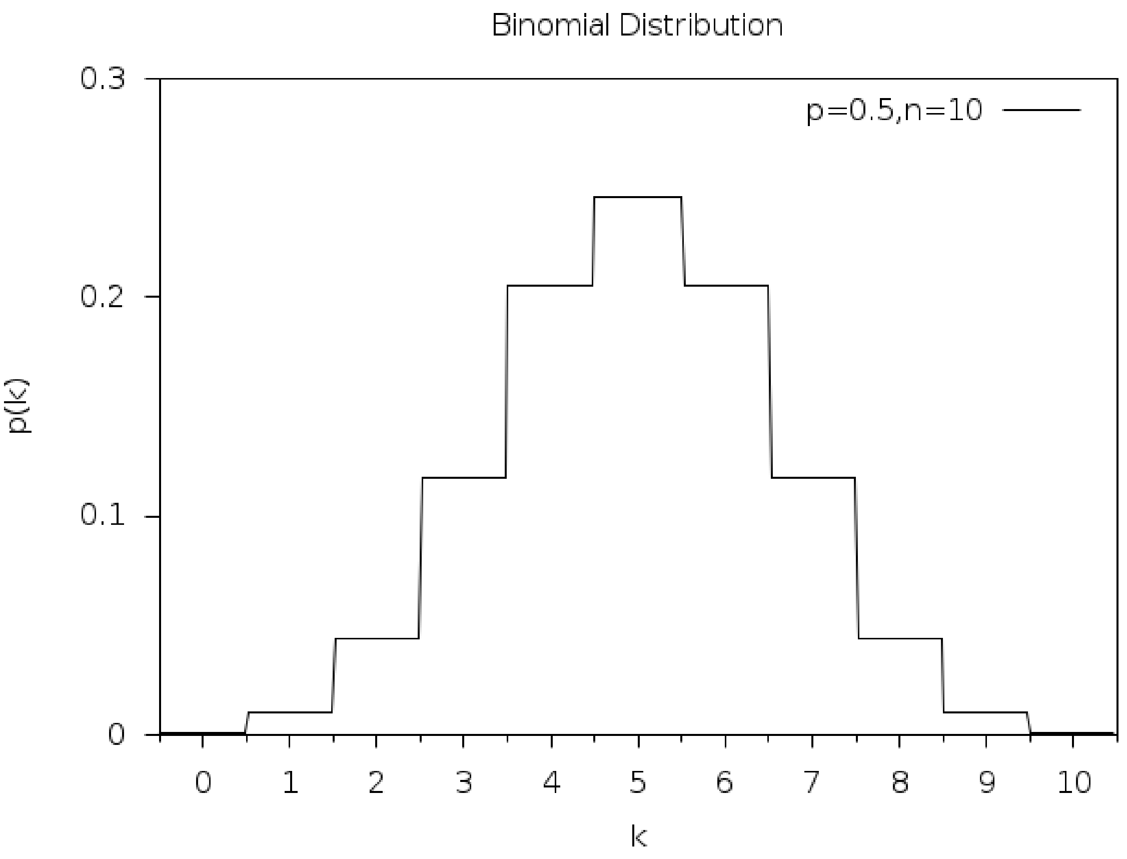
This function returns a random integer from the binomial distribution, the number of successes in *n* independent trials with probability *p*. The probability distribution for binomial variates is,

$$p(k) = \frac{n!}{k!(n-k)!} p^k (1-p)^{n-k}$$

for $0 \le k \le n$.

double **gsl_ran_binomial_pdf**(unsigned int k, double p, unsigned int n)

This function computes the probability $p(k)$ of obtaining *k* from a binomial distribution with parameters *p* and *n*, using the formula given above.



double **gsl_cdf_binomial_P**(unsigned int k, double p, unsigned int n)

double **gsl_cdf_binomial_Q**(unsigned int k, double p, unsigned int n)

These functions compute the cumulative distribution functions $P(k)$, $Q(k)$ for the binomial distribution with parameters *p* and *n*.

20.33 The Multinomial Distribution

void **gsl_ran_multinomial**(const *gsl_rng* *r, size_t K, unsigned int N, const double p[], unsigned int n[])

This function computes a random sample *n* from the multinomial distribution formed by *N* trials from an underlying distribution `p[K]`. The distribution function for *n* is,

$$P(n_1, n_2, \cdots, n_K) = \frac{N!}{n_1! n_2! \cdots n_K!} p_1^{n_1} p_2^{n_2} \cdots p_K^{n_K}$$

where $(n_1, n_2, \ldots, n_K)$ are nonnegative integers with $\sum_{k=1}^{K} n_k = N$, and $(p_1, p_2, \ldots, p_K)$ is a probability distribution with $\sum p_i = 1$. If the array `p[K]` is not normalized then its entries will be treated as weights and normalized appropriately. The arrays *n* and *p* must both be of length *K*.

Random variates are generated using the conditional binomial method (see C.S. Davis, *The computer generation of multinomial random variates*, Comp. Stat. Data Anal. 16 (1993) 205–217 for details).

double **gsl_ran_multinomial_pdf**(size_t K, const double p[], const unsigned int n[])

This function computes the probability $P(n_1, n_2, \ldots, n_K)$ of sampling `n[K]` from a multinomial distribution with parameters `p[K]`, using the formula given above.

double **gsl_ran_multinomial_lnpdf**(size_t K, const double p[], const unsigned int n[])

This function returns the logarithm of the probability for the multinomial distribution $P(n_1, n_2, \ldots, n_K)$ with parameters `p[K]`.

20.34 The Negative Binomial Distribution

unsigned int **gsl_ran_negative_binomial**(const *gsl_rng* *r, double p, double n)

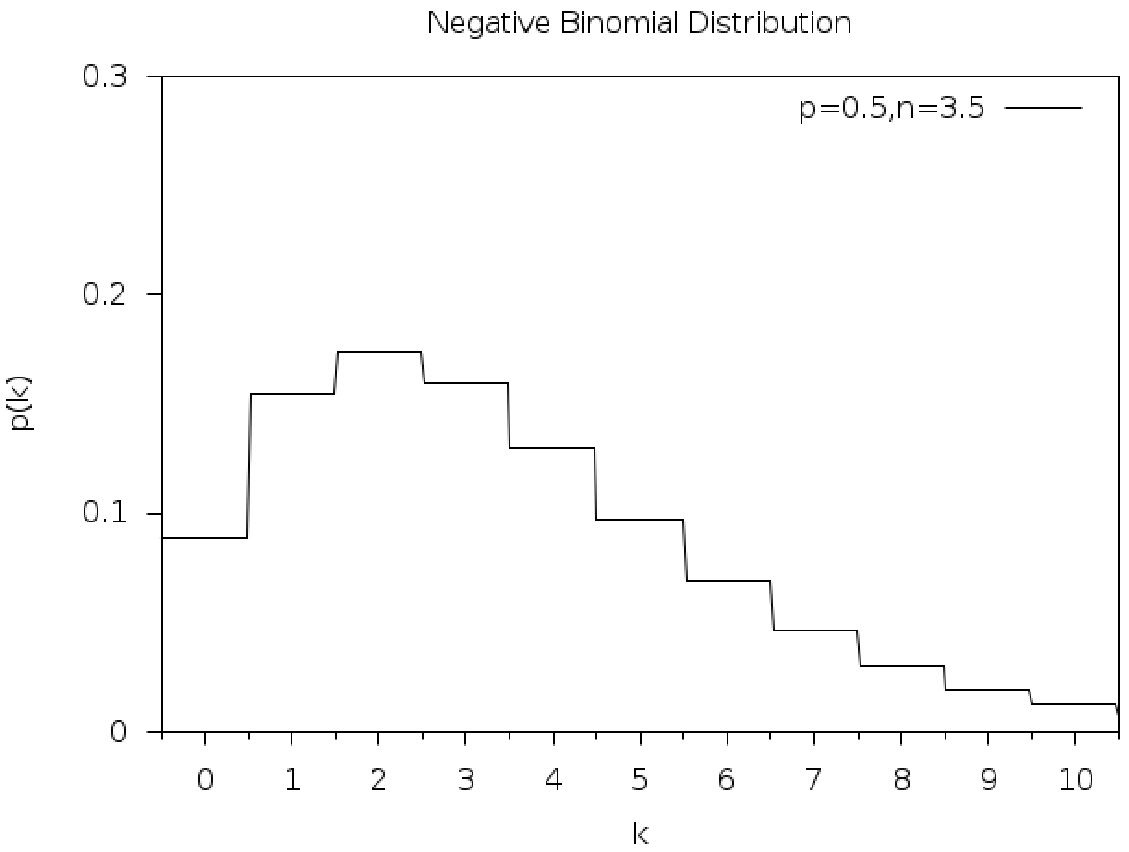
This function returns a random integer from the negative binomial distribution, the number of failures occurring before *n* successes in independent trials with probability *p* of success. The probability distribution for negative binomial variates is,

$$p(k) = \frac{\Gamma(n+k)}{\Gamma(k+1)\Gamma(n)} p^n (1-p)^k$$

Note that n is not required to be an integer.

double **gsl_ran_negative_binomial_pdf**(unsigned int k, double p, double n)

This function computes the probability $p(k)$ of obtaining *k* from a negative binomial distribution with parameters *p* and *n*, using the formula given above.



double **gsl_cdf_negative_binomial_P**(unsigned int k, double p, double n)

double **gsl_cdf_negative_binomial_Q**(unsigned int k, double p, double n)

These functions compute the cumulative distribution functions $P(k)$, $Q(k)$ for the negative binomial distribution with parameters *p* and *n*.

20.35 The Pascal Distribution

unsigned int **gsl_ran_pascal**(const *gsl_rng* *r, double p, unsigned int n)

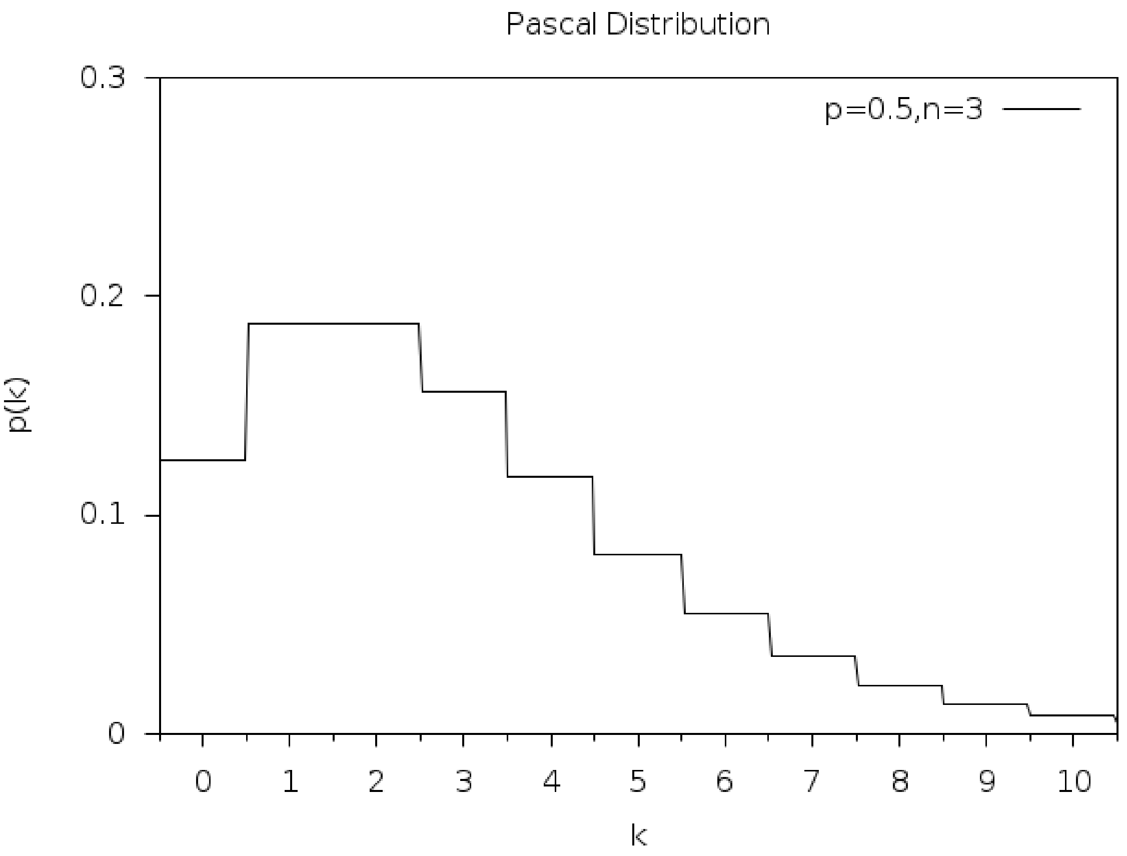
This function returns a random integer from the Pascal distribution. The Pascal distribution is simply a negative binomial distribution with an integer value of n.

$$p(k) = \frac{(n+k-1)!}{k!(n-1)!} p^n (1-p)^k$$

for $k \geq 0$.

double **gsl_ran_pascal_pdf**(unsigned int k, double p, unsigned int n)

This function computes the probability $p(k)$ of obtaining *k* from a Pascal distribution with parameters *p* and *n*, using the formula given above.



double **gsl_cdf_pascal_P**(unsigned int k, double p, unsigned int n)

double **gsl_cdf_pascal_Q**(unsigned int k, double p, unsigned int n)

These functions compute the cumulative distribution functions $P(k)$, $Q(k)$ for the Pascal distribution with parameters *p* and *n*.

20.36 The Geometric Distribution

unsigned int **gsl_ran_geometric**(const *gsl_rng* *r, double p)

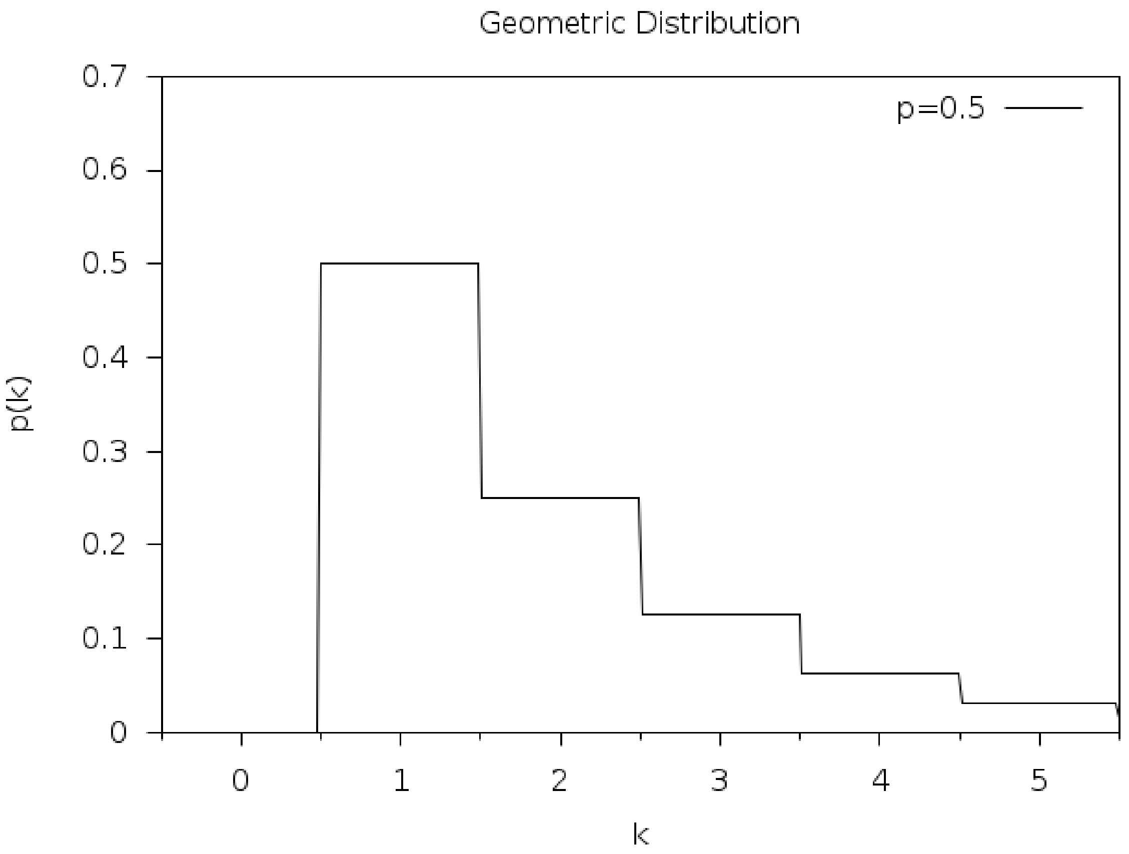
This function returns a random integer from the geometric distribution, the number of independent trials with probability *p* until the first success. The probability distribution for geometric variates is,

$$p(k) = p(1-p)^{k-1}$$

for $k \geq 1$. Note that the distribution begins with $k = 1$ with this definition. There is another convention in which the exponent $k - 1$ is replaced by k.

double **gsl_ran_geometric_pdf**(unsigned int k, double p)

This function computes the probability $p(k)$ of obtaining *k* from a geometric distribution with probability parameter *p*, using the formula given above.



double **gsl_cdf_geometric_P**(unsigned int k, double p)

double **gsl_cdf_geometric_Q**(unsigned int k, double p)

These functions compute the cumulative distribution functions $P(k)$, $Q(k)$ for the geometric distribution with parameter *p*.

20.37 The Hypergeometric Distribution

unsigned int **gsl_ran_hypergeometric**(const *gsl_rng* *r, unsigned int n1, unsigned int n2, unsigned int t)

This function returns a random integer from the hypergeometric distribution. The probability distribution for hypergeometric random variates is,

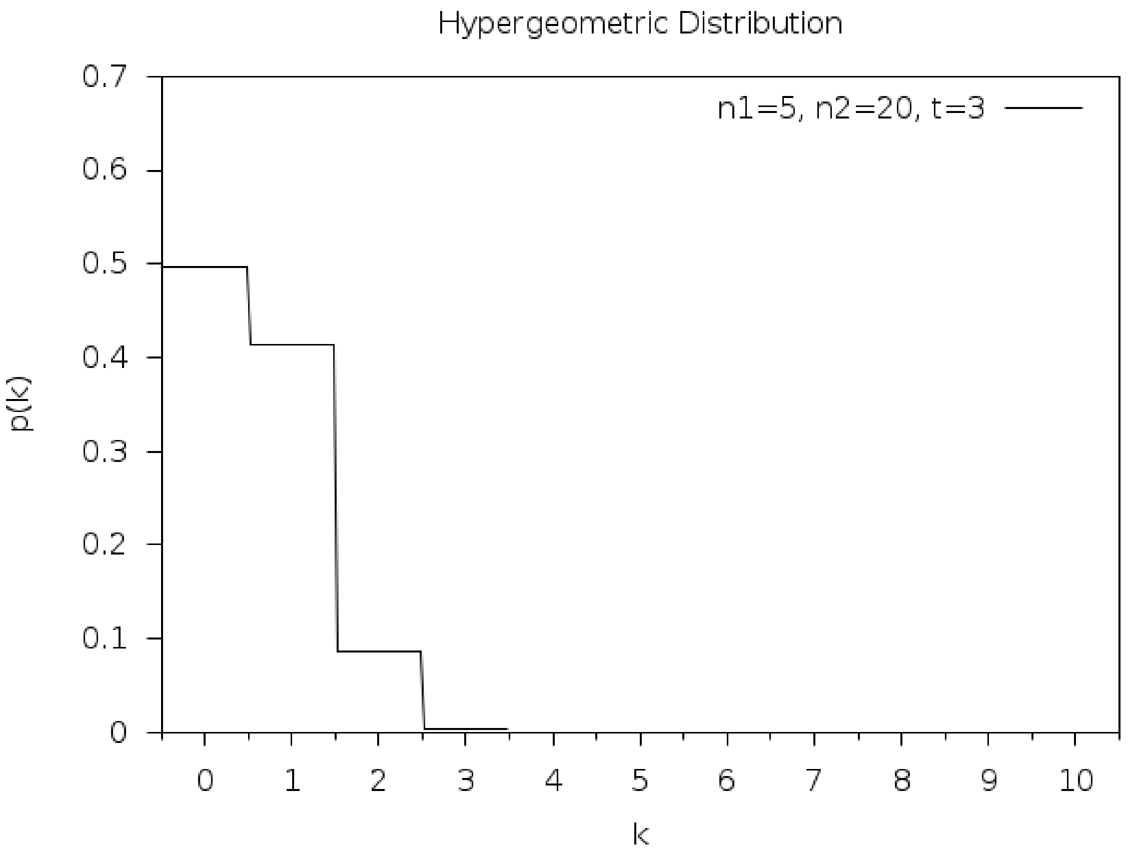
$$p(k) = C(n_1, k)C(n_2, t - k)/C(n_1 + n_2, t)$$

where $C(a, b) = a!/(b!(a - b)!)$ and $t \leq n_1 + n_2$. The domain of k is $\max(0, t - n_2), \ldots, \min(t, n_1)$

If a population contains n_1 elements of "type 1" and n_2 elements of "type 2" then the hypergeometric distribution gives the probability of obtaining k elements of "type 1" in t samples from the population without replacement.

double **gsl_ran_hypergeometric_pdf**(unsigned int k, unsigned int n1, unsigned int n2, unsigned int t)

This function computes the probability $p(k)$ of obtaining *k* from a hypergeometric distribution with parameters *n1*, *n2*, *t*, using the formula given above.



double **gsl_cdf_hypergeometric_P**(unsigned int k, unsigned int n1, unsigned int n2, unsigned int t)

double **gsl_cdf_hypergeometric_Q**(unsigned int k, unsigned int n1, unsigned int n2, unsigned int t)

These functions compute the cumulative distribution functions $P(k)$, $Q(k)$ for the hypergeometric distribution with parameters *n1*, *n2* and *t*.

20.38 The Logarithmic Distribution

unsigned int **gsl_ran_logarithmic**(const *gsl_rng* *r, double p)

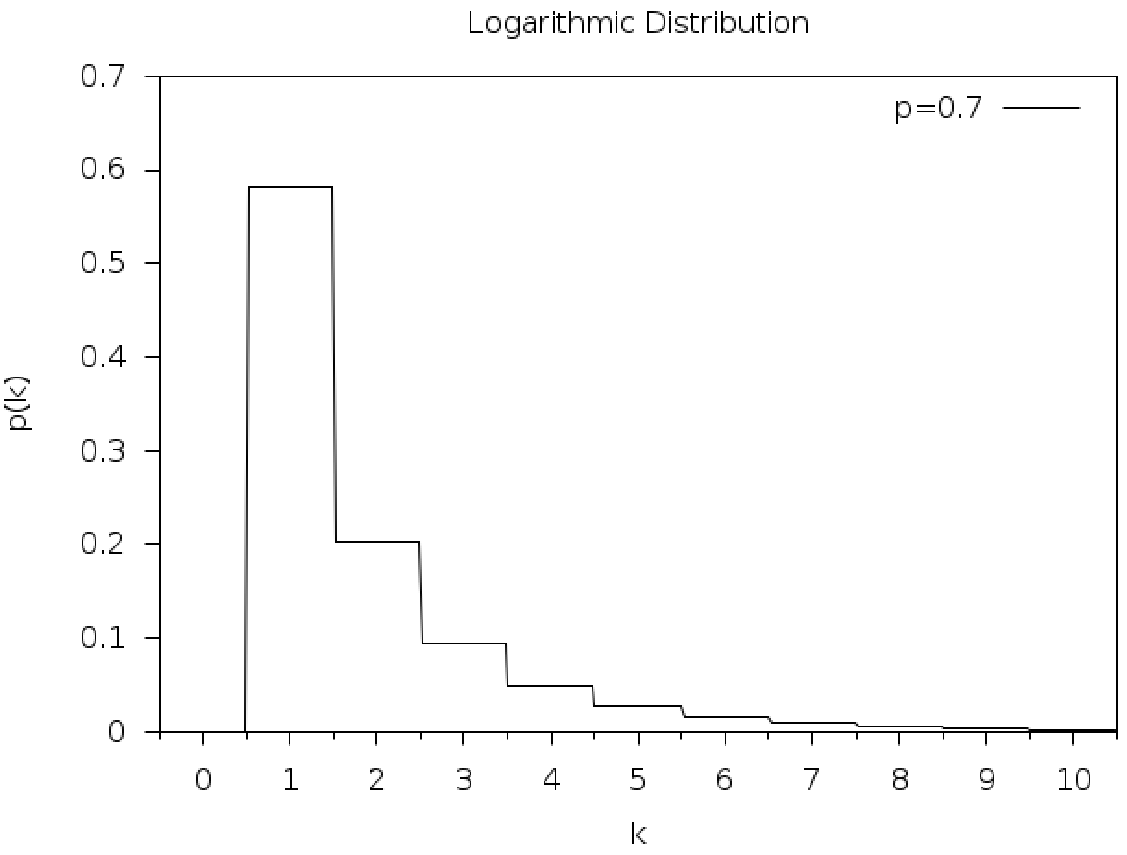
This function returns a random integer from the logarithmic distribution. The probability distribution for logarithmic random variates is,

$$p(k) = \frac{-1}{\log(1-p)} \left(\frac{p^k}{k}\right)$$

for $k \geq 1$.

double **gsl_ran_logarithmic_pdf**(unsigned int k, double p)

This function computes the probability $p(k)$ of obtaining k from a logarithmic distribution with probability parameter p, using the formula given above.



20.39 The Wishart Distribution

int **gsl_ran_wishart**(const *gsl_rng* *r, const double n, const *gsl_matrix* *L, *gsl_matrix* *result, *gsl_matrix* *work)

This function computes a random symmetric p-by-p matrix from the Wishart distribution. The probability distribution for Wishart random variates is,

$$p(X) = \frac{|X|^{(n-p-1)/2} e^{-\mathrm{tr}\left(V^{-1}X\right)/2}}{2^{\frac{np}{2}} |V|^{n/2} \Gamma_p(\frac{n}{2})}$$

Here, $n > p - 1$ is the number of degrees of freedom, V is a symmetric positive definite p-by-p scale matrix, whose Cholesky factor is specified by `L`, and `work` is p-by-p workspace. The p-by-p Wishart distributed matrix X is stored in `result` on output.

int **gsl_ran_wishart_pdf**(const *gsl_matrix* *X, const *gsl_matrix* *L_X, const double n, const *gsl_matrix* *L, double *result, *gsl_matrix* *work)

int **gsl_ran_wishart_log_pdf**(const *gsl_matrix* *X, const *gsl_matrix* *L_X, const double n, const *gsl_matrix* *L, double *result, *gsl_matrix* *work)

These functions compute $p(X)$ or $\log p(X)$ for the p-by-p matrix `X`, whose Cholesky factor is specified in `L_X`. The degrees of freedom is given by `n`, the Cholesky factor of the scale matrix V is specified in `L`, and `work` is p-by-p workspace. The probably density value is returned in `result`.

20.40 Shuffling and Sampling

The following functions allow the shuffling and sampling of a set of objects. The algorithms rely on a random number generator as a source of randomness and a poor quality generator can lead to correlations in the output. In particular it is important to avoid generators with a short period. For more information see Knuth, v2, 3rd ed, Section 3.4.2, "Random Sampling and Shuffling".

void **gsl_ran_shuffle**(const *gsl_rng* *r, void *base, size_t n, size_t size)

This function randomly shuffles the order of *n* objects, each of size *size*, stored in the array `base[0..n-1]`. The output of the random number generator *r* is used to produce the permutation. The algorithm generates all possible $n!$ permutations with equal probability, assuming a perfect source of random numbers.

The following code shows how to shuffle the numbers from 0 to 51:

```
int a[52];

for (i = 0; i < 52; i++)
  {
    a[i] = i;
  }

gsl_ran_shuffle (r, a, 52, sizeof (int));
```

int **gsl_ran_choose**(const *gsl_rng* *r, void *dest, size_t k, void *src, size_t n, size_t size)

This function fills the array `dest[k]` with *k* objects taken randomly from the *n* elements of the array `src[0..n-1]`. The objects are each of size *size*. The output of the random number generator *r* is used to make the selection. The algorithm ensures all possible samples are equally likely, assuming a perfect source of randomness.

The objects are sampled **without** replacement, thus each object can only appear once in *dest*. It is required that *k* be less than or equal to *n*. The objects in *dest* will be in the same relative order as those in *src*. You will need to call `gsl_ran_shuffle(r, dest, n, size)` if you want to randomize the order.

The following code shows how to select a random sample of three unique numbers from the set 0 to 99:

```
double a[3], b[100];

for (i = 0; i < 100; i++)
  {
    b[i] = (double) i;
  }

gsl_ran_choose (r, a, 3, b, 100, sizeof (double));
```

void **gsl_ran_sample**(const *gsl_rng* *r, void *dest, size_t k, void *src, size_t n, size_t size)

This function is like *gsl_ran_choose()* but samples *k* items from the original array of *n* items *src* with replacement, so the same object can appear more than once in the output sequence *dest*. There is no requirement that *k* be less than *n* in this case.

20.41 Examples

The following program demonstrates the use of a random number generator to produce variates from a distribution. It prints 10 samples from the Poisson distribution with a mean of 3.

```
#include <stdio.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>

int
main (void)
{
  const gsl_rng_type * T;
  gsl_rng * r;

  int i, n = 10;
  double mu = 3.0;

  /* create a generator chosen by the
     environment variable GSL_RNG_TYPE */

  gsl_rng_env_setup();

  T = gsl_rng_default;
  r = gsl_rng_alloc (T);

  /* print n random variates chosen from
     the poisson distribution with mean
     parameter mu */

  for (i = 0; i < n; i++)
    {
      unsigned int k = gsl_ran_poisson (r, mu);
      printf (" %u", k);
    }

  printf ("\n");
  gsl_rng_free (r);
  return 0;
}
```

If the library and header files are installed under `/usr/local` (the default location) then the program can be compiled with these options:

```
$ gcc -Wall demo.c -lgsl -lgslcblas -lm
```

Here is the output of the program,

```
 2 5 5 2 1 0 3 4 1 1
```

The variates depend on the seed used by the generator. The seed for the default generator type `gsl_rng_default` can be changed with the `GSL_RNG_SEED` environment variable to produce a different stream of variates:

```
$ GSL_RNG_SEED=123 ./a.out
```

giving output

```
 4 5 6 3 3 1 4 2 5 5
```

The following program generates a random walk in two dimensions.

```
#include <stdio.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>

int
main (void)
{
  int i;
  double x = 0, y = 0, dx, dy;

  const gsl_rng_type * T;
  gsl_rng * r;

  gsl_rng_env_setup();
  T = gsl_rng_default;
  r = gsl_rng_alloc (T);

  printf ("%g %g\n", x, y);

  for (i = 0; i < 10; i++)
    {
      gsl_ran_dir_2d (r, &dx, &dy);
      x += dx; y += dy;
      printf ("%g %g\n", x, y);
    }

  gsl_rng_free (r);
  return 0;
}
```

Fig. 20.1 shows the output from the program.

The following program computes the upper and lower cumulative distribution functions for the standard normal distribution at $x = 2$.

```
#include <stdio.h>
#include <gsl/gsl_cdf.h>

int
main (void)
{
  double P, Q;
  double x = 2.0;

  P = gsl_cdf_ugaussian_P (x);
  printf ("prob(x < %f) = %f\n", x, P);
```

(continues on next page)

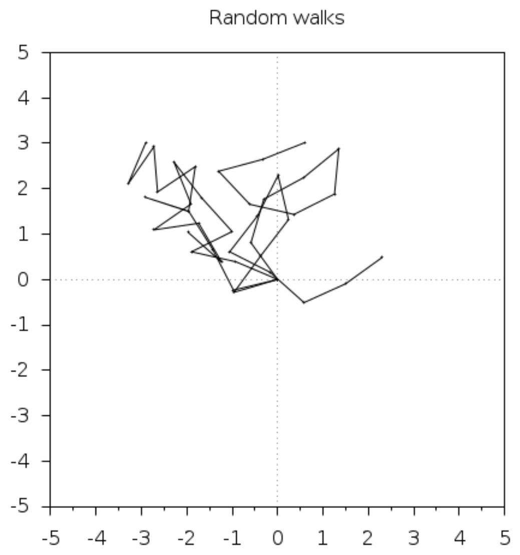


Fig. 20.1: Four 10-step random walks from the origin.

(continued from previous page)

```
  Q = gsl_cdf_ugaussian_Q (x);
  printf ("prob(x > %f) = %f\n", x, Q);

  x = gsl_cdf_ugaussian_Pinv (P);
  printf ("Pinv(%f) = %f\n", P, x);

  x = gsl_cdf_ugaussian_Qinv (Q);
  printf ("Qinv(%f) = %f\n", Q, x);

  return 0;
}
```

Here is the output of the program,

```
prob(x < 2.000000) = 0.977250
prob(x > 2.000000) = 0.022750
Pinv(0.977250) = 2.000000
Qinv(0.022750) = 2.000000
```

20.42 References and Further Reading

For an encyclopaedic coverage of the subject readers are advised to consult the book “Non-Uniform Random Variate Generation” by Luc Devroye. It covers every imaginable distribution and provides hundreds of algorithms.

- Luc Devroye, “Non-Uniform Random Variate Generation”, Springer-Verlag, ISBN 0-387-96305-7. Available online at http://cg.scs.carleton.ca/~luc/rnbookindex.html.

The subject of random variate generation is also reviewed by Knuth, who describes algorithms for all the major distributions.

- Donald E. Knuth, "The Art of Computer Programming: Seminumerical Algorithms" (Vol 2, 3rd Ed, 1997), Addison-Wesley, ISBN 0201896842.

The Particle Data Group provides a short review of techniques for generating distributions of random numbers in the "Monte Carlo" section of its Annual Review of Particle Physics.

- Review of Particle Properties, R.M. Barnett et al., Physical Review D54, 1 (1996) http://pdg.lbl.gov/.

The Review of Particle Physics is available online in postscript and pdf format.

An overview of methods used to compute cumulative distribution functions can be found in *Statistical Computing* by W.J. Kennedy and J.E. Gentle. Another general reference is *Elements of Statistical Computing* by R.A. Thisted.

- William E. Kennedy and James E. Gentle, Statistical Computing (1980), Marcel Dekker, ISBN 0-8247-6898-1.
- Ronald A. Thisted, Elements of Statistical Computing (1988), Chapman & Hall, ISBN 0-412-01371-1.

The cumulative distribution functions for the Gaussian distribution are based on the following papers,

- Rational Chebyshev Approximations Using Linear Equations, W.J. Cody, W. Fraser, J.F. Hart. Numerische Mathematik 12, 242–251 (1968).
- Rational Chebyshev Approximations for the Error Function, W.J. Cody. Mathematics of Computation 23, n107, 631–637 (July 1969).

CHAPTER

TWENTYONE

STATISTICS

This chapter describes the statistical functions in the library. The basic statistical functions include routines to compute the mean, variance and standard deviation. More advanced functions allow you to calculate absolute deviations, skewness, and kurtosis as well as the median and arbitrary percentiles. The algorithms use recurrence relations to compute average quantities in a stable way, without large intermediate values that might overflow.

The functions are available in versions for datasets in the standard floating-point and integer types. The versions for double precision floating-point data have the prefix `gsl_stats` and are declared in the header file `gsl_statistics_double.h`. The versions for integer data have the prefix `gsl_stats_int` and are declared in the header file `gsl_statistics_int.h`. All the functions operate on C arrays with a `stride` parameter specifying the spacing between elements.

21.1 Mean, Standard Deviation and Variance

double **gsl_stats_mean**(const double data[], size_t stride, size_t n)

This function returns the arithmetic mean of `data`, a dataset of length `n` with stride `stride`. The arithmetic mean, or *sample mean*, is denoted by $\hat{\mu}$ and defined as,

$$\hat{\mu} = \frac{1}{N} \sum x_i$$

where x_i are the elements of the dataset `data`. For samples drawn from a gaussian distribution the variance of $\hat{\mu}$ is σ^2/N.

double **gsl_stats_variance**(const double data[], size_t stride, size_t n)

This function returns the estimated, or *sample*, variance of `data`, a dataset of length `n` with stride `stride`. The estimated variance is denoted by $\hat{\sigma}^2$ and is defined by,

$$\hat{\sigma}^2 = \frac{1}{(N-1)} \sum (x_i - \hat{\mu})^2$$

where x_i are the elements of the dataset `data`. Note that the normalization factor of $1/(N-1)$ results from the derivation of $\hat{\sigma}^2$ as an unbiased estimator of the population variance σ^2. For samples drawn from a Gaussian distribution the variance of $\hat{\sigma}^2$ itself is $2\sigma^4/N$.

This function computes the mean via a call to `gsl_stats_mean()`. If you have already computed the mean then you can pass it directly to `gsl_stats_variance_m()`.

double **gsl_stats_variance_m**(const double data[], size_t stride, size_t n, double mean)

This function returns the sample variance of `data` relative to the given value of `mean`. The function is computed with $\hat{\mu}$ replaced by the value of `mean` that you supply,

$$\hat{\sigma}^2 = \frac{1}{(N-1)} \sum (x_i - mean)^2$$

double **gsl_stats_sd**(const double data[], size_t stride, size_t n)

double **gsl_stats_sd_m**(const double data[], size_t stride, size_t n, double mean)

The standard deviation is defined as the square root of the variance. These functions return the square root of the corresponding variance functions above.

double **gsl_stats_tss**(const double data[], size_t stride, size_t n)

double **gsl_stats_tss_m**(const double data[], size_t stride, size_t n, double mean)

These functions return the total sum of squares (TSS) of `data` about the mean. For `gsl_stats_tss_m()` the user-supplied value of `mean` is used, and for `gsl_stats_tss()` it is computed using `gsl_stats_mean()`.

$$\text{TSS} = \sum (x_i - mean)^2$$

double **gsl_stats_variance_with_fixed_mean**(const double data[], size_t stride, size_t n, double mean)

This function computes an unbiased estimate of the variance of `data` when the population mean `mean` of the underlying distribution is known *a priori*. In this case the estimator for the variance uses the factor $1/N$ and the sample mean $\hat{\mu}$ is replaced by the known population mean μ,

$$\hat{\sigma}^2 = \frac{1}{N} \sum (x_i - \mu)^2$$

double **gsl_stats_sd_with_fixed_mean**(const double data[], size_t stride, size_t n, double mean)

This function calculates the standard deviation of `data` for a fixed population mean `mean`. The result is the square root of the corresponding variance function.

21.2 Absolute deviation

double **gsl_stats_absdev**(const double data[], size_t stride, size_t n)

This function computes the absolute deviation from the mean of `data`, a dataset of length `n` with stride `stride`. The absolute deviation from the mean is defined as,

$$absdev = \frac{1}{N} \sum |x_i - \hat{\mu}|$$

where x_i are the elements of the dataset `data`. The absolute deviation from the mean provides a more robust measure of the width of a distribution than the variance. This function computes the mean of `data` via a call to `gsl_stats_mean()`.

double **gsl_stats_absdev_m**(const double data[], size_t stride, size_t n, double mean)

This function computes the absolute deviation of the dataset `data` relative to the given value of `mean`,

$$absdev = \frac{1}{N} \sum |x_i - mean|$$

This function is useful if you have already computed the mean of `data` (and want to avoid recomputing it), or wish to calculate the absolute deviation relative to another value (such as zero, or the median).

21.3 Higher moments (skewness and kurtosis)

double **gsl_stats_skew**(const double data[], size_t stride, size_t n)

This function computes the skewness of *data*, a dataset of length *n* with stride *stride*. The skewness is defined as,

$$skew = \frac{1}{N}\sum\left(\frac{x_i - \hat{\mu}}{\hat{\sigma}}\right)^3$$

where x_i are the elements of the dataset *data*. The skewness measures the asymmetry of the tails of a distribution.

The function computes the mean and estimated standard deviation of *data* via calls to *gsl_stats_mean()* and *gsl_stats_sd()*.

double **gsl_stats_skew_m_sd**(const double data[], size_t stride, size_t n, double mean, double sd)

This function computes the skewness of the dataset *data* using the given values of the mean *mean* and standard deviation *sd*,

$$skew = \frac{1}{N}\sum\left(\frac{x_i - mean}{sd}\right)^3$$

These functions are useful if you have already computed the mean and standard deviation of *data* and want to avoid recomputing them.

double **gsl_stats_kurtosis**(const double data[], size_t stride, size_t n)

This function computes the kurtosis of *data*, a dataset of length *n* with stride *stride*. The kurtosis is defined as,

$$kurtosis = \left(\frac{1}{N}\sum\left(\frac{x_i - \hat{\mu}}{\hat{\sigma}}\right)^4\right) - 3$$

The kurtosis measures how sharply peaked a distribution is, relative to its width. The kurtosis is normalized to zero for a Gaussian distribution.

double **gsl_stats_kurtosis_m_sd**(const double data[], size_t stride, size_t n, double mean, double sd)

This function computes the kurtosis of the dataset *data* using the given values of the mean *mean* and standard deviation *sd*,

$$kurtosis = \frac{1}{N}\left(\sum\left(\frac{x_i - mean}{sd}\right)^4\right) - 3$$

This function is useful if you have already computed the mean and standard deviation of *data* and want to avoid recomputing them.

21.4 Autocorrelation

double **gsl_stats_lag1_autocorrelation**(const double data[], const size_t stride, const size_t n)

This function computes the lag-1 autocorrelation of the dataset *data*.

$$a_1 = \frac{\sum_{i=2}^{n}(x_i - \hat{\mu})(x_{i-1} - \hat{\mu})}{\sum_{i=1}^{n}(x_i - \hat{\mu})(x_i - \hat{\mu})}$$

double **gsl_stats_lag1_autocorrelation_m**(const double data[], const size_t stride, const size_t n, const double mean)

This function computes the lag-1 autocorrelation of the dataset *data* using the given value of the mean *mean*.

21.5 Covariance

double **gsl_stats_covariance**(const double data1[], const size_t stride1, const double data2[], const size_t stride2, const size_t n)

This function computes the covariance of the datasets *data1* and *data2* which must both be of the same length *n*.

$$covar = \frac{1}{(n-1)} \sum_{i=1}^{n} (x_i - \hat{x})(y_i - \hat{y})$$

double **gsl_stats_covariance_m**(const double data1[], const size_t stride1, const double data2[], const size_t stride2, const size_t n, const double mean1, const double mean2)

This function computes the covariance of the datasets *data1* and *data2* using the given values of the means, *mean1* and *mean2*. This is useful if you have already computed the means of *data1* and *data2* and want to avoid recomputing them.

21.6 Correlation

double **gsl_stats_correlation**(const double data1[], const size_t stride1, const double data2[], const size_t stride2, const size_t n)

This function efficiently computes the Pearson correlation coefficient between the datasets *data1* and *data2* which must both be of the same length *n*.

$$r = \frac{cov(x,y)}{\hat{\sigma}_x \hat{\sigma}_y} = \frac{\frac{1}{n-1} \sum (x_i - \hat{x})(y_i - \hat{y})}{\sqrt{\frac{1}{n-1} \sum (x_i - \hat{x})^2} \sqrt{\frac{1}{n-1} \sum (y_i - \hat{y})^2}}$$

double **gsl_stats_spearman**(const double data1[], const size_t stride1, const double data2[], const size_t stride2, const size_t n, double work[])

This function computes the Spearman rank correlation coefficient between the datasets *data1* and *data2* which must both be of the same length *n*. Additional workspace of size 2 * *n* is required in *work*. The Spearman rank correlation between vectors x and y is equivalent to the Pearson correlation between the ranked vectors x_R and y_R, where ranks are defined to be the average of the positions of an element in the ascending order of the values.

21.7 Weighted Samples

The functions described in this section allow the computation of statistics for weighted samples. The functions accept an array of samples, x_i, with associated weights, w_i. Each sample x_i is considered as having been drawn from a Gaussian distribution with variance σ_i^2. The sample weight w_i is defined as the reciprocal of this variance, $w_i = 1/\sigma_i^2$. Setting a weight to zero corresponds to removing a sample from a dataset.

double **gsl_stats_wmean**(const double w[], size_t wstride, const double data[], size_t stride, size_t n)

This function returns the weighted mean of the dataset *data* with stride *stride* and length *n*, using the set of weights *w* with stride *wstride* and length *n*. The weighted mean is defined as,

$$\hat{\mu} = \frac{\sum w_i x_i}{\sum w_i}$$

double **gsl_stats_wvariance**(const double w[], size_t wstride, const double data[], size_t stride, size_t n)

This function returns the estimated variance of the dataset *data* with stride *stride* and length *n*, using the set of weights *w* with stride *wstride* and length *n*. The estimated variance of a weighted dataset is calculated as,

$$\hat{\sigma}^2 = \frac{\sum w_i}{(\sum w_i)^2 - \sum (w_i^2)} \sum w_i (x_i - \hat{\mu})^2$$

Note that this expression reduces to an unweighted variance with the familiar $1/(N-1)$ factor when there are N equal non-zero weights.

double **gsl_stats_wvariance_m**(const double w[], size_t wstride, const double data[], size_t stride, size_t n, double wmean)

This function returns the estimated variance of the weighted dataset *data* using the given weighted mean *wmean*.

double **gsl_stats_wsd**(const double w[], size_t wstride, const double data[], size_t stride, size_t n)

The standard deviation is defined as the square root of the variance. This function returns the square root of the corresponding variance function *gsl_stats_wvariance()* above.

double **gsl_stats_wsd_m**(const double w[], size_t wstride, const double data[], size_t stride, size_t n, double wmean)

This function returns the square root of the corresponding variance function *gsl_stats_wvariance_m()* above.

double **gsl_stats_wvariance_with_fixed_mean**(const double w[], size_t wstride, const double data[], size_t stride, size_t n, const double mean)

This function computes an unbiased estimate of the variance of the weighted dataset *data* when the population mean *mean* of the underlying distribution is known *a priori*. In this case the estimator for the variance replaces the sample mean $\hat{\mu}$ by the known population mean μ,

$$\hat{\sigma}^2 = \frac{\sum w_i (x_i - \mu)^2}{\sum w_i}$$

double **gsl_stats_wsd_with_fixed_mean**(const double w[], size_t wstride, const double data[], size_t stride, size_t n, const double mean)

The standard deviation is defined as the square root of the variance. This function returns the square root of the corresponding variance function above.

double **gsl_stats_wtss**(const double w[], const size_t wstride, const double data[], size_t stride, size_t n)

double **gsl_stats_wtss_m**(const double w[], const size_t wstride, const double data[], size_t stride, size_t n, double wmean)

These functions return the weighted total sum of squares (TSS) of *data* about the weighted mean. For *gsl_stats_wtss_m()* the user-supplied value of *wmean* is used, and for *gsl_stats_wtss()* it is computed using *gsl_stats_wmean()*.

$$\text{TSS} = \sum w_i (x_i - wmean)^2$$

double **gsl_stats_wabsdev**(const double w[], size_t wstride, const double data[], size_t stride, size_t n)

This function computes the weighted absolute deviation from the weighted mean of *data*. The absolute deviation from the mean is defined as,

$$absdev = \frac{\sum w_i |x_i - \hat{\mu}|}{\sum w_i}$$

double **gsl_stats_wabsdev_m**(const double w[], size_t wstride, const double data[], size_t stride, size_t n, double wmean)

This function computes the absolute deviation of the weighted dataset *data* about the given weighted mean *wmean*.

double **gsl_stats_wskew**(const double w[], size_t wstride, const double data[], size_t stride, size_t n)

This function computes the weighted skewness of the dataset *data*.

$$skew = \frac{\sum w_i((x_i - \hat{x})/\hat{\sigma})^3}{\sum w_i}$$

double **gsl_stats_wskew_m_sd**(const double w[], size_t wstride, const double data[], size_t stride, size_t n, double wmean, double wsd)

This function computes the weighted skewness of the dataset *data* using the given values of the weighted mean and weighted standard deviation, *wmean* and *wsd*.

double **gsl_stats_wkurtosis**(const double w[], size_t wstride, const double data[], size_t stride, size_t n)

This function computes the weighted kurtosis of the dataset *data*.

$$kurtosis = \frac{\sum w_i((x_i - \hat{x})/\hat{\sigma})^4}{\sum w_i} - 3$$

double **gsl_stats_wkurtosis_m_sd**(const double w[], size_t wstride, const double data[], size_t stride, size_t n, double wmean, double wsd)

This function computes the weighted kurtosis of the dataset *data* using the given values of the weighted mean and weighted standard deviation, *wmean* and *wsd*.

21.8 Maximum and Minimum values

The following functions find the maximum and minimum values of a dataset (or their indices). If the data contains `NaN`-s then a `NaN` will be returned, since the maximum or minimum value is undefined. For functions which return an index, the location of the first `NaN` in the array is returned.

double **gsl_stats_max**(const double data[], size_t stride, size_t n)

This function returns the maximum value in *data*, a dataset of length *n* with stride *stride*. The maximum value is defined as the value of the element x_i which satisfies $x_i \geq x_j$ for all j.

If you want instead to find the element with the largest absolute magnitude you will need to apply `fabs()` or `abs()` to your data before calling this function.

double **gsl_stats_min**(const double data[], size_t stride, size_t n)

This function returns the minimum value in *data*, a dataset of length *n* with stride *stride*. The minimum value is defined as the value of the element x_i which satisfies $x_i \leq x_j$ for all j.

If you want instead to find the element with the smallest absolute magnitude you will need to apply `fabs()` or `abs()` to your data before calling this function.

void **gsl_stats_minmax**(double *min, double *max, const double data[], size_t stride, size_t n)

This function finds both the minimum and maximum values *min*, *max* in *data* in a single pass.

size_t **gsl_stats_max_index**(const double data[], size_t stride, size_t n)

This function returns the index of the maximum value in *data*, a dataset of length *n* with stride *stride*. The maximum value is defined as the value of the element x_i which satisfies $x_i \geq x_j$ for all j. When there are several equal maximum elements then the first one is chosen.

size_t **gsl_stats_min_index**(const double data[], size_t stride, size_t n)

This function returns the index of the minimum value in *data*, a dataset of length *n* with stride *stride*. The minimum value is defined as the value of the element x_i which satisfies $x_i \geq x_j$ for all j. When there are several equal minimum elements then the first one is chosen.

void **gsl_stats_minmax_index**(size_t *min_index, size_t *max_index, const double data[], size_t stride, size_t n)

This function returns the indexes *min_index*, *max_index* of the minimum and maximum values in *data* in a single pass.

21.9 Median and Percentiles

The median and percentile functions described in this section operate on sorted data in $O(1)$ time. There is also a routine for computing the median of an unsorted input array in average $O(n)$ time using the quickselect algorithm. For convenience we use *quantiles*, measured on a scale of 0 to 1, instead of percentiles (which use a scale of 0 to 100).

double **gsl_stats_median_from_sorted_data**(const double sorted_data[], const size_t stride, const size_t n)

This function returns the median value of `sorted_data`, a dataset of length `n` with stride `stride`. The elements of the array must be in ascending numerical order. There are no checks to see whether the data are sorted, so the function `gsl_sort()` should always be used first.

When the dataset has an odd number of elements the median is the value of element $(n-1)/2$. When the dataset has an even number of elements the median is the mean of the two nearest middle values, elements $(n-1)/2$ and $n/2$. Since the algorithm for computing the median involves interpolation this function always returns a floating-point number, even for integer data types.

double **gsl_stats_median**(double data[], const size_t stride, const size_t n)

This function returns the median value of `data`, a dataset of length `n` with stride `stride`. The median is found using the quickselect algorithm. The input array does not need to be sorted, but note that the algorithm rearranges the array and so the input is not preserved on output.

double **gsl_stats_quantile_from_sorted_data**(const double sorted_data[], size_t stride, size_t n, double f)

This function returns a quantile value of `sorted_data`, a double-precision array of length `n` with stride `stride`. The elements of the array must be in ascending numerical order. The quantile is determined by the `f`, a fraction between 0 and 1. For example, to compute the value of the 75th percentile `f` should have the value 0.75.

There are no checks to see whether the data are sorted, so the function `gsl_sort()` should always be used first.

The quantile is found by interpolation, using the formula

$$\text{quantile} = (1-\delta)x_i + \delta x_{i+1}$$

where i is `floor((n - 1)f)` and δ is $(n-1)f - i$.

Thus the minimum value of the array (`data[0*stride]`) is given by `f` equal to zero, the maximum value (`data[(n-1)*stride]`) is given by `f` equal to one and the median value is given by `f` equal to 0.5. Since the algorithm for computing quantiles involves interpolation this function always returns a floating-point number, even for integer data types.

21.10 Order Statistics

The k-th *order statistic* of a sample is equal to its k-th smallest value. The k-th order statistic of a set of n values $x = \{x_i\}, 1 \le i \le n$ is denoted $x_{(k)}$. The median of the set x is equal to $x_{\left(\frac{n}{2}\right)}$ if n is odd, or the average of $x_{\left(\frac{n}{2}\right)}$ and $x_{\left(\frac{n}{2}+1\right)}$ if n is even. The k-th smallest element of a length n vector can be found in average $O(n)$ time using the quickselect algorithm.

double **gsl_stats_select**(double data[], const size_t stride, const size_t n, const size_t k)

This function finds the `k`-th smallest element of the input array `data` of length `n` and stride `stride` using the quickselect method. The algorithm rearranges the elements of `data` and so the input array is not preserved on output.

21.11 Robust Location Estimates

A *location estimate* refers to a typical or central value which best describes a given dataset. The mean and median are both examples of location estimators. However, the mean has a severe sensitivity to data outliers and can give erroneous values when even a small number of outliers are present. The median on the other hand, has a strong insensitivity to data outliers, but due to its non-smoothness it can behave unexpectedly in certain situations. GSL offers the following alternative location estimators, which are robust to the presence of outliers.

21.11.1 Trimmed Mean

The trimmed mean, or *truncated mean*, discards a certain number of smallest and largest samples from the input vector before computing the mean of the remaining samples. The amount of trimming is specified by a factor $\alpha \in [0, 0.5]$. Then the number of samples discarded from both ends of the input vector is $\lfloor \alpha n \rfloor$, where n is the length of the input. So to discard 25% of the samples from each end, one would set $\alpha = 0.25$.

double **gsl_stats_trmean_from_sorted_data**(const double alpha, const double sorted_data[], const size_t stride, const size_t n)

This function returns the trimmed mean of `sorted_data`, a dataset of length `n` with stride `stride`. The elements of the array must be in ascending numerical order. There are no checks to see whether the data are sorted, so the function `gsl_sort()` should always be used first. The trimming factor α is given in `alpha`. If $\alpha \geq 0.5$, then the median of the input is returned.

21.11.2 Gastwirth Estimator

Gastwirth's location estimator is a weighted sum of three order statistics,

$$gastwirth = 0.3 \times Q_{\frac{1}{3}} + 0.4 \times Q_{\frac{1}{2}} + 0.3 \times Q_{\frac{2}{3}}$$

where $Q_{\frac{1}{3}}$ is the one-third quantile, $Q_{\frac{1}{2}}$ is the one-half quantile (i.e. median), and $Q_{\frac{2}{3}}$ is the two-thirds quantile.

double **gsl_stats_gastwirth_from_sorted_data**(const double sorted_data[], const size_t stride, const size_t n)

This function returns the Gastwirth location estimator of `sorted_data`, a dataset of length `n` with stride `stride`. The elements of the array must be in ascending numerical order. There are no checks to see whether the data are sorted, so the function `gsl_sort()` should always be used first.

21.12 Robust Scale Estimates

A *robust scale estimate*, also known as a robust measure of scale, attempts to quantify the statistical dispersion (variability, scatter, spread) in a set of data which may contain outliers. In such datasets, the usual variance or standard deviation scale estimate can be rendered useless by even a single outlier.

21.12.1 Median Absolute Deviation (MAD)

The median absolute deviation (MAD) is defined as

$$MAD = 1.4826 \times \text{median}\left\{|x_i - \text{median}\left(x\right)|\right\}$$

In words, first the median of all samples is computed. Then the median is subtracted from all samples in the input to find the deviation of each sample from the median. The median of all absolute deviations is then the MAD. The factor 1.4826 makes the MAD an unbiased estimator of the standard deviation for Gaussian data. The median absolute deviation has an asymptotic efficiency of 37%.

double **gsl_stats_mad0**(const double data[], const size_t stride, const size_t n, double work[])

double **gsl_stats_mad**(const double data[], const size_t stride, const size_t n, double work[])

These functions return the median absolute deviation of *data*, a dataset of length *n* and stride *stride*. The `mad0` function calculates $\mathrm{median}\left\{\left|x_i - \mathrm{median}\left(x\right)\right|\right\}$ (i.e. the MAD statistic without the bias correction scale factor). These functions require additional workspace of size `n` provided in *work*.

21.12.2 S_n Statistic

The S_n statistic developed by Croux and Rousseeuw is defined as

$$S_n = 1.1926 \times c_n \times \mathrm{median}_i \left\{ \mathrm{median}_j \left(\left| x_i - x_j \right| \right) \right\}$$

For each sample $x_i, 1 \le i \le n$, the median of the values $\left|x_i - x_j\right|$ is computed for all $x_j, 1 \le j \le n$. This yields n values, whose median then gives the final S_n. The factor 1.1926 makes S_n an unbiased estimate of the standard deviation for Gaussian data. The factor c_n is a correction factor to correct bias in small sample sizes. S_n has an asymptotic efficiency of 58%.

double **gsl_stats_Sn0_from_sorted_data**(const double sorted_data[], const size_t stride, const size_t n, double work[])

double **gsl_stats_Sn_from_sorted_data**(const double sorted_data[], const size_t stride, const size_t n, double work[])

These functions return the S_n statistic of *sorted_data*, a dataset of length *n* with stride *stride*. The elements of the array must be in ascending numerical order. There are no checks to see whether the data are sorted, so the function *gsl_sort()* should always be used first. The `Sn0` function calculates $\mathrm{median}_i \left\{ \mathrm{median}_j \left(\left| x_i - x_j \right| \right) \right\}$ (i.e. the S_n statistic without the bias correction scale factors). These functions require additional workspace of size `n` provided in *work*.

21.12.3 Q_n Statistic

The Q_n statistic developed by Croux and Rousseeuw is defined as

$$Q_n = 2.21914 \times d_n \times \left\{ \left| x_i - x_j \right|, i < j \right\}_{(k)}$$

The factor 2.21914 makes Q_n an unbiased estimate of the standard deviation for Gaussian data. The factor d_n is a correction factor to correct bias in small sample sizes. The order statistic is

$$k = \begin{pmatrix} \left\lfloor \frac{n}{2} \right\rfloor + 1 \\ 2 \end{pmatrix}$$

Q_n has an asymptotic efficiency of 82%.

double **gsl_stats_Qn0_from_sorted_data**(const double sorted_data[], const size_t stride, const size_t n, double work[], int work_int[])

double **gsl_stats_Qn_from_sorted_data**(const double sorted_data[], const size_t stride, const size_t n, double work[], int work_int[])

These functions return the Q_n statistic of *sorted_data*, a dataset of length *n* with stride *stride*. The elements of the array must be in ascending numerical order. There are no checks to see whether the data are sorted, so the function *gsl_sort()* should always be used first. The `Qn0` function calculates $\left\{ \left| x_i - x_j \right|, i < j \right\}_{(k)}$ (i.e. Q_n without the bias correction scale factors). These functions require additional workspace of size `3n` provided in *work* and integer workspace of size `5n` provided in *work_int*.

21.13 Examples

Here is a basic example of how to use the statistical functions:

```
#include <stdio.h>
#include <gsl/gsl_statistics.h>

int
main(void)
{
  double data[5] = {17.2, 18.1, 16.5, 18.3, 12.6};
  double mean, variance, largest, smallest;

  mean     = gsl_stats_mean(data, 1, 5);
  variance = gsl_stats_variance(data, 1, 5);
  largest  = gsl_stats_max(data, 1, 5);
  smallest = gsl_stats_min(data, 1, 5);

  printf ("The dataset is %g, %g, %g, %g, %g\n",
         data[0], data[1], data[2], data[3], data[4]);

  printf ("The sample mean is %g\n", mean);
  printf ("The estimated variance is %g\n", variance);
  printf ("The largest value is %g\n", largest);
  printf ("The smallest value is %g\n", smallest);
  return 0;
}
```

The program should produce the following output,

```
The dataset is 17.2, 18.1, 16.5, 18.3, 12.6
The sample mean is 16.54
The estimated variance is 5.373
The largest value is 18.3
The smallest value is 12.6
```

Here is an example using sorted data,

```
#include <stdio.h>
#include <gsl/gsl_sort.h>
#include <gsl/gsl_statistics.h>

int
main(void)
{
  double data[5] = {17.2, 18.1, 16.5, 18.3, 12.6};
  double median, upperq, lowerq;

  printf ("Original dataset:  %g, %g, %g, %g, %g\n",
         data[0], data[1], data[2], data[3], data[4]);

  gsl_sort (data, 1, 5);
```

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```
  printf ("Sorted dataset: %g, %g, %g, %g, %g\n",
         data[0], data[1], data[2], data[3], data[4]);

  median
    = gsl_stats_median_from_sorted_data (data,
                                         1, 5);

  upperq
    = gsl_stats_quantile_from_sorted_data (data,
                                           1, 5,
                                           0.75);
  lowerq
    = gsl_stats_quantile_from_sorted_data (data,
                                           1, 5,
                                           0.25);

  printf ("The median is %g\n", median);
  printf ("The upper quartile is %g\n", upperq);
  printf ("The lower quartile is %g\n", lowerq);
  return 0;
}
```

This program should produce the following output,

```
Original dataset:  17.2, 18.1, 16.5, 18.3, 12.6
Sorted dataset: 12.6, 16.5, 17.2, 18.1, 18.3
The median is 17.2
The upper quartile is 18.1
The lower quartile is 16.5
```

21.14 References and Further Reading

The standard reference for almost any topic in statistics is the multi-volume *Advanced Theory of Statistics* by Kendall and Stuart.

- Maurice Kendall, Alan Stuart, and J. Keith Ord. *The Advanced Theory of Statistics* (multiple volumes) reprinted as *Kendall's Advanced Theory of Statistics*. Wiley, ISBN 047023380X.

Many statistical concepts can be more easily understood by a Bayesian approach. The following book by Gelman, Carlin, Stern and Rubin gives a comprehensive coverage of the subject.

- Andrew Gelman, John B. Carlin, Hal S. Stern, Donald B. Rubin. *Bayesian Data Analysis*. Chapman & Hall, ISBN 0412039915.

For physicists the Particle Data Group provides useful reviews of Probability and Statistics in the "Mathematical Tools" section of its Annual Review of Particle Physics.

- *Review of Particle Properties*, R.M. Barnett et al., Physical Review D54, 1 (1996)

The Review of Particle Physics is available online at the website http://pdg.lbl.gov/.

The following papers describe robust scale estimation,

- C. Croux and P. J. Rousseeuw, *Time-Efficient algorithms for two highly robust estimators of scale*, Comp. Stat., Physica, Heidelberg, 1992.

- P. J. Rousseeuw and C. Croux, *Explicit scale estimators with high breakdown point*, L1-Statistical Analysis and Related Methods, pp. 77-92, 1992.

CHAPTER

TWENTYTWO

RUNNING STATISTICS

This chapter describes routines for computing running statistics, also known as online statistics, of data. These routines are suitable for handling large datasets for which it may be inconvenient or impractical to store in memory all at once. The data can be processed in a single pass, one point at a time. Each time a data point is added to the accumulator, internal parameters are updated in order to compute the current mean, variance, standard deviation, skewness, and kurtosis. These statistics are exact, and are updated with numerically stable single-pass algorithms. The median and arbitrary quantiles are also available, however these calculations use algorithms which provide approximations, and grow more accurate as more data is added to the accumulator.

The functions described in this chapter are declared in the header file `gsl_rstat.h`.

22.1 Initializing the Accumulator

type **`gsl_rstat_workspace`**

This workspace contains parameters used to calculate various statistics and are updated after each data point is added to the accumulator.

gsl_rstat_workspace ***`gsl_rstat_alloc`**(void)

This function allocates a workspace for computing running statistics. The size of the workspace is $O(1)$.

void **`gsl_rstat_free`**(*gsl_rstat_workspace* *w)

This function frees the memory associated with the workspace *`w`*.

int **`gsl_rstat_reset`**(*gsl_rstat_workspace* *w)

This function resets the workspace *`w`* to its initial state, so it can begin working on a new set of data.

22.2 Adding Data to the Accumulator

int **`gsl_rstat_add`**(const double x, *gsl_rstat_workspace* *w)

This function adds the data point *`x`* to the statistical accumulator, updating calculations of the mean, variance, standard deviation, skewness, kurtosis, and median.

size_t **`gsl_rstat_n`**(const *gsl_rstat_workspace* *w)

This function returns the number of data so far added to the accumulator.

22.3 Current Statistics

double **gsl_rstat_min**(const *gsl_rstat_workspace* *w)

This function returns the minimum value added to the accumulator.

double **gsl_rstat_max**(const *gsl_rstat_workspace* *w)

This function returns the maximum value added to the accumulator.

double **gsl_rstat_mean**(const *gsl_rstat_workspace* *w)

This function returns the mean of all data added to the accumulator, defined as

$$\hat{\mu} = \frac{1}{N}\sum x_i$$

double **gsl_rstat_variance**(const *gsl_rstat_workspace* *w)

This function returns the variance of all data added to the accumulator, defined as

$$\hat{\sigma}^2 = \frac{1}{(N-1)}\sum (x_i - \hat{\mu})^2$$

double **gsl_rstat_sd**(const *gsl_rstat_workspace* *w)

This function returns the standard deviation of all data added to the accumulator, defined as the square root of the variance given above.

double **gsl_rstat_sd_mean**(const *gsl_rstat_workspace* *w)

This function returns the standard deviation of the mean, defined as

$$\hat{\sigma}_{\hat{\mu}} = \frac{\hat{\sigma}}{\sqrt{N}}$$

double **gsl_rstat_rms**(const *gsl_rstat_workspace* *w)

This function returns the root mean square of all data added to the accumulator, defined as

$$rms = \sqrt{\frac{1}{N}\sum x_i^2}$$

double **gsl_rstat_skew**(const *gsl_rstat_workspace* *w)

This function returns the skewness of all data added to the accumulator, defined as

$$skew = \frac{1}{N}\sum \left(\frac{x_i - \hat{\mu}}{\hat{\sigma}}\right)^3$$

double **gsl_rstat_kurtosis**(const *gsl_rstat_workspace* *w)

This function returns the kurtosis of all data added to the accumulator, defined as

$$kurtosis = \left(\frac{1}{N}\sum \left(\frac{x_i - \hat{\mu}}{\hat{\sigma}}\right)^4\right) - 3$$

double **gsl_rstat_median**(*gsl_rstat_workspace* *w)

This function returns an estimate of the median of the data added to the accumulator.

22.4 Quantiles

The functions in this section estimate quantiles dynamically without storing the entire dataset, using the algorithm of Jain and Chlamtec, 1985. Only five points (markers) are stored which represent the minimum and maximum of the data, as well as current estimates of the $p/2$-, p-, and $(1+p)/2$-quantiles. Each time a new data point is added, the marker positions and heights are updated.

type **gsl_rstat_quantile_workspace**

This workspace contains parameters for estimating quantiles of the current dataset

gsl_rstat_quantile_workspace ***gsl_rstat_quantile_alloc**(const double p)

This function allocates a workspace for the dynamic estimation of `p`-quantiles, where `p` is between 0 and 1. The median corresponds to $p = 0.5$. The size of the workspace is $O(1)$.

void **gsl_rstat_quantile_free**(*gsl_rstat_quantile_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_rstat_quantile_reset**(*gsl_rstat_quantile_workspace* *w)

This function resets the workspace `w` to its initial state, so it can begin working on a new set of data.

int **gsl_rstat_quantile_add**(const double x, *gsl_rstat_quantile_workspace* *w)

This function updates the estimate of the p-quantile with the new data point `x`.

double **gsl_rstat_quantile_get**(*gsl_rstat_quantile_workspace* *w)

This function returns the current estimate of the p-quantile.

22.5 Examples

Here is a basic example of how to use the statistical functions:

```
#include <stdio.h>
#include <gsl/gsl_rstat.h>

int
main(void)
{
  double data[5] = {17.2, 18.1, 16.5, 18.3, 12.6};
  double mean, variance, largest, smallest, sd,
         rms, sd_mean, median, skew, kurtosis;
  gsl_rstat_workspace *rstat_p = gsl_rstat_alloc();
  size_t i, n;

  /* add data to rstat accumulator */
  for (i = 0; i < 5; ++i)
    gsl_rstat_add(data[i], rstat_p);

  mean     = gsl_rstat_mean(rstat_p);
  variance = gsl_rstat_variance(rstat_p);
  largest  = gsl_rstat_max(rstat_p);
  smallest = gsl_rstat_min(rstat_p);
  median   = gsl_rstat_median(rstat_p);
  sd       = gsl_rstat_sd(rstat_p);
  sd_mean  = gsl_rstat_sd_mean(rstat_p);
  skew     = gsl_rstat_skew(rstat_p);
```

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```
  rms      = gsl_rstat_rms(rstat_p);
  kurtosis = gsl_rstat_kurtosis(rstat_p);
  n        = gsl_rstat_n(rstat_p);

  printf ("The dataset is %g, %g, %g, %g, %g\n",
         data[0], data[1], data[2], data[3], data[4]);

  printf ("The sample mean is %g\n", mean);
  printf ("The estimated variance is %g\n", variance);
  printf ("The largest value is %g\n", largest);
  printf ("The smallest value is %g\n", smallest);
  printf( "The median is %g\n", median);
  printf( "The standard deviation is %g\n", sd);
  printf( "The root mean square is %g\n", rms);
  printf( "The standard devation of the mean is %g\n", sd_mean);
  printf( "The skew is %g\n", skew);
  printf( "The kurtosis %g\n", kurtosis);
  printf( "There are %zu items in the accumulator\n", n);

  gsl_rstat_reset(rstat_p);
  n = gsl_rstat_n(rstat_p);
  printf( "There are %zu items in the accumulator\n", n);

  gsl_rstat_free(rstat_p);

  return 0;
}
```

The program should produce the following output,

```
The dataset is 17.2, 18.1, 16.5, 18.3, 12.6
The sample mean is 16.54
The estimated variance is 5.373
The largest value is 18.3
The smallest value is 12.6
The median is 17.2
The standard deviation is 2.31797
The root mean square is 16.6694
The standard devation of the mean is 1.03663
The skew is -0.829058
The kurtosis -1.2217
There are 5 items in the accumulator
There are 0 items in the accumulator
```

This next program estimates the lower quartile, median and upper quartile from 10,000 samples of a random Rayleigh distribution, using the P^2 algorithm of Jain and Chlamtec. For comparison, the exact values are also computed from the sorted dataset.

```
#include <stdio.h>
#include <stdlib.h>
#include <gsl/gsl_rstat.h>
#include <gsl/gsl_statistics.h>
```

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```
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_sort.h>

int
main(void)
{
  const size_t N = 10000;
  double *data = malloc(N * sizeof(double));
  gsl_rstat_quantile_workspace *work_25 = gsl_rstat_quantile_alloc(0.25);
  gsl_rstat_quantile_workspace *work_50 = gsl_rstat_quantile_alloc(0.5);
  gsl_rstat_quantile_workspace *work_75 = gsl_rstat_quantile_alloc(0.75);
  gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
  double exact_p25, exact_p50, exact_p75;
  double val_p25, val_p50, val_p75;
  size_t i;

  /* add data to quantile accumulators; also store data for exact
   * comparisons */
  for (i = 0; i < N; ++i)
    {
      data[i] = gsl_ran_rayleigh(r, 1.0);
      gsl_rstat_quantile_add(data[i], work_25);
      gsl_rstat_quantile_add(data[i], work_50);
      gsl_rstat_quantile_add(data[i], work_75);
    }

  /* exact values */
  gsl_sort(data, 1, N);
  exact_p25 = gsl_stats_quantile_from_sorted_data(data, 1, N, 0.25);
  exact_p50 = gsl_stats_quantile_from_sorted_data(data, 1, N, 0.5);
  exact_p75 = gsl_stats_quantile_from_sorted_data(data, 1, N, 0.75);

  /* estimated values */
  val_p25 = gsl_rstat_quantile_get(work_25);
  val_p50 = gsl_rstat_quantile_get(work_50);
  val_p75 = gsl_rstat_quantile_get(work_75);

  printf ("The dataset is %g, %g, %g, %g, %g, ...\n",
         data[0], data[1], data[2], data[3], data[4]);

  printf ("0.25 quartile: exact = %.5f, estimated = %.5f, error = %.6e\n",
          exact_p25, val_p25, (val_p25 - exact_p25) / exact_p25);
  printf ("0.50 quartile: exact = %.5f, estimated = %.5f, error = %.6e\n",
          exact_p50, val_p50, (val_p50 - exact_p50) / exact_p50);
  printf ("0.75 quartile: exact = %.5f, estimated = %.5f, error = %.6e\n",
          exact_p75, val_p75, (val_p75 - exact_p75) / exact_p75);

  gsl_rstat_quantile_free(work_25);
  gsl_rstat_quantile_free(work_50);
  gsl_rstat_quantile_free(work_75);
  gsl_rng_free(r);
```

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```
  free(data);

  return 0;
}
```

The program should produce the following output,

```
The dataset is 0.00645272, 0.0074002, 0.0120706, 0.0207256, 0.0227282, ...
0.25 quartile: exact = 0.75766, estimated = 0.75580, error = -2.450209e-03
0.50 quartile: exact = 1.17508, estimated = 1.17438, error = -5.995912e-04
0.75 quartile: exact = 1.65347, estimated = 1.65696, error = 2.110571e-03
```

22.6 References and Further Reading

The algorithm used to dynamically estimate p-quantiles is described in the paper,

- R. Jain and I. Chlamtac. *The P^2 algorithm for dynamic calculation of quantiles and histograms without storing observations*, Communications of the ACM, Volume 28 (October), Number 10, 1985, p. 1076-1085.

CHAPTER

TWENTYTHREE

MOVING WINDOW STATISTICS

This chapter describes routines for computing *moving window statistics* (also called rolling statistics and running statistics), using a window around a sample which is used to calculate various local statistical properties of an input data stream. The window is then slid forward by one sample to process the next data point and so on.

The functions described in this chapter are declared in the header file `gsl_movstat.h`.

23.1 Introduction

This chapter is concerned with calculating various statistics from subsets of a given dataset. The main idea is to compute statistics in the vicinity of a given data sample by defining a *window* which includes the sample itself as well as some specified number of samples before and after the sample in question. For a sample x_i, we define a window $W_i^{H,J}$ as

$$W_i^{H,J} = \{x_{i-H}, \dots, x_i, \dots, x_{i+J}\}$$

The parameters H and J are non-negative integers specifying the number of samples to include before and after the sample x_i. Statistics such as the mean and standard deviation of the window $W_i^{H,J}$ may be computed, and then the window is shifted forward by one sample to focus on x_{i+1}. The total number of samples in the window is $K = H + J + 1$. To define a symmetric window centered on x_i, one would set $H = J = \lfloor K/2 \rfloor$.

23.2 Handling Endpoints

When processing samples near the ends of the input signal, there will not be enough samples to fill the window $W_i^{H,J}$ defined above. Therefore the user must specify how to construct the windows near the end points. This is done by passing an input argument of type *`gsl_movstat_end_t`*:

type **`gsl_movstat_end_t`**

This data type specifies how to construct windows near end points and can be selected from the following choices:

`GSL_MOVSTAT_END_PADZERO`

With this option, a full window of length K will be constructed by inserting zeros into the window near the signal end points. Effectively, the input signal is modified to

$$\tilde{x} = \{\underbrace{0, \dots, 0}_{H \text{ zeros}}, x_1, x_2, \dots, x_{n-1}, x_n, \underbrace{0, \dots, 0}_{J \text{ zeros}}\}$$

to ensure a well-defined window for all x_i.

GSL_MOVSTAT_END_PADVALUE
With this option, a full window of length K will be constructed by padding the window with the first and last sample in the input signal. Effectively, the input signal is modified to

$$\tilde{x} = \{\underbrace{x_1, \dots, x_1}_{H}, x_1, x_2, \dots, x_{n-1}, x_n, \underbrace{x_n, \dots, x_n}_{J}\}$$

GSL_MOVSTAT_END_TRUNCATE
With this option, no padding is performed, and the windows are simply truncated as the end points are approached.

23.3 Allocation for Moving Window Statistics

type **gsl_movstat_workspace**
The moving window statistical routines use a common workspace.

gsl_movstat_workspace ***gsl_movstat_alloc**(const size_t K)
This function allocates a workspace for computing symmetric, centered moving statistics with a window length of K samples. In this case, $H = J = \lfloor K/2 \rfloor$. The size of the workspace is $O(7K)$.

gsl_movstat_workspace ***gsl_movstat_alloc2**(const size_t H, const size_t J)
This function allocates a workspace for computing moving statistics using a window with H samples prior to the current sample, and J samples after the current sample. The total window size is $K = H + J + 1$. The size of the workspace is $O(7K)$.

void ***gsl_movstat_free**(*gsl_movstat_workspace* *w)
This function frees the memory associated with `w`.

23.4 Moving Mean

The moving window mean calculates the mean of the values of each window $W_i^{H,J}$.

$$\hat{\mu}_i = \frac{1}{\left|W_i^{H,J}\right|} \sum_{x_m \in W_i^{H,J}} x_m$$

Here, $\left|W_i^{H,J}\right|$ represents the number of elements in the window $W_i^{H,J}$. This will normally be K, unless the `GSL_MOVSTAT_END_TRUNCATE` option is selected, in which case it could be less than K near the signal end points.

int **gsl_movstat_mean**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y, *gsl_movstat_workspace* *w)
This function computes the moving window mean of the input vector `x`, storing the output in `y`. The parameter `endtype` specifies how windows near the ends of the input should be handled. It is allowed to have `x = y` for an in-place moving mean.

23.5 Moving Variance and Standard Deviation

The moving window variance calculates the *sample variance* of the values of each window $W_i^{H,J}$, defined by

$$\hat{\sigma}_i^2 = \frac{1}{\left(\left| W_i^{H,J} \right| - 1 \right)} \sum_{x_m \in W_i^{H,J}} \left(x_m - \hat{\mu}_i \right)^2$$

where $\hat{\mu}_i$ is the mean of $W_i^{H,J}$ defined above. The standard deviation $\hat{\sigma}_i$ is the square root of the variance.

int **gsl_movstat_variance**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y, *gsl_movstat_workspace* *w)

This function computes the moving window variance of the input vector `x`, storing the output in `y`. The parameter `endtype` specifies how windows near the ends of the input should be handled. It is allowed to have `x` = `y` for an in-place moving variance.

int **gsl_movstat_sd**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y, *gsl_movstat_workspace* *w)

This function computes the moving window standard deviation of the input vector `x`, storing the output in `y`. The parameter `endtype` specifies how windows near the ends of the input should be handled. It is allowed to have `x` = `y` for an in-place moving standard deviation.

23.6 Moving Minimum and Maximum

The moving minimum/maximum calculates the minimum and maximum values of each window $W_i^{H,J}$.

$$y_i^{min} = \min \left(W_i^{H,J} \right)$$
$$y_i^{max} = \max \left(W_i^{H,J} \right)$$

int **gsl_movstat_min**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y, *gsl_movstat_workspace* *w)

This function computes the moving minimum of the input vector `x`, storing the result in `y`. The parameter `endtype` specifies how windows near the ends of the input should be handled. It is allowed to have `x` = `y` for an in-place moving minimum.

int **gsl_movstat_max**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y, *gsl_movstat_workspace* *w)

This function computes the moving maximum of the input vector `x`, storing the result in `y`. The parameter `endtype` specifies how windows near the ends of the input should be handled. It is allowed to have `x` = `y` for an in-place moving maximum.

int **gsl_movstat_minmax**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y_min, *gsl_vector* *y_max, *gsl_movstat_workspace* *w)

This function computes the moving minimum and maximum of the input vector `x`, storing the window minimums in `y_min` and the window maximums in `y_max`. The parameter `endtype` specifies how windows near the ends of the input should be handled.

23.7 Moving Sum

The moving window sum calculates the sum of the values of each window $W_i^{H,J}$.

$$y_i = \sum_{x_m \in W_i^{H,J}} x_m$$

int **gsl_movstat_sum**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y, *gsl_movstat_workspace* *w)

This function computes the moving window sum of the input vector `x`, storing the output in `y`. The parameter `endtype` specifies how windows near the ends of the input should be handled. It is allowed to have `x` = `y` for an in-place moving sum.

23.8 Moving Median

The moving median calculates the median of the window $W_i^{H,J}$ for each sample x_i:

$$y_i = \text{median}\left(W_i^{H,J}\right)$$

int **gsl_movstat_median**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y, *gsl_movstat_workspace* *w)

This function computes the moving median of the input vector `x`, storing the output in `y`. The parameter `endtype` specifies how windows near the ends of the input should be handled. It is allowed for `x` = `y` for an in-place moving window median.

23.9 Robust Scale Estimation

A common problem in statistics is to quantify the dispersion (also known as the variability, scatter, and spread) of a set of data. Often this is done by calculating the variance or standard deviation. However these statistics are strongly influenced by outliers, and can often provide erroneous results when even a small number of outliers are present.

Several useful statistics have emerged to provide robust estimates of scale which are not as susceptible to data outliers. A few of these statistical scale estimators are described below.

23.9.1 Moving MAD

The median absolute deviation (MAD) for the window $W_i^{H,J}$ is defined to be the median of the absolute deviations from the window's median:

$$MAD_i = 1.4826 \times \text{median}\left(\left|W_i^{H,J} - \text{median}\left(W_i^{H,J}\right)\right|\right)$$

The factor of 1.4826 makes the MAD an unbiased estimator of the standard deviation for Gaussian data. The MAD has an efficiency of 37%. See *here* for more information.

int **gsl_movstat_mad0**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *xmedian, *gsl_vector* *xmad, *gsl_movstat_workspace* *w) int **gsl_movstat_mad**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *xmedian, *gsl_vector* *xmad, *gsl_movstat_workspace* *w)

These functions compute the moving MAD of the input vector `x` and store the result in `xmad`. The medians of each window $W_i^{H,J}$ are stored in `xmedian` on output. The inputs `x`, `xmedian`, and `xmad` must all be the same length. The parameter `endtype` specifies how windows near the ends of the input should be handled. The function `mad0` does not include the scale factor of 1.4826, while the function `mad` does include this factor.

23.9.2 Moving QQR

The q-quantile range (QQR) is the difference between the $(1 - q)$ and q quantiles of a set of data,

$$QQR = Q_{1-q} - Q_q$$

The case $q = 0.25$ corresponds to the well-known *interquartile range (IQR)*, which is the difference between the 75th and 25th percentiles of a set of data. The QQR is a *trimmed estimator*, the main idea being to discard the largest and smallest values in a data window and compute a scale estimate from the remaining middle values. In the case of the IQR, the largest and smallest 25% of the data are discarded and the scale is estimated from the remaining (middle) 50%.

int **gsl_movstat_qqr**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, const double q, *gsl_vector* *xqqr, *gsl_movstat_workspace* *w)

This function computes the moving QQR of the input vector `x` and stores the q-quantile ranges of each window $W_i^{H,J}$ in `xqqr`. The quantile parameter `q` must be between 0 and 0.5. The input $q = 0.25$ corresponds to the IQR. The inputs `x` and `xqqr` must be the same length. The parameter `endtype` specifies how windows near the ends of the input should be handled.

23.9.3 Moving S_n

The S_n statistic proposed by Croux and Rousseeuw is based on pairwise differences between all samples in the window. It has an efficiency of 58%, significantly higher than the MAD. See *here* for more information.

int **gsl_movstat_Sn**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *xscale, *gsl_movstat_workspace* *w)

This function computes the moving S_n of the input vector `x` and stores the output in `xscale`. The inputs `x` and `xscale` must be the same length. The parameter `endtype` specifies how windows near the ends of the input should be handled. It is allowed for `x` = `xscale` for an in-place moving window S_n.

23.9.4 Moving Q_n

The Q_n statistic proposed by Croux and Rousseeuw is loosely based on the Hodges-Lehmann location estimator. It has a relatively high efficiency of 82%. See *here* for more information.

int **gsl_movstat_Qn**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *xscale, *gsl_movstat_workspace* *w)

This function computes the moving Q_n of the input vector `x` and stores the output in `xscale`. The inputs `x` and `xscale` must be the same length. The parameter `endtype` specifies how windows near the ends of the input should be handled. It is allowed for `x` = `xscale` for an in-place moving window Q_n.

23.10 User-defined Moving Statistics

GSL offers an interface for users to define their own moving window statistics functions, without needing to implement the edge-handling and accumulator machinery. This can be done by explicitly constructing the windows $W_i^{H,J}$ for a given input signal (*gsl_movstat_fill()*), or by calculating a user-defined function for each window automatically. In order to apply a user-defined function to each window, users must define a variable of type *gsl_movstat_function* to pass into *gsl_movstat_apply()*. This structure is defined as follows.

type **gsl_movstat_function**

Structure specifying user-defined moving window statistical function:

```
typedef struct
{
  double (* function) (const size_t n, double x[], void * params);
  void * params;
} gsl_movstat_function;
```

This structure contains a pointer to the user-defined function as well as possible parameters to pass to the function.

double (***function**)(const size_t n, double x[], void *params)

This function returns the user-defined statistic of the array `x` of length `n`. User-specified parameters are passed in via *params*. It is allowed to modify the array `x`.

void ***params**

User-specified parameters to be passed into the function.

int **gsl_movstat_apply**(const *gsl_movstat_end_t* endtype, const *gsl_movstat_function* *F, const *gsl_vector* *x, *gsl_vector* *y, *gsl_movstat_workspace* *w)

This function applies the user-defined moving window statistic specified in *F* to the input vector *x*, storing the output in *y*. The parameter *endtype* specifies how windows near the ends of the input should be handled. It is allowed for *x* = *y* for an in-place moving window calculation.

size_t **gsl_movstat_fill**(const *gsl_movstat_end_t* endtype, const *gsl_vector* *x, const size_t idx, const size_t H, const size_t J, double *window)

This function explicitly constructs the sliding window for the input vector *x* which is centered on the sample *idx*. On output, the array *window* will contain $W_{idx}^{H,J}$. The number of samples to the left and right of the sample *idx* are specified by *H* and *J* respectively. The parameter *endtype* specifies how windows near the ends of the input should be handled. The function returns the size of the window.

23.11 Accumulators

Many of the algorithms of this chapter are based on an accumulator design, which process the input vector one sample at a time, updating calculations of the desired statistic for the current window. Each accumulator is stored in the following structure:

type **gsl_movstat_accum**

Structure specifying accumulator for moving window statistics:

```
typedef struct
{
  size_t (* size) (const size_t n);
  int (* init) (const size_t n, void * vstate);
  int (* insert) (const double x, void * vstate);
```

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```
  int (* delete) (void * vstate);
  int (* get) (void * params, double * result, const void * vstate);
} gsl_movstat_accum;
```

The structure contains function pointers responsible for performing different tasks for the accumulator.

size_t (***size**)(const size_t n)
: This function returns the size of the workspace (in bytes) needed by the accumulator for a moving window of length `n`.

int (***init**)(const size_t n, void *vstate)
: This function initializes the workspace `vstate` for a moving window of length `n`.

int (***insert**)(const double x, void *vstate)
: This function inserts a single sample `x` into the accumulator, updating internal calculations of the desired statistic. If the accumulator is full (i.e. n samples have already been inserted), then the oldest sample is deleted from the accumulator.

int (***delete**)(void *vstate)
: This function deletes the oldest sample from the accumulator, updating internal calculations of the desired statistic.

int (***get**)(void *params, double *result, const void *vstate)
: This function stores the desired statistic for the current window in `result`. The input `params` specifies optional parameters for calculating the statistic.

The following accumulators of type `gsl_movstat_accum` are defined by GSL to perform moving window statistics calculations.

gsl_movstat_accum ***gsl_movstat_accum_min**

gsl_movstat_accum ***gsl_movstat_accum_max**

gsl_movstat_accum ***gsl_movstat_accum_minmax**

These accumulators calculate moving window minimum/maximums efficiently, using the algorithm of D. Lemire.

gsl_movstat_accum ***gsl_movstat_accum_mean**

gsl_movstat_accum ***gsl_movstat_accum_sd**

gsl_movstat_accum ***gsl_movstat_accum_variance**

These accumulators calculate the moving window mean, standard deviation, and variance, using the algorithm of B. P. Welford.

gsl_movstat_accum ***gsl_movstat_accum_median**

This accumulator calculates the moving window median using the min/max heap algorithm of Härdle and Steiger.

gsl_movstat_accum ***gsl_movstat_accum_Sn**

gsl_movstat_accum ***gsl_movstat_accum_Qn**

These accumulators calculate the moving window S_n and Q_n statistics developed by Croux and Rousseeuw.

gsl_movstat_accum ***gsl_movstat_accum_sum**

This accumulator calculates the moving window sum.

gsl_movstat_accum ***gsl_movstat_accum_qqr**

This accumulator calculates the moving window q-quantile range.

23.12 Examples

23.12.1 Example 1

The following example program computes the moving mean, minimum and maximum of a noisy sinusoid signal of length $N = 500$ with a symmetric moving window of size $K = 11$.

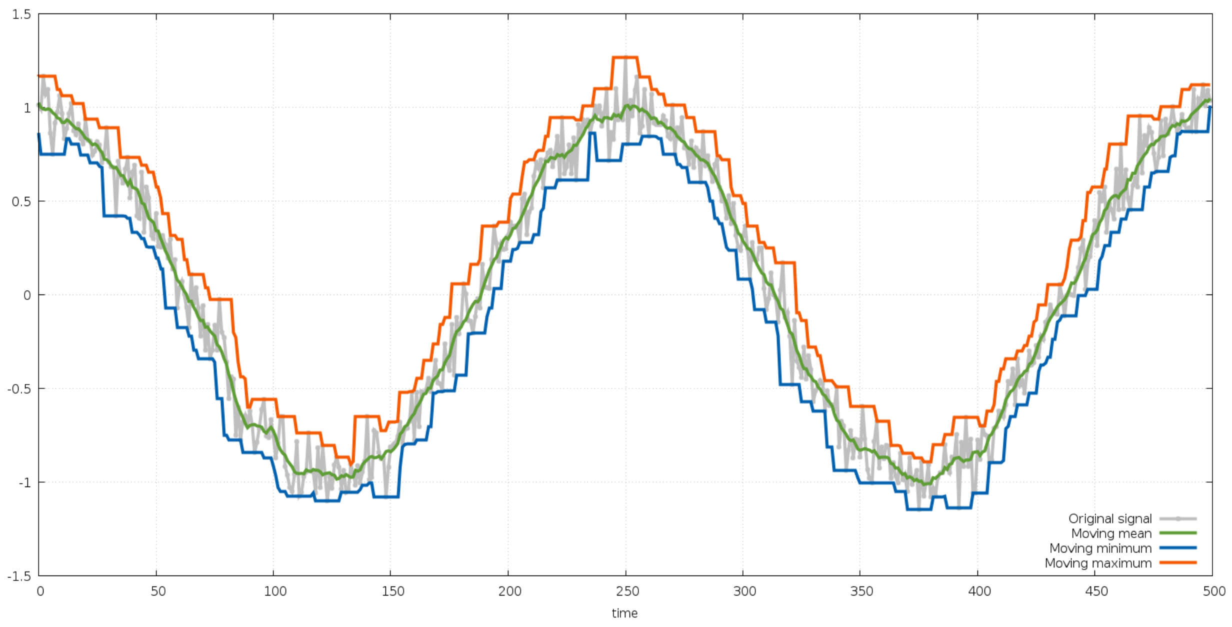

Fig. 23.1: Original signal time series (gray) with moving mean (green), moving minimum (blue), and moving maximum (orange).

The program is given below.

```
#include <stdio.h>
#include <stdlib.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_movstat.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_vector.h>

int
main(void)
{
  const size_t N = 500;                      /* length of time series */
  const size_t K = 11;                       /* window size */
  gsl_movstat_workspace * w = gsl_movstat_alloc(K);
  gsl_vector *x = gsl_vector_alloc(N);
  gsl_vector *xmean = gsl_vector_alloc(N);
  gsl_vector *xmin = gsl_vector_alloc(N);
  gsl_vector *xmax = gsl_vector_alloc(N);
  gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
```

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```
  size_t i;

  for (i = 0; i < N; ++i)
    {
      double xi = cos(4.0 * M_PI * i / (double) N);
      double ei = gsl_ran_gaussian(r, 0.1);

      gsl_vector_set(x, i, xi + ei);
    }

  /* compute moving statistics */
  gsl_movstat_mean(GSL_MOVSTAT_END_PADVALUE, x, xmean, w);
  gsl_movstat_minmax(GSL_MOVSTAT_END_PADVALUE, x, xmin, xmax, w);

  /* print results */
  for (i = 0; i < N; ++i)
    {
      printf("%zu %f %f %f %f\n",
             i,
             gsl_vector_get(x, i),
             gsl_vector_get(xmean, i),
             gsl_vector_get(xmin, i),
             gsl_vector_get(xmax, i));
    }

  gsl_vector_free(x);
  gsl_vector_free(xmean);
  gsl_rng_free(r);
  gsl_movstat_free(w);

  return 0;
}
```

23.12.2 Example 2: Robust Scale

The following example program analyzes a time series of length $N = 1000$ composed of Gaussian random variates with zero mean whose standard deviation changes in a piecewise constant fashion as shown in the table below.

Sample Range	σ
1-200	1.0
201-450	5.0
451-600	1.0
601-850	3.0
851-1000	5.0

Additionally, about 1% of the samples are perturbed to represent outliers by adding ± 15 to the random Gaussian variate. The program calculates the moving statistics MAD, IQR, S_n, Q_n, and the standard deviation using a symmetric moving window of length $K = 41$. The results are shown in Fig. 23.2.

The robust statistics follow the true standard deviation piecewise changes well, without being influenced by the outliers. The moving standard deviation (gray curve) is heavily influenced by the presence of the outliers. The program is given

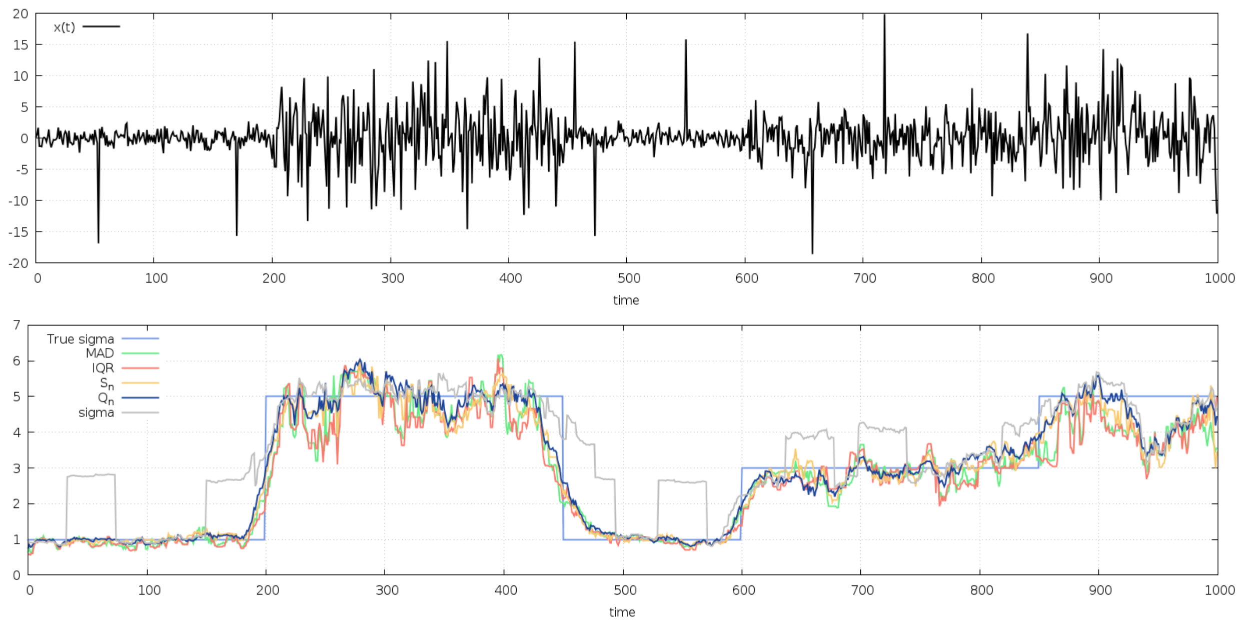

Fig. 23.2: Top: time series of piecewise constant variance. Bottom: scale estimates using a moving window; the true sigma value is in light blue, MAD in green, IQR in red, S_n in yellow, and Q_n in dark blue. The moving standard deviation is shown in gray.

below.

```
#include <stdio.h>
#include <stdlib.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_movstat.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_vector.h>

int
main(void)
{
  const size_t N = 1000;                              /* length of time series */
  const double sigma[] = { 1.0, 5.0, 1.0, 3.0, 5.0 };    /* variances */
  const size_t N_sigma[] = { 200, 450, 600, 850, 1000 }; /* samples where variance␣
↪changes */
  const size_t K = 41;                                /* window size */
  gsl_vector *x = gsl_vector_alloc(N);
  gsl_vector *xmedian = gsl_vector_alloc(N);
  gsl_vector *xmad = gsl_vector_alloc(N);
  gsl_vector *xiqr = gsl_vector_alloc(N);
  gsl_vector *xSn = gsl_vector_alloc(N);
  gsl_vector *xQn = gsl_vector_alloc(N);
  gsl_vector *xsd = gsl_vector_alloc(N);
  gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
  gsl_movstat_workspace * w = gsl_movstat_alloc(K);
```

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```
  size_t idx = 0;
  size_t i;

  for (i = 0; i < N; ++i)
    {
      double gi = gsl_ran_gaussian(r, sigma[idx]);
      double u = gsl_rng_uniform(r);
      double outlier = (u < 0.01) ? 15.0*GSL_SIGN(gi) : 0.0;
      double xi = gi + outlier;

      gsl_vector_set(x, i, xi);

      if (i == N_sigma[idx] - 1)
        ++idx;
    }

  /* compute moving statistics */
  gsl_movstat_mad(GSL_MOVSTAT_END_TRUNCATE, x, xmedian, xmad, w);
  gsl_movstat_qqr(GSL_MOVSTAT_END_TRUNCATE, x, 0.25, xiqr, w);
  gsl_movstat_Sn(GSL_MOVSTAT_END_TRUNCATE, x, xSn, w);
  gsl_movstat_Qn(GSL_MOVSTAT_END_TRUNCATE, x, xQn, w);
  gsl_movstat_sd(GSL_MOVSTAT_END_TRUNCATE, x, xsd, w);

  /* scale IQR by factor to approximate standard deviation */
  gsl_vector_scale(xiqr, 0.7413);

  /* print results */
  idx = 0;
  for (i = 0; i < N; ++i)
    {
      printf("%zu %f %f %f %f %f %f %f\n",
             i,
             gsl_vector_get(x, i),
             sigma[idx],
             gsl_vector_get(xmad, i),
             gsl_vector_get(xiqr, i),
             gsl_vector_get(xSn, i),
             gsl_vector_get(xQn, i),
             gsl_vector_get(xsd, i));

      if (i == N_sigma[idx] - 1)
        ++idx;
    }

  gsl_vector_free(x);
  gsl_vector_free(xmedian);
  gsl_vector_free(xmad);
  gsl_vector_free(xiqr);
  gsl_vector_free(xSn);
  gsl_vector_free(xQn);
  gsl_vector_free(xsd);
  gsl_rng_free(r);
```

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```
  gsl_movstat_free(w);

  return 0;
}
```

23.12.3 Example 3: User-defined Moving Window

This example program illustrates how a user can define their own moving window function to apply to an input vector. It constructs a random noisy time series of length $N = 1000$ with some outliers added. Then it applies a moving window trimmed mean to the time series with trim parameter $\alpha = 0.1$. The length of the moving window is $K = 11$, so the smallest and largest sample of each window is discarded prior to computing the mean. The results are shown in Fig. 23.3.

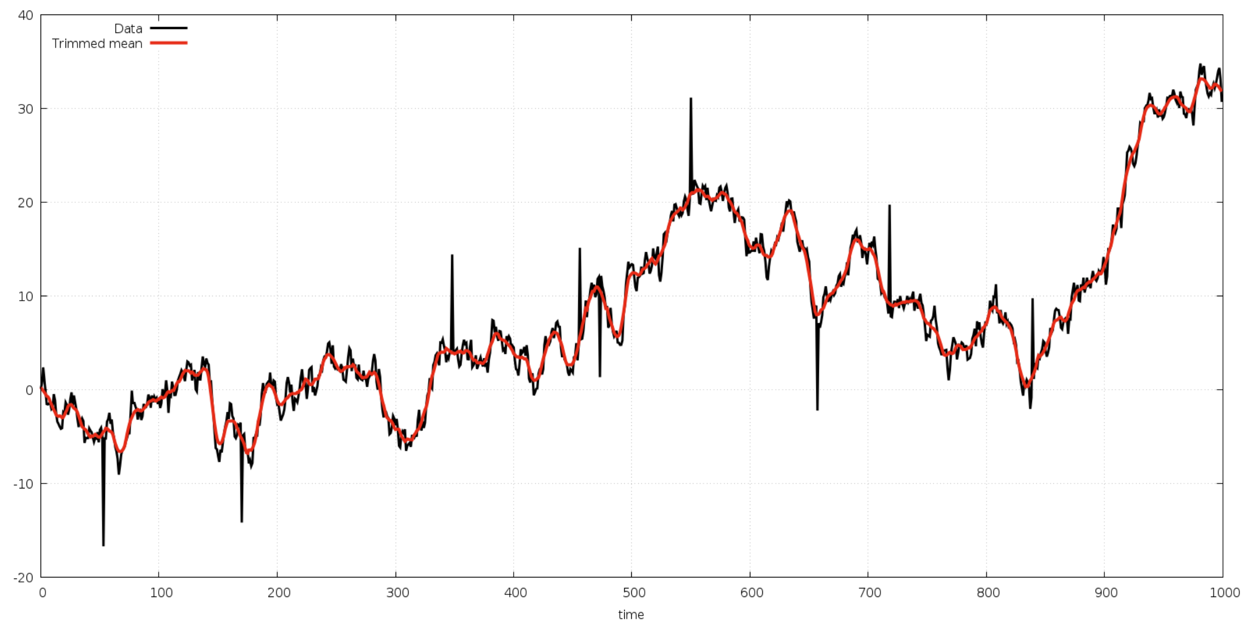

Fig. 23.3: Noisy time series data (black) with moving window trimmed mean (red)

The program is given below.

```
#include <stdio.h>
#include <stdlib.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_movstat.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_sort.h>
#include <gsl/gsl_statistics.h>

double
func(const size_t n, double x[], void * params)
```

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```
{
  const double alpha = *(double *) params;

  gsl_sort(x, 1, n);

  return gsl_stats_trmean_from_sorted_data(alpha, x, 1, n);
}

int
main(void)
{
  const size_t N = 1000;                 /* length of time series */
  const size_t K = 11;                   /* window size */
  double alpha = 0.1;                    /* trimmed mean parameter */
  gsl_vector *x = gsl_vector_alloc(N);  /* input vector */
  gsl_vector *y = gsl_vector_alloc(N);  /* filtered output vector for alpha1 */
  gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
  gsl_movstat_workspace *w = gsl_movstat_alloc(K);
  gsl_movstat_function F;
  size_t i;
  double sum = 0.0;

  /* generate input signal */
  for (i = 0; i < N; ++i)
    {
      double ui = gsl_ran_gaussian(r, 1.0);
      double outlier = (gsl_rng_uniform(r) < 0.01) ? 10.0*GSL_SIGN(ui) : 0.0;
      sum += ui;
      gsl_vector_set(x, i, sum + outlier);
    }

  /* apply moving window function */
  F.function = func;
  F.params = &alpha;
  gsl_movstat_apply(GSL_MOVSTAT_END_PADVALUE, &F, x, y, w);

  /* print results */
  for (i = 0; i < N; ++i)
    {
      double xi = gsl_vector_get(x, i);
      double yi = gsl_vector_get(y, i);

      printf("%f %f\n", xi, yi);
    }

  gsl_vector_free(x);
  gsl_vector_free(y);
  gsl_rng_free(r);
  gsl_movstat_free(w);

  return 0;
}
```

23.13 References and Further Reading

The following publications are relevant to the algorithms described in this chapter,

- W.Hardle and W. Steiger, *Optimal Median Smoothing*, Appl. Statist., 44 (2), 1995.
- D. Lemire, *Streaming Maximum-Minimum Filter Using No More than Three Comparisons per Element*, Nordic Journal of Computing, 13 (4), 2006 (https://arxiv.org/abs/cs/0610046).
- B. P. Welford, *Note on a method for calculating corrected sums of squares and products*, Technometrics, 4 (3), 1962.

CHAPTER

TWENTYFOUR

DIGITAL FILTERING

24.1 Introduction

The filters discussed in this chapter are based on the following moving data window which is centered on i-th sample:

$$W_i^H = \{x_{i-H}, \dots, x_i, \dots, x_{i+H}\}$$

Here, H is a non-negative integer called the *window half-length*, which represents the number of samples before and after sample i. The total window length is $K = 2H + 1$.

24.2 Handling Endpoints

When processing samples near the ends of the input signal, there will not be enough samples to fill the window W_i^H defined above. Therefore the user must specify how to construct the windows near the end points. This is done by passing an input argument of type *gsl_filter_end_t*:

type **gsl_filter_end_t**

This data type specifies how to construct windows near end points and can be selected from the following choices:

GSL_FILTER_END_PADZERO

With this option, a full window of length K will be constructed by inserting zeros into the window near the signal end points. Effectively, the input signal is modified to

$$\tilde{x} = \{\underbrace{0, \dots, 0}_{H \text{ zeros}}, x_1, x_2, \dots, x_{n-1}, x_n, \underbrace{0, \dots, 0}_{H \text{ zeros}}\}$$

to ensure a well-defined window for all x_i.

GSL_FILTER_END_PADVALUE

With this option, a full window of length K will be constructed by padding the window with the first and last sample in the input signal. Effectively, the input signal is modified to

$$\tilde{x} = \{\underbrace{x_1, \dots, x_1}_{H}, x_1, x_2, \dots, x_{n-1}, x_n, \underbrace{x_n, \dots, x_n}_{H}\}$$

GSL_FILTER_END_TRUNCATE

With this option, no padding is performed, and the windows are simply truncated as the end points are approached.

24.3 Linear Digital Filters

24.3.1 Gaussian Filter

The Gaussian filter convolves the input signal with a Gaussian kernel or window. This filter is often used as a smoothing or noise reduction filter. The Gaussian kernel is defined by

$$G(k) = e^{-\frac{1}{2}\left(\alpha \frac{k}{(K-1)/2}\right)^2} = e^{-k^2/2\sigma^2}$$

for $-(K-1)/2 \le k \le (K-1)/2$, and K is the size of the kernel. The parameter α specifies the number of standard deviations σ desired in the kernel. So for example setting $\alpha = 3$ would define a Gaussian window of length K which spans $\pm 3\sigma$. It is often more convenient to specify the parameter α rather than the standard deviation σ when constructing the kernel, since a fixed value of α would correspond to the same shape of Gaussian regardless of the size K. The appropriate value of the standard deviation depends on K and is related to α as

$$\sigma = \frac{K-1}{2\alpha}$$

The routines below accept α as an input argument instead of σ.

The Gaussian filter offers a convenient way of differentiating and smoothing an input signal in a single pass. Using the derivative property of a convolution,

$$\frac{d}{dt}(G * x) = \frac{dG}{dt} * x$$

the input signal $x(t)$ can be smoothed and differentiated at the same time by convolution with a derivative Gaussian kernel, which can be readily computed from the analytic expression above. The same principle applies to higher order derivatives.

gsl_filter_gaussian_workspace ***gsl_filter_gaussian_alloc**(const size_t K)

This function initializes a workspace for Gaussian filtering using a kernel of size `K`. Here, $H = K/2$. If K is even, it is rounded up to the next odd integer to ensure a symmetric window. The size of the workspace is $O(K)$.

void **gsl_filter_gaussian_free**(gsl_filter_gaussian_workspace *w)

This function frees the memory associated with `w`.

int **gsl_filter_gaussian**(const *gsl_filter_end_t* endtype, const double alpha, const size_t order, const *gsl_vector* *x, *gsl_vector* *y, gsl_filter_gaussian_workspace *w)

This function applies a Gaussian filter parameterized by `alpha` to the input vector `x`, storing the output in `y`. The derivative order is specified by `order`, with `0` corresponding to a Gaussian, `1` corresponding to a first derivative Gaussian, and so on. The parameter `endtype` specifies how the signal end points are handled. It is allowed for `x` = `y` for an in-place filter.

int **gsl_filter_gaussian_kernel**(const double alpha, const size_t order, const int normalize, *gsl_vector* *kernel)

This function constructs a Gaussian kernel parameterized by `alpha` and stores the output in `kernel`. The parameter `order` specifies the derivative order, with `0` corresponding to a Gaussian, `1` corresponding to a first derivative Gaussian, and so on. If `normalize` is set to `1`, then the kernel will be normalized to sum to one on output. If `normalize` is set to `0`, no normalization is performed.

24.4 Nonlinear Digital Filters

The nonlinear digital filters described below are based on the window median, which is given by

$$m_i = \text{median} \left\{ W_i^H \right\} = \text{median} \left\{ x_{i-H}, \dots, x_i, \dots, x_{i+H} \right\}$$

The median is considered robust to local outliers, unlike the mean. Median filters can preserve sharp edges while at the same removing signal noise, and are used in a wide range of applications.

24.4.1 Standard Median Filter

The *standard median filter* (SMF) simply replaces the sample x_i by the median m_i of the window W_i^H: This filter has one tuning parameter given by H. The standard median filter is considered highly resistant to local outliers and local noise in the data sequence $\{x_i\}$.

gsl_filter_median_workspace ***gsl_filter_median_alloc**(const size_t K)

This function initializes a workspace for standard median filtering using a symmetric centered moving window of size `K`. Here, $H = K/2$. If K is even, it is rounded up to the next odd integer to ensure a symmetric window. The size of the workspace is $O(7K)$.

void **gsl_filter_median_free**(gsl_filter_median_workspace *w)

This function frees the memory associated with `w`.

int **gsl_filter_median**(const *gsl_filter_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y, gsl_filter_median_workspace *w)

This function applies a standard median filter to the input `x`, storing the output in `y`. The parameter `endtype` specifies how the signal end points are handled. It is allowed to have `x` = `y` for an in-place filter.

24.4.2 Recursive Median Filter

The *recursive median filter* (RMF) is a modification of the SMF to include previous filter outputs in the window before computing the median. The filter's response is

$$y_i = \text{median} \left(y_{i-H}, \dots, y_{i-1}, x_i, x_{i+1}, \dots, x_{i+H} \right)$$

Sometimes, the SMF must be applied several times in a row to achieve adequate smoothing (i.e. a cascade filter). The RMF, on the other hand, converges to a *root sequence* in one pass, and can sometimes provide a smoother result than several passes of the SMF. A root sequence is an input which is left unchanged by the filter. So there is no need to apply a recursive median filter twice to an input vector.

gsl_filter_rmedian_workspace ***gsl_filter_rmedian_alloc**(const size_t K)

This function initializes a workspace for recursive median filtering using a symmetric centered moving window of size `K`. Here, $H = K/2$. If K is even, it is rounded up to the next odd integer to ensure a symmetric window. The size of the workspace is $O(K)$.

void **gsl_filter_rmedian_free**(gsl_filter_rmedian_workspace *w)

This function frees the memory associated with `w`.

int **gsl_filter_rmedian**(const *gsl_filter_end_t* endtype, const *gsl_vector* *x, *gsl_vector* *y, gsl_filter_rmedian_workspace *w)

This function applies a recursive median filter to the input `x`, storing the output in `y`. The parameter `endtype` specifies how the signal end points are handled. It is allowed to have `x` = `y` for an in-place filter.

24.4.3 Impulse Detection Filter

Impulsive noise is characterized by short sequences of data points distinct from those in the surrounding neighborhood. This section describes a powerful class of filters, also known as *impulse rejection filters* and *decision-based filters*, designed to detect and remove such outliers from data. The filter's response is given by

$$y_i = \left\{ \begin{array}{cc} x_i, & |x_i - m_i| \le t S_i \\ m_i, & |x_i - m_i| > t S_i \end{array} \right.$$

where m_i is the median value of the window W_i^H, S_i is a robust estimate of the scatter or dispersion for the window W_i^H, and t is a tuning parameter specifying the number of scale factors needed to determine that a point is an outlier. The main idea is that the median m_i will be unaffected by a small number of outliers in the window, and so a given sample x_i is tested to determine how far away it is from the median in terms of the local scale estimate S_i. Samples which are more than t scale estimates away from the median are labeled as outliers and replaced by the window median m_i. Samples which are less than t scale estimates from the median are left unchanged by the filter.

Note that when $t = 0$, the impulse detection filter is equivalent to the standard median filter. When $t \rightarrow \infty$, it becomes the identity filter. This means the impulse detection filter can be viewed as a "less aggressive" version of the standard median filter, becoming less aggressive as t is increased. Note that this filter modifies only samples identified as outliers, while the standard median filter changes all samples to the local median, regardless of whether they are outliers. This fact, plus the additional flexibility offered by the additional tuning parameter t can make the impulse detection filter a better choice for some applications.

It is important to have a robust and accurate scale estimate S_i in order to detect impulse outliers even in the presence of noise. The window standard deviation is not typically a good choice, as it can be significantly perturbed by the presence of even one outlier. GSL offers the following choices (specified by a parameter of type `gsl_filter_scale_t`) for computing the scale estimate S_i, all of which are robust to the presence of impulse outliers.

type **`gsl_filter_scale_t`**

This type specifies how the scale estimate S_i of the window W_i^H is calculated.

`GSL_FILTER_SCALE_MAD`

This option specifies the median absolute deviation (MAD) scale estimate, defined by

$$S_i = 1.4826 \times \text{median} \left\{ |W_i^H - m_i| \right\}$$

This choice of scale estimate is also known as the *Hampel filter* in the statistical literature. See *here* for more information.

`GSL_FILTER_SCALE_IQR`

This option specifies the interquartile range (IQR) scale estimate, defined as the difference between the 75th and 25th percentiles of the window W_i^H,

$$S_i = 0.7413 \left(Q_{0.75} - Q_{0.25} \right)$$

where Q_p is the p-quantile of the window W_i^H. The idea is to throw away the largest and smallest 25% of the window samples (where the outliers would be), and estimate a scale from the middle 50%. The factor 0.7413 provides an unbiased estimate of the standard deviation for Gaussian data.

`GSL_FILTER_SCALE_SN`

This option specifies the so-called S_n statistic proposed by Croux and Rousseeuw. See *here* for more information.

`GSL_FILTER_SCALE_QN`

This option specifies the so-called Q_n statistic proposed by Croux and Rousseeuw. See *here* for more information.

Warning: While the scale estimates defined above are much less sensitive to outliers than the standard deviation, they can suffer from an effect called *implosion*. The standard deviation of a window W_i^H will be zero if and only if all samples in the window are equal. However, it is possible for the MAD of a window to be zero even if all the samples in the window are not equal. For example, if $K/2+1$ or more of the K samples in the window are equal to some value x^*, then the window median will be equal to x^*. Consequently, at least $K/2+1$ of the absolute deviations $|x_j - x^*|$ will be zero, and so the MAD will be zero. In such a case, the Hampel filter will act like the standard median filter regardless of the value of t. Caution should also be exercised if dividing by S_i.

gsl_filter_impulse_workspace ***gsl_filter_impulse_alloc**(const size_t K)

This function initializes a workspace for impulse detection filtering using a symmetric moving window of size `K`. Here, $H = K/2$. If K is even, it is rounded up to the next odd integer to ensure a symmetric window. The size of the workspace is $O(6K)$.

void **gsl_filter_impulse_free**(gsl_filter_impulse_workspace *w)

This function frees the memory associated with `w`.

int **gsl_filter_impulse**(const *gsl_filter_end_t* endtype, const *gsl_filter_scale_t* scale_type, const double t, const *gsl_vector* *x, *gsl_vector* *y, *gsl_vector* *xmedian, *gsl_vector* *xsigma, size_t *noutlier, gsl_vector_int *ioutlier, gsl_filter_impulse_workspace *w)

These functions apply an impulse detection filter to the input vector `x`, storing the filtered output in `y`. The tuning parameter t is provided in `t`. The window medians m_i are stored in `xmedian` and the S_i are stored in `xsigma` on output. The number of outliers detected is stored in `noutlier` on output, while the locations of flagged outliers are stored in the boolean array `ioutlier`. The input `ioutlier` may be `NULL` if not desired. It is allowed to have `x` = `y` for an in-place filter.

24.5 Examples

24.5.1 Gaussian Example 1

This example program illustrates the Gaussian filter applied to smoothing a time series of length $N = 500$ with a kernel size of $K = 51$. Three filters are applied with parameters $\alpha = 0.5, 3, 10$. The results are shown in Fig. 24.1.

We see that the filter corresponding to $\alpha = 0.5$ applies the most smoothing, while $\alpha = 10$ corresponds to the least amount of smoothing. The program is given below.

```
#include <stdio.h>
#include <stdlib.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_filter.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_vector.h>

int
main(void)
{
  const size_t N = 500;                        /* length of time series */
  const size_t K = 51;                         /* window size */
  const double alpha[3] = { 0.5, 3.0, 10.0 };  /* alpha values */
  gsl_vector *x = gsl_vector_alloc(N);         /* input vector */
  gsl_vector *y1 = gsl_vector_alloc(N);        /* filtered output vector for alpha1 */
```

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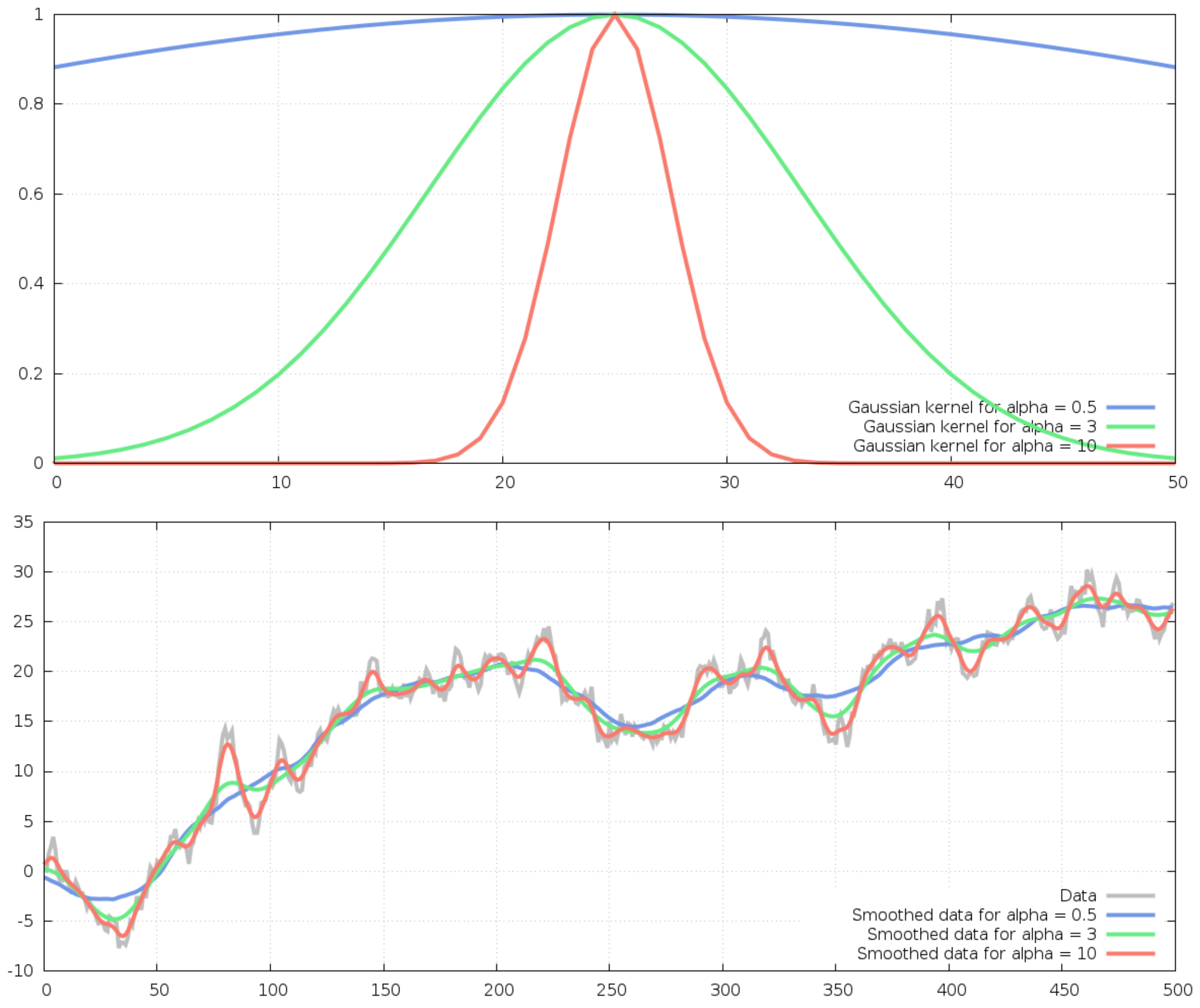

Fig. 24.1: Top panel: Gaussian kernels (unnormalized) for $\alpha = 0.5, 3, 10$. Bottom panel: Time series (gray) with Gaussian filter output for same α values.

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```
gsl_vector *y2 = gsl_vector_alloc(N);        /* filtered output vector for alpha2 */
gsl_vector *y3 = gsl_vector_alloc(N);        /* filtered output vector for alpha3 */
gsl_vector *k1 = gsl_vector_alloc(K);        /* Gaussian kernel for alpha1 */
gsl_vector *k2 = gsl_vector_alloc(K);        /* Gaussian kernel for alpha2 */
gsl_vector *k3 = gsl_vector_alloc(K);        /* Gaussian kernel for alpha3 */
gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
gsl_filter_gaussian_workspace *gauss_p = gsl_filter_gaussian_alloc(K);
size_t i;
double sum = 0.0;

/* generate input signal */
for (i = 0; i < N; ++i)
  {
    double ui = gsl_ran_gaussian(r, 1.0);
    sum += ui;
    gsl_vector_set(x, i, sum);
  }

/* compute kernels without normalization */
gsl_filter_gaussian_kernel(alpha[0], 0, 0, k1);
gsl_filter_gaussian_kernel(alpha[1], 0, 0, k2);
gsl_filter_gaussian_kernel(alpha[2], 0, 0, k3);

/* apply filters */
gsl_filter_gaussian(GSL_FILTER_END_PADVALUE, alpha[0], 0, x, y1, gauss_p);
gsl_filter_gaussian(GSL_FILTER_END_PADVALUE, alpha[1], 0, x, y2, gauss_p);
gsl_filter_gaussian(GSL_FILTER_END_PADVALUE, alpha[2], 0, x, y3, gauss_p);

/* print kernels */
for (i = 0; i < K; ++i)
  {
    double k1i = gsl_vector_get(k1, i);
    double k2i = gsl_vector_get(k2, i);
    double k3i = gsl_vector_get(k3, i);

    printf("%e %e %e\n", k1i, k2i, k3i);
  }

printf("\n\n");

/* print filter results */
for (i = 0; i < N; ++i)
  {
    double xi = gsl_vector_get(x, i);
    double y1i = gsl_vector_get(y1, i);
    double y2i = gsl_vector_get(y2, i);
    double y3i = gsl_vector_get(y3, i);

    printf("%.12e %.12e %.12e %.12e\n", xi, y1i, y2i, y3i);
  }

gsl_vector_free(x);
```

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```
  gsl_vector_free(y1);
  gsl_vector_free(y2);
  gsl_vector_free(y3);
  gsl_vector_free(k1);
  gsl_vector_free(k2);
  gsl_vector_free(k3);
  gsl_rng_free(r);
  gsl_filter_gaussian_free(gauss_p);

  return 0;
}
```

24.5.2 Gaussian Example 2

A common application of the Gaussian filter is to detect edges, or sudden jumps, in a noisy input signal. It is used both for 1D edge detection in time series, as well as 2D edge detection in images. Here we will examine a noisy time series of length $N = 1000$ with a single edge. The input signal is defined as

$$x(n) = e(n) + \begin{cases} 0, & n \le N/2 \\ 0.5, & n > N/2 \end{cases}$$

where $e(n)$ is Gaussian random noise. The program smooths the input signal with order $0, 1,$ and 2 Gaussian filters of length $K = 61$ with $\alpha = 3$. For comparison, the program also computes finite differences of the input signal without smoothing. The results are shown in Fig. 24.2.

The finite difference approximation of the first derivative (second row) shows the common problem with differentiating a noisy signal. The noise is amplified and makes it extremely difficult to detect the sharp gradient at sample 500. The third row shows the first order Gaussian smoothed signal with a clear peak at the location of the edge. Alternatively, one could examine the second order Gaussian smoothed signal (fourth row) and look for zero crossings to determine the edge location.

The program is given below.

```
#include <stdio.h>
#include <stdlib.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_filter.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_vector.h>

int
main(void)
{
  const size_t N = 1000;                        /* length of time series */
  const size_t K = 61;                          /* window size */
  const double alpha = 3.0;                     /* Gaussian kernel has +/- 3 standard␣
↪deviations */
  gsl_vector *x = gsl_vector_alloc(N);          /* input vector */
  gsl_vector *y = gsl_vector_alloc(N);          /* filtered output vector */
  gsl_vector *dy = gsl_vector_alloc(N);         /* first derivative filtered vector */
```

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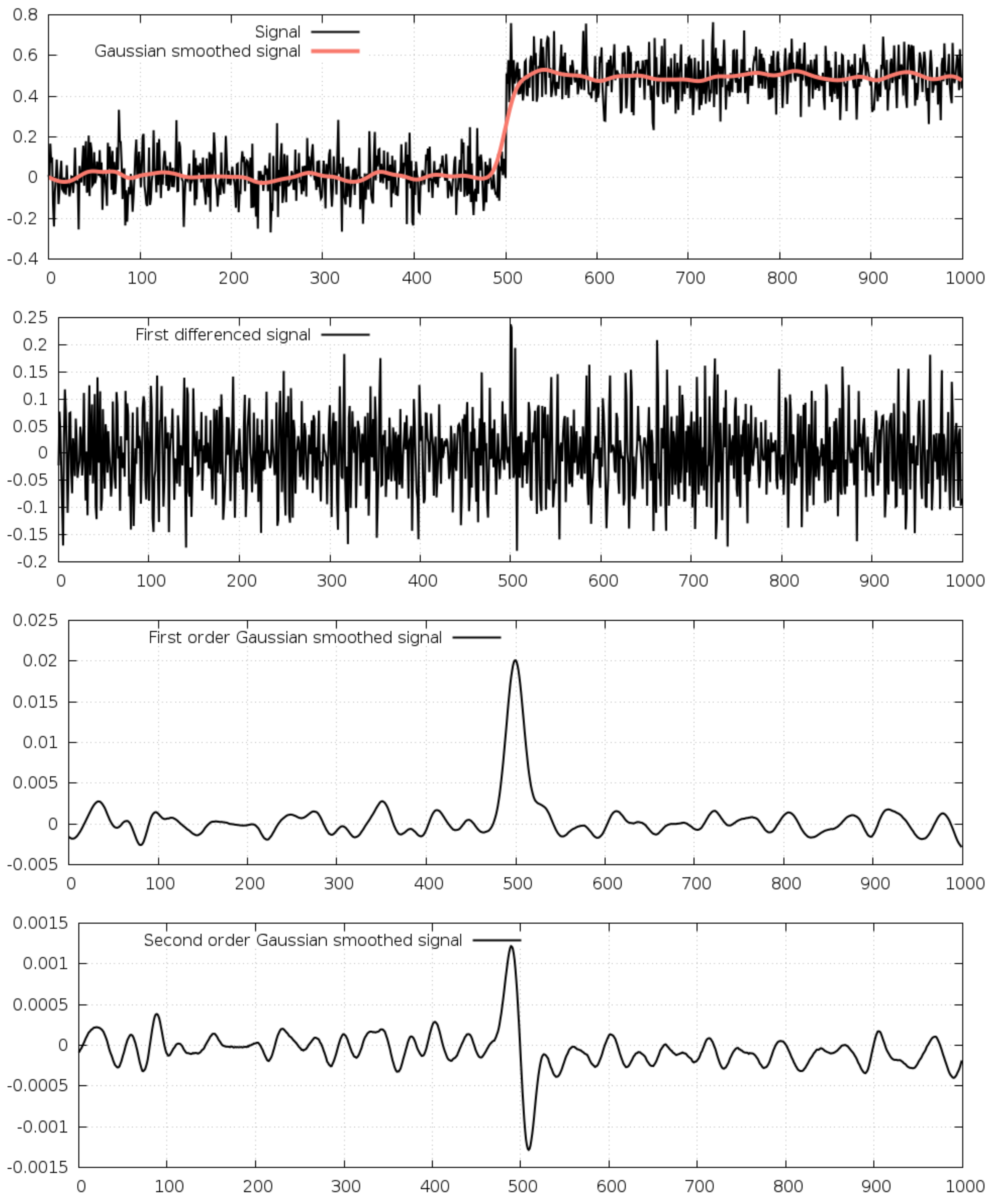

Fig. 24.2: Top row: original input signal $x(n)$ (black) with Gaussian smoothed signal in red. Second row: First finite differences of input signal. Third row: Input signal smoothed with a first order Gaussian filter. Fourth row: Input signal smoothed with a second order Gaussian filter.

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```
  gsl_vector *d2y = gsl_vector_alloc(N);       /* second derivative filtered vector */
  gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
  gsl_filter_gaussian_workspace *gauss_p = gsl_filter_gaussian_alloc(K);
  size_t i;

  /* generate input signal */
  for (i = 0; i < N; ++i)
    {
      double xi = (i > N / 2) ? 0.5 : 0.0;
      double ei = gsl_ran_gaussian(r, 0.1);

      gsl_vector_set(x, i, xi + ei);
    }

  /* apply filters */
  gsl_filter_gaussian(GSL_FILTER_END_PADVALUE, alpha, 0, x, y, gauss_p);
  gsl_filter_gaussian(GSL_FILTER_END_PADVALUE, alpha, 1, x, dy, gauss_p);
  gsl_filter_gaussian(GSL_FILTER_END_PADVALUE, alpha, 2, x, d2y, gauss_p);

  /* print results */
  for (i = 0; i < N; ++i)
    {
      double xi = gsl_vector_get(x, i);
      double yi = gsl_vector_get(y, i);
      double dyi = gsl_vector_get(dy, i);
      double d2yi = gsl_vector_get(d2y, i);
      double dxi;

      /* compute finite difference of x vector */
      if (i == 0)
        dxi = gsl_vector_get(x, i + 1) - xi;
      else if (i == N - 1)
        dxi = gsl_vector_get(x, i) - gsl_vector_get(x, i - 1);
      else
        dxi = 0.5 * (gsl_vector_get(x, i + 1) - gsl_vector_get(x, i - 1));

      printf("%.12e %.12e %.12e %.12e %.12e\n",
             xi,
             yi,
             dxi,
             dyi,
             d2yi);
    }

  gsl_vector_free(x);
  gsl_vector_free(y);
  gsl_vector_free(dy);
  gsl_vector_free(d2y);
  gsl_rng_free(r);
  gsl_filter_gaussian_free(gauss_p);

  return 0;
```

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```
}
```

24.5.3 Square Wave Signal Example

The following example program illustrates the median filters on a noisy square wave signal. Median filters are well known for preserving sharp edges in the input signal while reducing noise. The program constructs a 5 Hz square wave signal with Gaussian noise added. Then the signal is filtered with a standard median filter and recursive median filter using a symmetric window of length $K = 7$. The results are shown in Fig. 24.3.

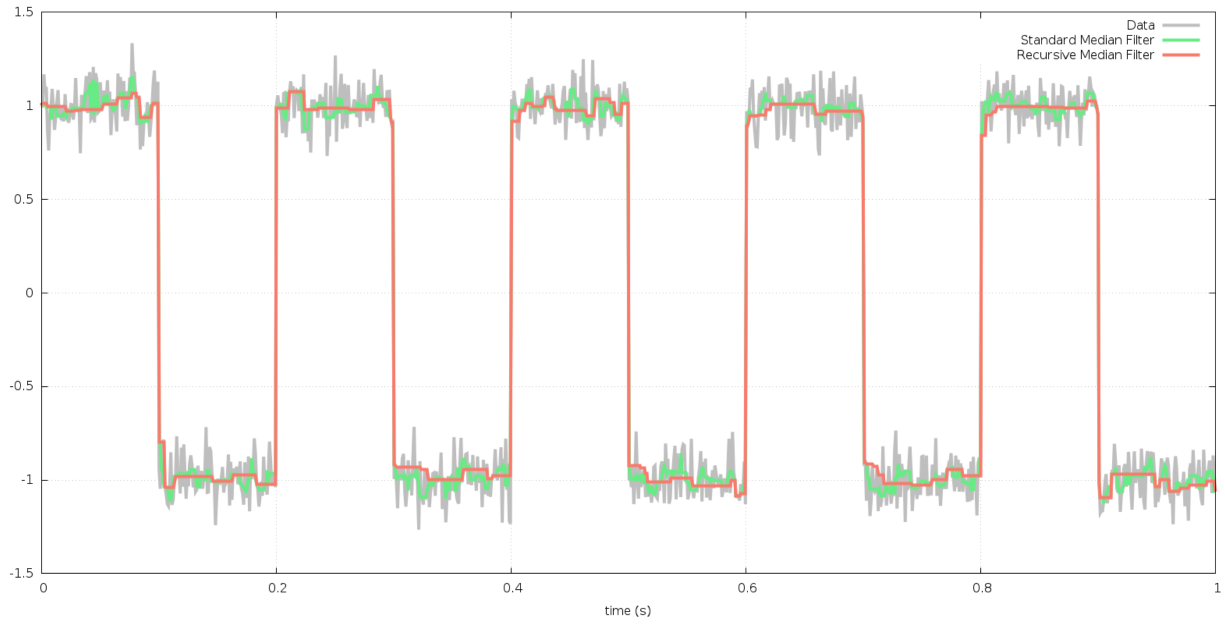

Fig. 24.3: Original time series is in gray. The standard median filter output is in green and the recursive median filter output is in red.

Both filters preserve the sharp signal edges while reducing the noise. The recursive median filter achieves a smoother result than the standard median filter. The "blocky" nature of the output is characteristic of all median filters. The program is given below.

```
#include <stdio.h>
#include <stdlib.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_filter.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_vector.h>

int
main(void)
{
  const size_t N = 1000;                              /* length of time series */
  const size_t K = 7;                                 /* window size */
```

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```
  const double f = 5.0;                                 /* frequency of square wave in Hz␣
↪*/
  gsl_filter_median_workspace *median_p = gsl_filter_median_alloc(K);
  gsl_filter_rmedian_workspace *rmedian_p = gsl_filter_rmedian_alloc(K);
  gsl_vector *t = gsl_vector_alloc(N);                  /* time */
  gsl_vector *x = gsl_vector_alloc(N);                  /* input vector */
  gsl_vector *y_median = gsl_vector_alloc(N);           /* median filtered output */
  gsl_vector *y_rmedian = gsl_vector_alloc(N);          /* recursive median filtered␣
↪output */
  gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
  size_t i;

  /* generate input signal */
  for (i = 0; i < N; ++i)
    {
      double ti = (double) i / (N - 1.0);
      double tmp = sin(2.0 * M_PI * f * ti);
      double xi = (tmp >= 0.0) ? 1.0 : -1.0;
      double ei = gsl_ran_gaussian(r, 0.1);

      gsl_vector_set(t, i, ti);
      gsl_vector_set(x, i, xi + ei);
    }

  gsl_filter_median(GSL_FILTER_END_PADVALUE, x, y_median, median_p);
  gsl_filter_rmedian(GSL_FILTER_END_PADVALUE, x, y_rmedian, rmedian_p);

  /* print results */
  for (i = 0; i < N; ++i)
    {
      double ti = gsl_vector_get(t, i);
      double xi = gsl_vector_get(x, i);
      double medi = gsl_vector_get(y_median, i);
      double rmedi = gsl_vector_get(y_rmedian, i);

      printf("%f %f %f %f\n",
             ti,
             xi,
             medi,
             rmedi);
    }

  gsl_vector_free(t);
  gsl_vector_free(x);
  gsl_vector_free(y_median);
  gsl_vector_free(y_rmedian);
  gsl_rng_free(r);
  gsl_filter_median_free(median_p);

  return 0;
}
```

24.5.4 Impulse Detection Example

The following example program illustrates the impulse detection filter. First, it constructs a sinusoid signal of length $N = 1000$ with Gaussian noise added. Then, about 1% of the data are perturbed to represent large outliers. An impulse detecting filter is applied with a window size $K = 25$ and tuning parameter $t = 4$, using the Q_n statistic as the robust measure of scale. The results are plotted in Fig. 24.4.

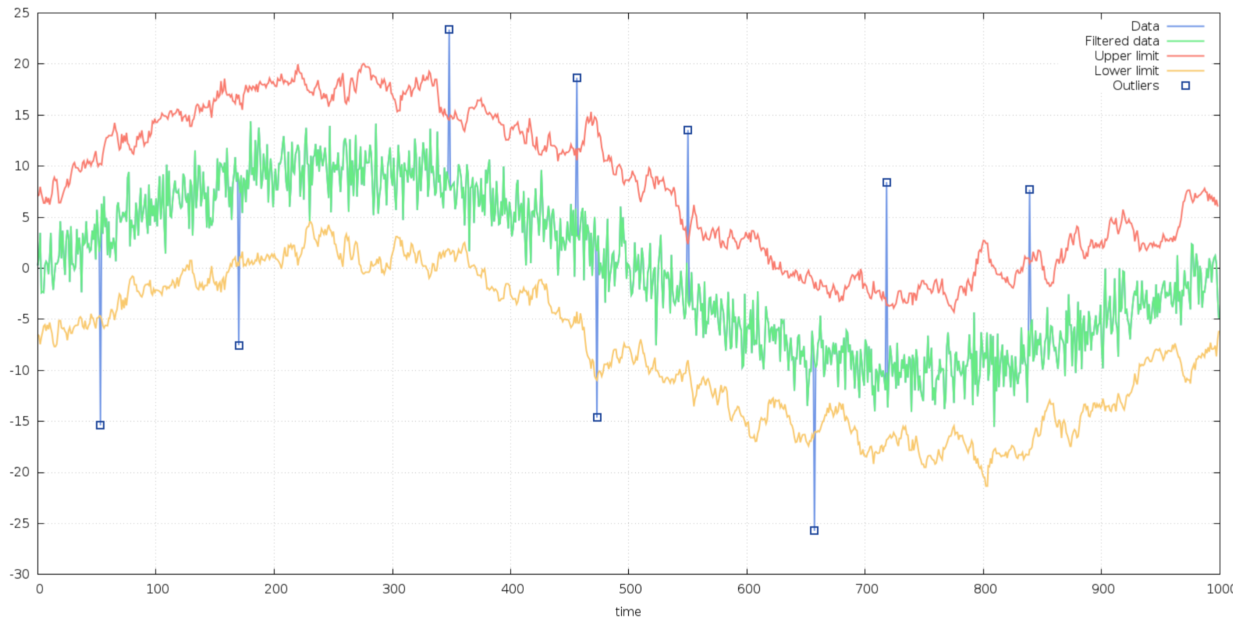

Fig. 24.4: Original time series is in blue, filter output is in green, upper and lower intervals for detecting outliers are in red and yellow respectively. Detected outliers are marked with squares.

The program is given below.

```
#include <stdio.h>
#include <stdlib.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_filter.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_vector.h>

int
main(void)
{
  const size_t N = 1000;                                 /* length of time series */
  const size_t K = 25;                                   /* window size */
  const double t = 4.0;                                  /* number of scale factors for␣
↪outlier detection */
  gsl_vector *x = gsl_vector_alloc(N);                   /* input vector */
  gsl_vector *y = gsl_vector_alloc(N);                   /* output (filtered) vector */
  gsl_vector *xmedian = gsl_vector_alloc(N);             /* window medians */
  gsl_vector *xsigma = gsl_vector_alloc(N);              /* window scale estimates */
  gsl_vector_int *ioutlier = gsl_vector_int_alloc(N);    /* outlier detected? */
```

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```
  gsl_filter_impulse_workspace * w = gsl_filter_impulse_alloc(K);
  gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
  size_t noutlier;
  size_t i;

  /* generate input signal */
  for (i = 0; i < N; ++i)
    {
      double xi = 10.0 * sin(2.0 * M_PI * i / (double) N);
      double ei = gsl_ran_gaussian(r, 2.0);
      double u = gsl_rng_uniform(r);
      double outlier = (u < 0.01) ? 15.0*GSL_SIGN(ei) : 0.0;

      gsl_vector_set(x, i, xi + ei + outlier);
    }

  /* apply impulse detection filter */
  gsl_filter_impulse(GSL_FILTER_END_TRUNCATE, GSL_FILTER_SCALE_QN, t, x, y,
                     xmedian, xsigma, &noutlier, ioutlier, w);

  /* print results */
  for (i = 0; i < N; ++i)
    {
      double xi = gsl_vector_get(x, i);
      double yi = gsl_vector_get(y, i);
      double xmedi = gsl_vector_get(xmedian, i);
      double xsigmai = gsl_vector_get(xsigma, i);
      int outlier = gsl_vector_int_get(ioutlier, i);

      printf("%zu %f %f %f %f %d\n",
             i,
             xi,
             yi,
             xmedi + t * xsigmai,
             xmedi - t * xsigmai,
             outlier);
    }

  gsl_vector_free(x);
  gsl_vector_free(y);
  gsl_vector_free(xmedian);
  gsl_vector_free(xsigma);
  gsl_vector_int_free(ioutlier);
  gsl_filter_impulse_free(w);
  gsl_rng_free(r);

  return 0;
}
```

24.6 References and Further Reading

The following publications are relevant to the algorithms described in this chapter,

- F. J. Harris, *On the use of windows for harmonic analysis with the discrete Fourier transform*, Proceedings of the IEEE, 66 (1), 1978.
- S-J. Ko, Y-H. Lee, and A. T. Fam. *Efficient implementation of one-dimensional recursive median filters*, IEEE transactions on circuits and systems 37.11 (1990): 1447-1450.
- R. K. Pearson and M. Gabbouj, *Nonlinear Digital Filtering with Python: An Introduction*. CRC Press, 2015.

CHAPTER TWENTYFIVE

HISTOGRAMS

This chapter describes functions for creating histograms. Histograms provide a convenient way of summarizing the distribution of a set of data. A histogram consists of a set of *bins* which count the number of events falling into a given range of a continuous variable x. In GSL the bins of a histogram contain floating-point numbers, so they can be used to record both integer and non-integer distributions. The bins can use arbitrary sets of ranges (uniformly spaced bins are the default). Both one and two-dimensional histograms are supported.

Once a histogram has been created it can also be converted into a probability distribution function. The library provides efficient routines for selecting random samples from probability distributions. This can be useful for generating simulations based on real data.

The functions are declared in the header files `gsl_histogram.h` and `gsl_histogram2d.h`.

25.1 The histogram struct

A histogram is defined by the following struct,

type **`gsl_histogram`**

size_t n	This is the number of histogram bins
double * range	The ranges of the bins are stored in an array of `n+1` elements pointed to by range.
double * bin	The counts for each bin are stored in an array of `n` elements pointed to by `bin`. The bins are floating-point numbers, so you can increment them by non-integer values if necessary.

The range for `bin[i]` is given by `range[i]` to `range[i+1]`. For n bins there are `n+1` entries in the array `range`. Each bin is inclusive at the lower end and exclusive at the upper end. Mathematically this means that the bins are defined by the following inequality,

$$\text{bin[i] corresponds to range[i]} \leq x < \text{range[i+1]}$$

Here is a diagram of the correspondence between ranges and bins on the number-line for x:

```
   [ bin[0] )[ bin[1] )[ bin[2] )[ bin[3] )[ bin[4] )
---|---------|---------|---------|---------|---------|---  x
 r[0]      r[1]      r[2]      r[3]      r[4]      r[5]
```

In this picture the values of the `range` array are denoted by r. On the left-hand side of each bin the square bracket `[` denotes an inclusive lower bound ($r \leq x$), and the round parentheses `)` on the right-hand side denote an exclusive upper bound ($x < r$). Thus any samples which fall on the upper end of the histogram are excluded. If you want to include this value for the last bin you will need to add an extra bin to your histogram.

The *gsl_histogram* struct and its associated functions are defined in the header file `gsl_histogram.h`.

25.2 Histogram allocation

The functions for allocating memory to a histogram follow the style of `malloc()` and `free()`. In addition they also perform their own error checking. If there is insufficient memory available to allocate a histogram then the functions call the error handler (with an error number of *GSL_ENOMEM*) in addition to returning a null pointer. Thus if you use the library error handler to abort your program then it isn't necessary to check every histogram `alloc`.

gsl_histogram ***gsl_histogram_alloc**(size_t n)

This function allocates memory for a histogram with *n* bins, and returns a pointer to a newly created *gsl_histogram* struct. If insufficient memory is available a null pointer is returned and the error handler is invoked with an error code of *GSL_ENOMEM*. The bins and ranges are not initialized, and should be prepared using one of the range-setting functions below in order to make the histogram ready for use.

int **gsl_histogram_set_ranges**(*gsl_histogram* *h, const double range[], size_t size)

This function sets the ranges of the existing histogram *h* using the array *range* of size *size*. The values of the histogram bins are reset to zero. The *range* array should contain the desired bin limits. The ranges can be arbitrary, subject to the restriction that they are monotonically increasing.

The following example shows how to create a histogram with logarithmic bins with ranges [1,10), [10,100) and [100,1000):

```
gsl_histogram * h = gsl_histogram_alloc (3);

/* bin[0] covers the range 1 <= x < 10 */
/* bin[1] covers the range 10 <= x < 100 */
/* bin[2] covers the range 100 <= x < 1000 */

double range[4] = { 1.0, 10.0, 100.0, 1000.0 };

gsl_histogram_set_ranges (h, range, 4);
```

Note that the size of the *range* array should be defined to be one element bigger than the number of bins. The additional element is required for the upper value of the final bin.

int **gsl_histogram_set_ranges_uniform**(*gsl_histogram* *h, double xmin, double xmax)

This function sets the ranges of the existing histogram *h* to cover the range *xmin* to *xmax* uniformly. The values of the histogram bins are reset to zero. The bin ranges are shown in the table below,

bin[0]	corresponds to	$xmin \le x < xmin + d$
bin[1]	corresponds to	$xmin + d \le x < xmin + 2d$
...	...	...
bin[n-1]	corresponds to	$xmin + (n-1)d \le x < xmax$

where d is the bin spacing, $d = (xmax - xmin)/n$.

void **gsl_histogram_free**(*gsl_histogram* *h)

This function frees the histogram *h* and all of the memory associated with it.

25.3 Copying Histograms

int **gsl_histogram_memcpy**(*gsl_histogram* *dest, const *gsl_histogram* *src)

This function copies the histogram `src` into the pre-existing histogram `dest`, making `dest` into an exact copy of `src`. The two histograms must be of the same size.

gsl_histogram ***gsl_histogram_clone**(const *gsl_histogram* *src)

This function returns a pointer to a newly created histogram which is an exact copy of the histogram `src`.

25.4 Updating and accessing histogram elements

There are two ways to access histogram bins, either by specifying an x coordinate or by using the bin-index directly. The functions for accessing the histogram through x coordinates use a binary search to identify the bin which covers the appropriate range.

int **gsl_histogram_increment**(*gsl_histogram* *h, double x)

This function updates the histogram `h` by adding one (1.0) to the bin whose range contains the coordinate `x`.

If `x` lies in the valid range of the histogram then the function returns zero to indicate success. If `x` is less than the lower limit of the histogram then the function returns `GSL_EDOM`, and none of bins are modified. Similarly, if the value of `x` is greater than or equal to the upper limit of the histogram then the function returns `GSL_EDOM`, and none of the bins are modified. The error handler is not called, however, since it is often necessary to compute histograms for a small range of a larger dataset, ignoring the values outside the range of interest.

int **gsl_histogram_accumulate**(*gsl_histogram* *h, double x, double weight)

This function is similar to `gsl_histogram_increment()` but increases the value of the appropriate bin in the histogram `h` by the floating-point number `weight`.

double **gsl_histogram_get**(const *gsl_histogram* *h, size_t i)

This function returns the contents of the `i`-th bin of the histogram `h`. If `i` lies outside the valid range of indices for the histogram then the error handler is called with an error code of `GSL_EDOM` and the function returns 0.

int **gsl_histogram_get_range**(const *gsl_histogram* *h, size_t i, double *lower, double *upper)

This function finds the upper and lower range limits of the `i`-th bin of the histogram `h`. If the index `i` is valid then the corresponding range limits are stored in `lower` and `upper`. The lower limit is inclusive (i.e. events with this coordinate are included in the bin) and the upper limit is exclusive (i.e. events with the coordinate of the upper limit are excluded and fall in the neighboring higher bin, if it exists). The function returns 0 to indicate success. If `i` lies outside the valid range of indices for the histogram then the error handler is called and the function returns an error code of `GSL_EDOM`.

double **gsl_histogram_max**(const *gsl_histogram* *h)

double **gsl_histogram_min**(const *gsl_histogram* *h)

size_t **gsl_histogram_bins**(const *gsl_histogram* *h)

These functions return the maximum upper and minimum lower range limits and the number of bins of the histogram `h`. They provide a way of determining these values without accessing the `gsl_histogram` struct directly.

void **gsl_histogram_reset**(*gsl_histogram* *h)

This function resets all the bins in the histogram `h` to zero.

25.5 Searching histogram ranges

The following functions are used by the access and update routines to locate the bin which corresponds to a given x coordinate.

int **gsl_histogram_find**(const *gsl_histogram* *h, double x, size_t *i)

This function finds and sets the index *i* to the bin number which covers the coordinate *x* in the histogram *h*. The bin is located using a binary search. The search includes an optimization for histograms with uniform range, and will return the correct bin immediately in this case. If *x* is found in the range of the histogram then the function sets the index *i* and returns GSL_SUCCESS. If *x* lies outside the valid range of the histogram then the function returns *GSL_EDOM* and the error handler is invoked.

25.6 Histogram Statistics

double **gsl_histogram_max_val**(const *gsl_histogram* *h)

This function returns the maximum value contained in the histogram bins.

size_t **gsl_histogram_max_bin**(const *gsl_histogram* *h)

This function returns the index of the bin containing the maximum value. In the case where several bins contain the same maximum value the smallest index is returned.

double **gsl_histogram_min_val**(const *gsl_histogram* *h)

This function returns the minimum value contained in the histogram bins.

size_t **gsl_histogram_min_bin**(const *gsl_histogram* *h)

This function returns the index of the bin containing the minimum value. In the case where several bins contain the same minimum value the smallest index is returned.

double **gsl_histogram_mean**(const *gsl_histogram* *h)

This function returns the mean of the histogrammed variable, where the histogram is regarded as a probability distribution. Negative bin values are ignored for the purposes of this calculation. The accuracy of the result is limited by the bin width.

double **gsl_histogram_sigma**(const *gsl_histogram* *h)

This function returns the standard deviation of the histogrammed variable, where the histogram is regarded as a probability distribution. Negative bin values are ignored for the purposes of this calculation. The accuracy of the result is limited by the bin width.

double **gsl_histogram_sum**(const *gsl_histogram* *h)

This function returns the sum of all bin values. Negative bin values are included in the sum.

25.7 Histogram Operations

int **gsl_histogram_equal_bins_p**(const *gsl_histogram* *h1, const *gsl_histogram* *h2)

This function returns 1 if the all of the individual bin ranges of the two histograms are identical, and 0 otherwise.

int **gsl_histogram_add**(*gsl_histogram* *h1, const *gsl_histogram* *h2)

This function adds the contents of the bins in histogram *h2* to the corresponding bins of histogram *h1*, i.e. $h'_1(i) = h_1(i) + h_2(i)$. The two histograms must have identical bin ranges.

int **gsl_histogram_sub**(*gsl_histogram* *h1, const *gsl_histogram* *h2)

This function subtracts the contents of the bins in histogram *h2* from the corresponding bins of histogram *h1*, i.e. $h'_1(i) = h_1(i) - h_2(i)$. The two histograms must have identical bin ranges.

int **gsl_histogram_mul**(*gsl_histogram* *h1, const *gsl_histogram* *h2)
This function multiplies the contents of the bins of histogram `h1` by the contents of the corresponding bins in histogram `h2`, i.e. $h'_1(i) = h_1(i) * h_2(i)$. The two histograms must have identical bin ranges.

int **gsl_histogram_div**(*gsl_histogram* *h1, const *gsl_histogram* *h2)
This function divides the contents of the bins of histogram `h1` by the contents of the corresponding bins in histogram `h2`, i.e. $h'_1(i) = h_1(i)/h_2(i)$. The two histograms must have identical bin ranges.

int **gsl_histogram_scale**(*gsl_histogram* *h, double scale)
This function multiplies the contents of the bins of histogram `h` by the constant `scale`, i.e.

$$h'_1(i) = h_1(i) * scale$$

int **gsl_histogram_shift**(*gsl_histogram* *h, double offset)
This function shifts the contents of the bins of histogram `h` by the constant `offset`, i.e.

$$h'_1(i) = h_1(i) + offset$$

25.8 Reading and writing histograms

The library provides functions for reading and writing histograms to a file as binary data or formatted text.

int **gsl_histogram_fwrite**(FILE *stream, const *gsl_histogram* *h)
This function writes the ranges and bins of the histogram `h` to the stream `stream` in binary format. The return value is 0 for success and `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

int **gsl_histogram_fread**(FILE *stream, *gsl_histogram* *h)
This function reads into the histogram `h` from the open stream `stream` in binary format. The histogram `h` must be preallocated with the correct size since the function uses the number of bins in `h` to determine how many bytes to read. The return value is 0 for success and `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

int **gsl_histogram_fprintf**(FILE *stream, const *gsl_histogram* *h, const char *range_format, const char *bin_format)
This function writes the ranges and bins of the histogram `h` line-by-line to the stream `stream` using the format specifiers `range_format` and `bin_format`. These should be one of the `%g`, `%e` or `%f` formats for floating point numbers. The function returns 0 for success and `GSL_EFAILED` if there was a problem writing to the file. The histogram output is formatted in three columns, and the columns are separated by spaces, like this:

```
range[0] range[1] bin[0]
range[1] range[2] bin[1]
range[2] range[3] bin[2]
....
range[n-1] range[n] bin[n-1]
```

The values of the ranges are formatted using `range_format` and the value of the bins are formatted using `bin_format`. Each line contains the lower and upper limit of the range of the bins and the value of the bin itself. Since the upper limit of one bin is the lower limit of the next there is duplication of these values between lines but this allows the histogram to be manipulated with line-oriented tools.

int **gsl_histogram_fscanf**(FILE *stream, *gsl_histogram* *h)
This function reads formatted data from the stream `stream` into the histogram `h`. The data is assumed to be in the three-column format used by `gsl_histogram_fprintf()`. The histogram `h` must be preallocated with the correct length since the function uses the size of `h` to determine how many numbers to read. The function returns 0 for success and `GSL_EFAILED` if there was a problem reading from the file.

25.9 Resampling from histograms

A histogram made by counting events can be regarded as a measurement of a probability distribution. Allowing for statistical error, the height of each bin represents the probability of an event where the value of x falls in the range of that bin. The probability distribution function has the one-dimensional form $p(x)dx$ where,

$$p(x) = n_i/(Nw_i)$$

In this equation n_i is the number of events in the bin which contains x, w_i is the width of the bin and N is the total number of events. The distribution of events within each bin is assumed to be uniform.

25.10 The histogram probability distribution struct

The probability distribution function for a histogram consists of a set of *bins* which measure the probability of an event falling into a given range of a continuous variable x. A probability distribution function is defined by the following struct, which actually stores the cumulative probability distribution function. This is the natural quantity for generating samples via the inverse transform method, because there is a one-to-one mapping between the cumulative probability distribution and the range [0,1]. It can be shown that by taking a uniform random number in this range and finding its corresponding coordinate in the cumulative probability distribution we obtain samples with the desired probability distribution.

type **`gsl_histogram_pdf`**

`size_t n`	This is the number of bins used to approximate the probability distribution function.
`double * range`	The ranges of the bins are stored in an array of $n+1$ elements pointed to by `range`.
`double * sum`	The cumulative probability for the bins is stored in an array of `n` elements pointed to by `sum`.

The following functions allow you to create a `gsl_histogram_pdf` struct which represents this probability distribution and generate random samples from it.

gsl_histogram_pdf ***gsl_histogram_pdf_alloc**(size_t n)

This function allocates memory for a probability distribution with `n` bins and returns a pointer to a newly initialized `gsl_histogram_pdf` struct. If insufficient memory is available a null pointer is returned and the error handler is invoked with an error code of `GSL_ENOMEM`.

int **gsl_histogram_pdf_init**(*gsl_histogram_pdf* *p, const *gsl_histogram* *h)

This function initializes the probability distribution `p` with the contents of the histogram `h`. If any of the bins of `h` are negative then the error handler is invoked with an error code of `GSL_EDOM` because a probability distribution cannot contain negative values.

void **gsl_histogram_pdf_free**(*gsl_histogram_pdf* *p)

This function frees the probability distribution function `p` and all of the memory associated with it.

double **gsl_histogram_pdf_sample**(const *gsl_histogram_pdf* *p, double r)

This function uses `r`, a uniform random number between zero and one, to compute a single random sample from the probability distribution `p`. The algorithm used to compute the sample s is given by the following formula,

$$s = \text{range}[i] + \delta * (\text{range}[i+1] - \text{range}[i])$$

where i is the index which satisfies $sum[i] \leq r < sum[i+1]$ and $delta$ is $(r - sum[i])/(sum[i+1] - sum[i])$.

25.11 Example programs for histograms

The following program shows how to make a simple histogram of a column of numerical data supplied on `stdin`. The program takes three arguments, specifying the upper and lower bounds of the histogram and the number of bins. It then reads numbers from `stdin`, one line at a time, and adds them to the histogram. When there is no more data to read it prints out the accumulated histogram using *gsl_histogram_fprintf()*.

```
#include <stdio.h>
#include <stdlib.h>
#include <gsl/gsl_histogram.h>

int
main (int argc, char **argv)
{
  double a, b;
  size_t n;

  if (argc != 4)
    {
      printf ("Usage: gsl-histogram xmin xmax n\n"
              "Computes a histogram of the data "
              "on stdin using n bins from xmin "
              "to xmax\n");
      exit (0);
    }

  a = atof (argv[1]);
  b = atof (argv[2]);
  n = atoi (argv[3]);

  {
    double x;
    gsl_histogram * h = gsl_histogram_alloc (n);
    gsl_histogram_set_ranges_uniform (h, a, b);

    while (fscanf (stdin, "%lg", &x) == 1)
      {
        gsl_histogram_increment (h, x);
      }
    gsl_histogram_fprintf (stdout, h, "%g", "%g");
    gsl_histogram_free (h);
  }
  exit (0);
}
```

Here is an example of the program in use. We generate 10000 random samples from a Cauchy distribution with a width of 30 and histogram them over the range -100 to 100, using 200 bins:

```
$ gsl-randist 0 10000 cauchy 30
   | gsl-histogram -- -100 100 200 > histogram.dat
```

Fig. 25.1 shows the familiar shape of the Cauchy distribution and the fluctuations caused by the finite sample size.

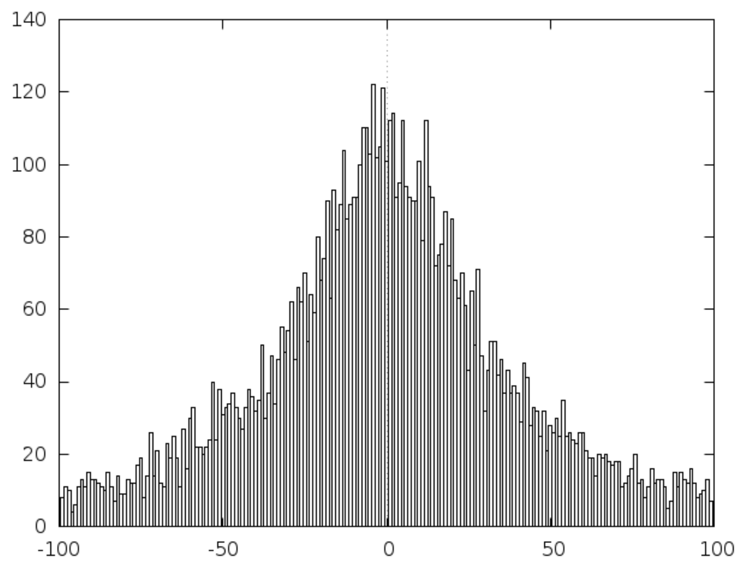

Fig. 25.1: Histogram output from example program

25.12 Two dimensional histograms

A two dimensional histogram consists of a set of *bins* which count the number of events falling in a given area of the (x, y) plane. The simplest way to use a two dimensional histogram is to record two-dimensional position information, $n(x, y)$. Another possibility is to form a *joint distribution* by recording related variables. For example a detector might record both the position of an event (x) and the amount of energy it deposited E. These could be histogrammed as the joint distribution $n(x, E)$.

25.13 The 2D histogram struct

Two dimensional histograms are defined by the following struct,

type **gsl_histogram2d**

`size_t nx, ny`	This is the number of histogram bins in the x and y directions.
`double * xrange`	The ranges of the bins in the x-direction are stored in an array of `nx + 1` elements pointed to by `xrange`.
`double * yrange`	The ranges of the bins in the y-direction are stored in an array of `ny + 1` elements pointed to by `yrange`.
`double * bin`	The counts for each bin are stored in an array pointed to by `bin`. The bins are floating-point numbers, so you can increment them by non-integer values if necessary. The array `bin` stores the two dimensional array of bins in a single block of memory according to the mapping `bin(i,j)` = `bin[i * ny + j]`.

The range for `bin(i,j)` is given by `xrange[i]` to `xrange[i+1]` in the x-direction and `yrange[j]` to `yrange[j+1]` in the y-direction. Each bin is inclusive at the lower end and exclusive at the upper end. Mathematically this means that the bins are defined by the following inequality,

$$\begin{array}{cc} \text{bin(i,j) corresponds to} & \mathit{xrange}[i] \le x < \mathit{xrange}[i+1] \\ \text{and} & \mathit{yrange}[j] \le y < \mathit{yrange}[j+1] \end{array}$$

Note that any samples which fall on the upper sides of the histogram are excluded. If you want to include these values for the side bins you will need to add an extra row or column to your histogram.

The *gsl_histogram2d* struct and its associated functions are defined in the header file `gsl_histogram2d.h`.

25.14 2D Histogram allocation

The functions for allocating memory to a 2D histogram follow the style of `malloc()` and `free()`. In addition they also perform their own error checking. If there is insufficient memory available to allocate a histogram then the functions call the error handler (with an error number of *GSL_ENOMEM*) in addition to returning a null pointer. Thus if you use the library error handler to abort your program then it isn't necessary to check every 2D histogram `alloc`.

gsl_histogram2d ***gsl_histogram2d_alloc**(size_t nx, size_t ny)

This function allocates memory for a two-dimensional histogram with *nx* bins in the x direction and *ny* bins in the y direction. The function returns a pointer to a newly created *gsl_histogram2d* struct. If insufficient memory is available a null pointer is returned and the error handler is invoked with an error code of *GSL_ENOMEM*. The bins and ranges must be initialized with one of the functions below before the histogram is ready for use.

int **gsl_histogram2d_set_ranges**(*gsl_histogram2d* *h, const double xrange[], size_t xsize, const double yrange[], size_t ysize)

This function sets the ranges of the existing histogram *h* using the arrays *xrange* and *yrange* of size *xsize* and *ysize* respectively. The values of the histogram bins are reset to zero.

int **gsl_histogram2d_set_ranges_uniform**(*gsl_histogram2d* *h, double xmin, double xmax, double ymin, double ymax)

This function sets the ranges of the existing histogram *h* to cover the ranges *xmin* to *xmax* and *ymin* to *ymax* uniformly. The values of the histogram bins are reset to zero.

void **gsl_histogram2d_free**(*gsl_histogram2d* *h)

This function frees the 2D histogram *h* and all of the memory associated with it.

25.15 Copying 2D Histograms

int **gsl_histogram2d_memcpy**(*gsl_histogram2d* *dest, const *gsl_histogram2d* *src)

This function copies the histogram *src* into the pre-existing histogram *dest*, making *dest* into an exact copy of *src*. The two histograms must be of the same size.

gsl_histogram2d ***gsl_histogram2d_clone**(const *gsl_histogram2d* *src)

This function returns a pointer to a newly created histogram which is an exact copy of the histogram *src*.

25.16 Updating and accessing 2D histogram elements

You can access the bins of a two-dimensional histogram either by specifying a pair of (x, y) coordinates or by using the bin indices (i, j) directly. The functions for accessing the histogram through (x, y) coordinates use binary searches in the x and y directions to identify the bin which covers the appropriate range.

int **gsl_histogram2d_increment**(*gsl_histogram2d* *h, double x, double y)

This function updates the histogram `h` by adding one (1.0) to the bin whose x and y ranges contain the coordinates (`x`, `y`).

If the point (x, y) lies inside the valid ranges of the histogram then the function returns zero to indicate success. If (x, y) lies outside the limits of the histogram then the function returns `GSL_EDOM`, and none of the bins are modified. The error handler is not called, since it is often necessary to compute histograms for a small range of a larger dataset, ignoring any coordinates outside the range of interest.

int **gsl_histogram2d_accumulate**(*gsl_histogram2d* *h, double x, double y, double weight)

This function is similar to `gsl_histogram2d_increment()` but increases the value of the appropriate bin in the histogram `h` by the floating-point number `weight`.

double **gsl_histogram2d_get**(const *gsl_histogram2d* *h, size_t i, size_t j)

This function returns the contents of the (`i`, `j`)-th bin of the histogram `h`. If (`i`, `j`) lies outside the valid range of indices for the histogram then the error handler is called with an error code of `GSL_EDOM` and the function returns 0.

int **gsl_histogram2d_get_xrange**(const *gsl_histogram2d* *h, size_t i, double *xlower, double *xupper)

int **gsl_histogram2d_get_yrange**(const *gsl_histogram2d* *h, size_t j, double *ylower, double *yupper)

These functions find the upper and lower range limits of the `i`-th and `j`-th bins in the x and y directions of the histogram `h`. The range limits are stored in `xlower` and `xupper` or `ylower` and `yupper`. The lower limits are inclusive (i.e. events with these coordinates are included in the bin) and the upper limits are exclusive (i.e. events with the value of the upper limit are not included and fall in the neighboring higher bin, if it exists). The functions return 0 to indicate success. If `i` or `j` lies outside the valid range of indices for the histogram then the error handler is called with an error code of `GSL_EDOM`.

double **gsl_histogram2d_xmax**(const *gsl_histogram2d* *h)

double **gsl_histogram2d_xmin**(const *gsl_histogram2d* *h)

size_t **gsl_histogram2d_nx**(const *gsl_histogram2d* *h)

double **gsl_histogram2d_ymax**(const *gsl_histogram2d* *h)

double **gsl_histogram2d_ymin**(const *gsl_histogram2d* *h)

size_t **gsl_histogram2d_ny**(const *gsl_histogram2d* *h)

These functions return the maximum upper and minimum lower range limits and the number of bins for the x and y directions of the histogram `h`. They provide a way of determining these values without accessing the `gsl_histogram2d` struct directly.

void **gsl_histogram2d_reset**(*gsl_histogram2d* *h)

This function resets all the bins of the histogram `h` to zero.

25.17 Searching 2D histogram ranges

The following functions are used by the access and update routines to locate the bin which corresponds to a given (x, y) coordinate.

int **gsl_histogram2d_find**(const *gsl_histogram2d* *h, double x, double y, size_t *i, size_t *j)

This function finds and sets the indices *i* and *j* to the bin which covers the coordinates (*x*, *y*). The bin is located using a binary search. The search includes an optimization for histograms with uniform ranges, and will return the correct bin immediately in this case. If (x, y) is found then the function sets the indices (*i*, *j*) and returns GSL_SUCCESS. If (x, y) lies outside the valid range of the histogram then the function returns *GSL_EDOM* and the error handler is invoked.

25.18 2D Histogram Statistics

double **gsl_histogram2d_max_val**(const *gsl_histogram2d* *h)

This function returns the maximum value contained in the histogram bins.

void **gsl_histogram2d_max_bin**(const *gsl_histogram2d* *h, size_t *i, size_t *j)

This function finds the indices of the bin containing the maximum value in the histogram *h* and stores the result in (*i*, *j*). In the case where several bins contain the same maximum value the first bin found is returned.

double **gsl_histogram2d_min_val**(const *gsl_histogram2d* *h)

This function returns the minimum value contained in the histogram bins.

void **gsl_histogram2d_min_bin**(const *gsl_histogram2d* *h, size_t *i, size_t *j)

This function finds the indices of the bin containing the minimum value in the histogram *h* and stores the result in (*i*, *j*). In the case where several bins contain the same maximum value the first bin found is returned.

double **gsl_histogram2d_xmean**(const *gsl_histogram2d* *h)

This function returns the mean of the histogrammed x variable, where the histogram is regarded as a probability distribution. Negative bin values are ignored for the purposes of this calculation.

double **gsl_histogram2d_ymean**(const *gsl_histogram2d* *h)

This function returns the mean of the histogrammed y variable, where the histogram is regarded as a probability distribution. Negative bin values are ignored for the purposes of this calculation.

double **gsl_histogram2d_xsigma**(const *gsl_histogram2d* *h)

This function returns the standard deviation of the histogrammed x variable, where the histogram is regarded as a probability distribution. Negative bin values are ignored for the purposes of this calculation.

double **gsl_histogram2d_ysigma**(const *gsl_histogram2d* *h)

This function returns the standard deviation of the histogrammed y variable, where the histogram is regarded as a probability distribution. Negative bin values are ignored for the purposes of this calculation.

double **gsl_histogram2d_cov**(const *gsl_histogram2d* *h)

This function returns the covariance of the histogrammed x and y variables, where the histogram is regarded as a probability distribution. Negative bin values are ignored for the purposes of this calculation.

double **gsl_histogram2d_sum**(const *gsl_histogram2d* *h)

This function returns the sum of all bin values. Negative bin values are included in the sum.

25.19 2D Histogram Operations

int **gsl_histogram2d_equal_bins_p**(const *gsl_histogram2d* *h1, const *gsl_histogram2d* *h2)

This function returns 1 if all the individual bin ranges of the two histograms are identical, and 0 otherwise.

int **gsl_histogram2d_add**(*gsl_histogram2d* *h1, const *gsl_histogram2d* *h2)

This function adds the contents of the bins in histogram `h2` to the corresponding bins of histogram `h1`, i.e. $h'_1(i,j) = h_1(i,j) + h_2(i,j)$. The two histograms must have identical bin ranges.

int **gsl_histogram2d_sub**(*gsl_histogram2d* *h1, const *gsl_histogram2d* *h2)

This function subtracts the contents of the bins in histogram `h2` from the corresponding bins of histogram `h1`, i.e. $h'_1(i,j) = h_1(i,j) - h_2(i,j)$. The two histograms must have identical bin ranges.

int **gsl_histogram2d_mul**(*gsl_histogram2d* *h1, const *gsl_histogram2d* *h2)

This function multiplies the contents of the bins of histogram `h1` by the contents of the corresponding bins in histogram `h2`, i.e. $h'_1(i,j) = h_1(i,j) * h_2(i,j)$. The two histograms must have identical bin ranges.

int **gsl_histogram2d_div**(*gsl_histogram2d* *h1, const *gsl_histogram2d* *h2)

This function divides the contents of the bins of histogram `h1` by the contents of the corresponding bins in histogram `h2`, i.e. $h'_1(i,j) = h_1(i,j)/h_2(i,j)$. The two histograms must have identical bin ranges.

int **gsl_histogram2d_scale**(*gsl_histogram2d* *h, double scale)

This function multiplies the contents of the bins of histogram `h` by the constant `scale`, i.e.

$$h'_1(i,j) = h_1(i,j) * scale$$

int **gsl_histogram2d_shift**(*gsl_histogram2d* *h, double offset)

This function shifts the contents of the bins of histogram `h` by the constant `offset`, i.e.

$$h'_1(i,j) = h_1(i,j) + offset$$

25.20 Reading and writing 2D histograms

The library provides functions for reading and writing two dimensional histograms to a file as binary data or formatted text.

int **gsl_histogram2d_fwrite**(FILE *stream, const *gsl_histogram2d* *h)

This function writes the ranges and bins of the histogram `h` to the stream `stream` in binary format. The return value is 0 for success and `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

int **gsl_histogram2d_fread**(FILE *stream, *gsl_histogram2d* *h)

This function reads into the histogram `h` from the stream `stream` in binary format. The histogram `h` must be preallocated with the correct size since the function uses the number of x and y bins in `h` to determine how many bytes to read. The return value is 0 for success and `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

int **gsl_histogram2d_fprintf**(FILE *stream, const *gsl_histogram2d* *h, const char *range_format, const char *bin_format)

This function writes the ranges and bins of the histogram `h` line-by-line to the stream `stream` using the format specifiers `range_format` and `bin_format`. These should be one of the `%g`, `%e` or `%f` formats for floating point numbers. The function returns 0 for success and `GSL_EFAILED` if there was a problem writing to the file. The histogram output is formatted in five columns, and the columns are separated by spaces, like this:

```
xrange[0] xrange[1] yrange[0] yrange[1] bin(0,0)
xrange[0] xrange[1] yrange[1] yrange[2] bin(0,1)
xrange[0] xrange[1] yrange[2] yrange[3] bin(0,2)
....
xrange[0] xrange[1] yrange[ny-1] yrange[ny] bin(0,ny-1)

xrange[1] xrange[2] yrange[0] yrange[1] bin(1,0)
xrange[1] xrange[2] yrange[1] yrange[2] bin(1,1)
xrange[1] xrange[2] yrange[1] yrange[2] bin(1,2)
....
xrange[1] xrange[2] yrange[ny-1] yrange[ny] bin(1,ny-1)

....

xrange[nx-1] xrange[nx] yrange[0] yrange[1] bin(nx-1,0)
xrange[nx-1] xrange[nx] yrange[1] yrange[2] bin(nx-1,1)
xrange[nx-1] xrange[nx] yrange[1] yrange[2] bin(nx-1,2)
....
xrange[nx-1] xrange[nx] yrange[ny-1] yrange[ny] bin(nx-1,ny-1)
```

Each line contains the lower and upper limits of the bin and the contents of the bin. Since the upper limits of the each bin are the lower limits of the neighboring bins there is duplication of these values but this allows the histogram to be manipulated with line-oriented tools.

int **gsl_histogram2d_fscanf**(FILE *stream, *gsl_histogram2d* *h)

This function reads formatted data from the stream *stream* into the histogram *h*. The data is assumed to be in the five-column format used by *gsl_histogram2d_fprintf()*. The histogram *h* must be preallocated with the correct lengths since the function uses the sizes of *h* to determine how many numbers to read. The function returns 0 for success and `GSL_EFAILED` if there was a problem reading from the file.

25.21 Resampling from 2D histograms

As in the one-dimensional case, a two-dimensional histogram made by counting events can be regarded as a measurement of a probability distribution. Allowing for statistical error, the height of each bin represents the probability of an event where (x, y) falls in the range of that bin. For a two-dimensional histogram the probability distribution takes the form $p(x,y)dxdy$ where,

$$p(x,y) = n_{ij}/(NA_{ij})$$

In this equation n_{ij} is the number of events in the bin which contains (x,y), A_{ij} is the area of the bin and N is the total number of events. The distribution of events within each bin is assumed to be uniform.

type **gsl_histogram2d_pdf**

`size_t nx, ny`	This is the number of histogram bins used to approximate the probability distribution function in the x and y directions.
`double * xrange`	The ranges of the bins in the x-direction are stored in an array of `nx + 1` elements pointed to by `xrange`.
`double * yrange`	The ranges of the bins in the y-direction are stored in an array of `ny + 1` pointed to by `yrange`.
`double * sum`	The cumulative probability for the bins is stored in an array of `nx` * `ny` elements pointed to by `sum`.

The following functions allow you to create a *gsl_histogram2d_pdf* struct which represents a two dimensional probability distribution and generate random samples from it.

gsl_histogram2d_pdf ***gsl_histogram2d_pdf_alloc**(size_t nx, size_t ny)

This function allocates memory for a two-dimensional probability distribution of size *nx*-by-*ny* and returns a pointer to a newly initialized *gsl_histogram2d_pdf* struct. If insufficient memory is available a null pointer is returned and the error handler is invoked with an error code of *GSL_ENOMEM*.

int **gsl_histogram2d_pdf_init**(*gsl_histogram2d_pdf* *p, const *gsl_histogram2d* *h)

This function initializes the two-dimensional probability distribution calculated *p* from the histogram *h*. If any of the bins of *h* are negative then the error handler is invoked with an error code of *GSL_EDOM* because a probability distribution cannot contain negative values.

void **gsl_histogram2d_pdf_free**(*gsl_histogram2d_pdf* *p)

This function frees the two-dimensional probability distribution function *p* and all of the memory associated with it.

int **gsl_histogram2d_pdf_sample**(const *gsl_histogram2d_pdf* *p, double r1, double r2, double *x, double *y)

This function uses two uniform random numbers between zero and one, *r1* and *r2*, to compute a single random sample from the two-dimensional probability distribution *p*.

25.22 Example programs for 2D histograms

This program demonstrates two features of two-dimensional histograms. First a 10-by-10 two-dimensional histogram is created with x and y running from 0 to 1. Then a few sample points are added to the histogram, at (0.3,0.3) with a height of 1, at (0.8,0.1) with a height of 5 and at (0.7,0.9) with a height of 0.5. This histogram with three events is used to generate a random sample of 1000 simulated events, which are printed out.

```
#include <stdio.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_histogram2d.h>

int
main (void)
{
  const gsl_rng_type * T;
  gsl_rng * r;

  gsl_histogram2d * h = gsl_histogram2d_alloc (10, 10);

  gsl_histogram2d_set_ranges_uniform (h,
                                      0.0, 1.0,
                                      0.0, 1.0);

  gsl_histogram2d_accumulate (h, 0.3, 0.3, 1);
  gsl_histogram2d_accumulate (h, 0.8, 0.1, 5);
  gsl_histogram2d_accumulate (h, 0.7, 0.9, 0.5);

  gsl_rng_env_setup ();

  T = gsl_rng_default;
  r = gsl_rng_alloc (T);

  {
```

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```
    int i;
    gsl_histogram2d_pdf * p
      = gsl_histogram2d_pdf_alloc (h->nx, h->ny);

    gsl_histogram2d_pdf_init (p, h);

    for (i = 0; i < 1000; i++) {
      double x, y;
      double u = gsl_rng_uniform (r);
      double v = gsl_rng_uniform (r);

      gsl_histogram2d_pdf_sample (p, u, v, &x, &y);

      printf ("%g %g\n", x, y);
    }

    gsl_histogram2d_pdf_free (p);
  }

  gsl_histogram2d_free (h);
  gsl_rng_free (r);

  return 0;
}
```

The following plot shows the distribution of the simulated events. Using a higher resolution grid we can see the original underlying histogram and also the statistical fluctuations caused by the events being uniformly distributed over the area of the original bins.

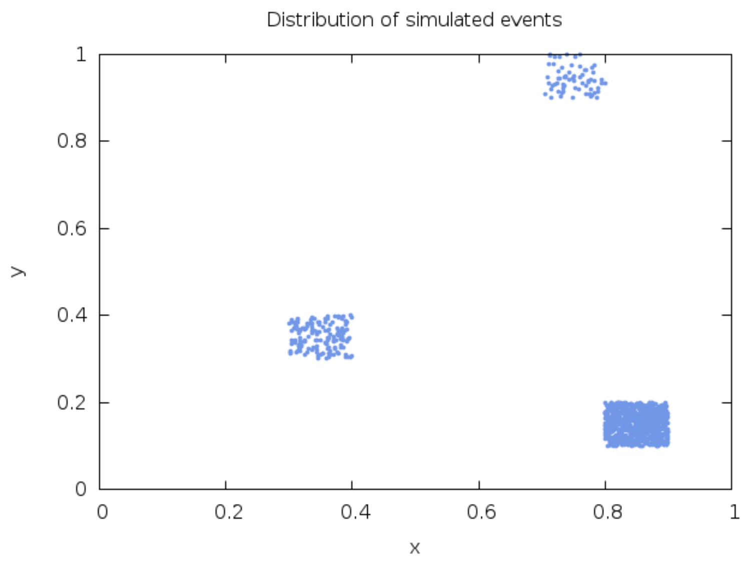

Fig. 25.2: Distribution of simulated events from example program

CHAPTER

TWENTYSIX

N-TUPLES

This chapter describes functions for creating and manipulating *ntuples*, sets of values associated with events. The ntuples are stored in files. Their values can be extracted in any combination and *booked* in a histogram using a selection function.

The values to be stored are held in a user-defined data structure, and an ntuple is created associating this data structure with a file. The values are then written to the file (normally inside a loop) using the ntuple functions described below.

A histogram can be created from ntuple data by providing a selection function and a value function. The selection function specifies whether an event should be included in the subset to be analyzed or not. The value function computes the entry to be added to the histogram for each event.

All the ntuple functions are defined in the header file `gsl_ntuple.h`.

26.1 The ntuple struct

type **`gsl_ntuple`**

Ntuples are manipulated using the *`gsl_ntuple`* struct. This struct contains information on the file where the ntuple data is stored, a pointer to the current ntuple data row and the size of the user-defined ntuple data struct:

```
typedef struct
  {
    FILE * file;
    void * ntuple_data;
    size_t size;
  } gsl_ntuple;
```

26.2 Creating ntuples

gsl_ntuple ***`gsl_ntuple_create`**(char *filename, void *ntuple_data, size_t size)

This function creates a new write-only ntuple file *`filename`* for ntuples of size *`size`* and returns a pointer to the newly created ntuple struct. Any existing file with the same name is truncated to zero length and overwritten. A pointer to memory for the current ntuple row *`ntuple_data`* must be supplied—this is used to copy ntuples in and out of the file.

26.3 Opening an existing ntuple file

gsl_ntuple ***gsl_ntuple_open**(char *filename, void *ntuple_data, size_t size)

This function opens an existing ntuple file `filename` for reading and returns a pointer to a corresponding ntuple struct. The ntuples in the file must have size `size`. A pointer to memory for the current ntuple row `ntuple_data` must be supplied—this is used to copy ntuples in and out of the file.

26.4 Writing ntuples

int **gsl_ntuple_write**(*gsl_ntuple* *ntuple)

This function writes the current ntuple `ntuple->ntuple_data` of size `ntuple->size` to the corresponding file.

int **gsl_ntuple_bookdata**(*gsl_ntuple* *ntuple)

This function is a synonym for `gsl_ntuple_write()`.

26.5 Reading ntuples

int **gsl_ntuple_read**(*gsl_ntuple* *ntuple)

This function reads the current row of the ntuple file for `ntuple` and stores the values in `ntuple->data`.

26.6 Closing an ntuple file

int **gsl_ntuple_close**(*gsl_ntuple* *ntuple)

This function closes the ntuple file `ntuple` and frees its associated allocated memory.

26.7 Histogramming ntuple values

Once an ntuple has been created its contents can be histogrammed in various ways using the function `gsl_ntuple_project()`. Two user-defined functions must be provided, a function to select events and a function to compute scalar values. The selection function and the value function both accept the ntuple row as a first argument and other parameters as a second argument.

type **gsl_ntuple_select_fn**

The *selection function* determines which ntuple rows are selected for histogramming. It is defined by the following struct:

```
typedef struct
  {
    int (* function) (void * ntuple_data, void * params);
    void * params;
  } gsl_ntuple_select_fn;
```

The struct component `function` should return a non-zero value for each ntuple row that is to be included in the histogram.

type **gsl_ntuple_value_fn**

The *value function* computes scalar values for those ntuple rows selected by the selection function:

```
typedef struct
  {
    double (* function) (void * ntuple_data, void * params);
    void * params;
  } gsl_ntuple_value_fn;
```

In this case the struct component `function` should return the value to be added to the histogram for the ntuple row.

int **gsl_ntuple_project**(*gsl_histogram* *h, *gsl_ntuple* *ntuple, *gsl_ntuple_value_fn* *value_func, *gsl_ntuple_select_fn* *select_func)

This function updates the histogram `h` from the ntuple `ntuple` using the functions `value_func` and `select_func`. For each ntuple row where the selection function `select_func` is non-zero the corresponding value of that row is computed using the function `value_func` and added to the histogram. Those ntuple rows where `select_func` returns zero are ignored. New entries are added to the histogram, so subsequent calls can be used to accumulate further data in the same histogram.

26.8 Examples

The following example programs demonstrate the use of ntuples in managing a large dataset. The first program creates a set of 10,000 simulated "events", each with 3 associated values (x, y, z). These are generated from a Gaussian distribution with unit variance, for demonstration purposes, and written to the ntuple file `test.dat`.

```
#include <gsl/gsl_ntuple.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>

struct data
{
  double x;
  double y;
  double z;
};

int
main (void)
{
  const gsl_rng_type * T;
  gsl_rng * r;

  struct data ntuple_row;
  int i;

  gsl_ntuple *ntuple
    = gsl_ntuple_create ("test.dat", &ntuple_row,
                         sizeof (ntuple_row));

  gsl_rng_env_setup ();

  T = gsl_rng_default;
  r = gsl_rng_alloc (T);
```

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```
  for (i = 0; i < 10000; i++)
    {
      ntuple_row.x = gsl_ran_ugaussian (r);
      ntuple_row.y = gsl_ran_ugaussian (r);
      ntuple_row.z = gsl_ran_ugaussian (r);

      gsl_ntuple_write (ntuple);
    }

  gsl_ntuple_close (ntuple);
  gsl_rng_free (r);

  return 0;
}
```

The next program analyses the ntuple data in the file `test.dat`. The analysis procedure is to compute the squared-magnitude of each event, $E^2 = x^2 + y^2 + z^2$, and select only those which exceed a lower limit of 1.5. The selected events are then histogrammed using their E^2 values.

```
#include <math.h>
#include <gsl/gsl_ntuple.h>
#include <gsl/gsl_histogram.h>

struct data
{
  double x;
  double y;
  double z;
};

int sel_func (void *ntuple_data, void *params);
double val_func (void *ntuple_data, void *params);

int
main (void)
{
  struct data ntuple_row;

  gsl_ntuple *ntuple
    = gsl_ntuple_open ("test.dat", &ntuple_row,
                       sizeof (ntuple_row));
  double lower = 1.5;

  gsl_ntuple_select_fn S;
  gsl_ntuple_value_fn V;

  gsl_histogram *h = gsl_histogram_alloc (100);
  gsl_histogram_set_ranges_uniform(h, 0.0, 10.0);

  S.function = &sel_func;
  S.params = &lower;
```

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```
  V.function = &val_func;
  V.params = 0;

  gsl_ntuple_project (h, ntuple, &V, &S);
  gsl_histogram_fprintf (stdout, h, "%f", "%f");
  gsl_histogram_free (h);
  gsl_ntuple_close (ntuple);

  return 0;
}

int
sel_func (void *ntuple_data, void *params)
{
  struct data * data = (struct data *) ntuple_data;
  double x, y, z, E2, scale;
  scale = *(double *) params;

  x = data->x;
  y = data->y;
  z = data->z;

  E2 = x * x + y * y + z * z;

  return E2 > scale;
}

double
val_func (void *ntuple_data, void *params)
{
  (void)(params); /* avoid unused parameter warning */
  struct data * data = (struct data *) ntuple_data;
  double x, y, z;

  x = data->x;
  y = data->y;
  z = data->z;

  return x * x + y * y + z * z;
}
```

Fig. 26.1 shows the distribution of the selected events. Note the cut-off at the lower bound.

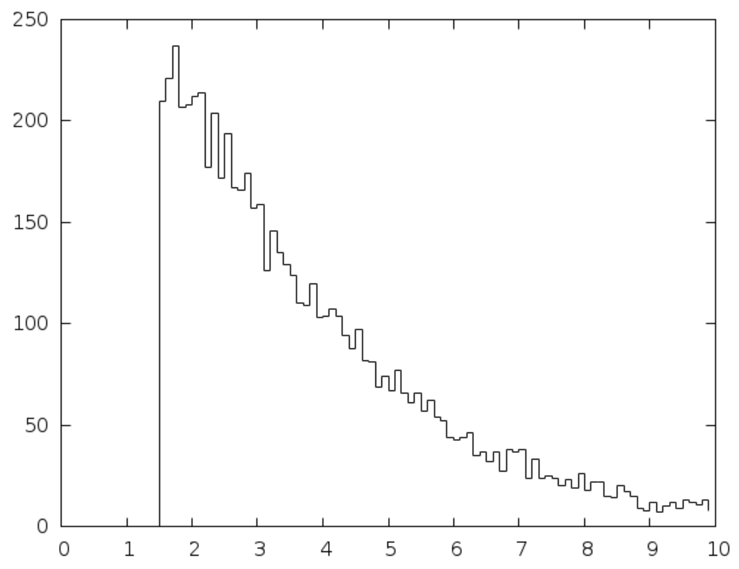

Fig. 26.1: Distribution of selected events

26.9 References and Further Reading

Further information on the use of ntuples can be found in the documentation for the CERN packages PAW and HBOOK (available online).

CHAPTER

TWENTYSEVEN

MONTE CARLO INTEGRATION

This chapter describes routines for multidimensional Monte Carlo integration. These include the traditional Monte Carlo method and adaptive algorithms such as VEGAS and MISER which use importance sampling and stratified sampling techniques. Each algorithm computes an estimate of a multidimensional definite integral of the form,

$$I = \int_{x_l}^{x_u} dx \int_{y_l}^{y_u} dy ... f(x, y, ...)$$

over a hypercubic region $((x_l, x_u)$, $(y_l, y_u), ...)$ using a fixed number of function calls. The routines also provide a statistical estimate of the error on the result. This error estimate should be taken as a guide rather than as a strict error bound—random sampling of the region may not uncover all the important features of the function, resulting in an underestimate of the error.

The functions are defined in separate header files for each routine, `gsl_monte_plain.h`, `gsl_monte_miser.h` and `gsl_monte_vegas.h`.

27.1 Interface

All of the Monte Carlo integration routines use the same general form of interface. There is an allocator to allocate memory for control variables and workspace, a routine to initialize those control variables, the integrator itself, and a function to free the space when done.

Each integration function requires a random number generator to be supplied, and returns an estimate of the integral and its standard deviation. The accuracy of the result is determined by the number of function calls specified by the user. If a known level of accuracy is required this can be achieved by calling the integrator several times and averaging the individual results until the desired accuracy is obtained.

Random sample points used within the Monte Carlo routines are always chosen strictly within the integration region, so that endpoint singularities are automatically avoided.

The function to be integrated has its own datatype, defined in the header file `gsl_monte.h`.

type **`gsl_monte_function`**

This data type defines a general function with parameters for Monte Carlo integration.

`double (* f) (double * x, size_t dim, void * params)`	this function should return the value $f(x, params)$ for the argument `x` and parameters `params`, where `x` is an array of size `dim` giving the coordinates of the point where the function is to be evaluated.
`size_t dim`	the number of dimensions for `x`.
`void * params`	a pointer to the parameters of the function.

Here is an example for a quadratic function in two dimensions,

$$f(x, y) = ax^2 + bxy + cy^2$$

with $a = 3, b = 2, c = 1$. The following code defines a *gsl_monte_function* `F` which you could pass to an integrator:

```
struct my_f_params { double a; double b; double c; };

double
my_f (double x[], size_t dim, void * p) {
   struct my_f_params * fp = (struct my_f_params *)p;

   if (dim != 2)
      {
        fprintf (stderr, "error: dim != 2");
        abort ();
      }

   return  fp->a * x[0] * x[0]
             + fp->b * x[0] * x[1]
               + fp->c * x[1] * x[1];
}

gsl_monte_function F;
struct my_f_params params = { 3.0, 2.0, 1.0 };

F.f = &my_f;
F.dim = 2;
F.params = &params;
```

The function $f(x)$ can be evaluated using the following macro:

```
#define GSL_MONTE_FN_EVAL(F,x)
    (*((F)->f))(x,(F)->dim,(F)->params)
```

27.2 PLAIN Monte Carlo

The plain Monte Carlo algorithm samples points randomly from the integration region to estimate the integral and its error. Using this algorithm the estimate of the integral $E(f; N)$ for N randomly distributed points x_i is given by,

$$E(f; N) = V\langle f\rangle = \frac{V}{N}\sum_i^N f(x_i)$$

where V is the volume of the integration region. The error on this estimate $\sigma(E; N)$ is calculated from the estimated variance of the mean,

$$\sigma^2(E; N) = \frac{V^2}{N^2}\sum_i^N (f(x_i) - \langle f\rangle)^2.$$

For large N this variance decreases asymptotically as $\mathrm{Var}(f)/N$, where $\mathrm{Var}(f)$ is the true variance of the function over the integration region. The error estimate itself should decrease as $\sigma(f)/\sqrt{N}$. The familiar law of errors decreasing as $1/\sqrt{N}$ applies—to reduce the error by a factor of 10 requires a 100-fold increase in the number of sample points.

The functions described in this section are declared in the header file `gsl_monte_plain.h`.

type **`gsl_monte_plain_state`**

   This is a workspace for plain Monte Carlo integration *gsl_monte_plain_state* ***gsl_monte_plain_alloc**(size_t dim)

This function allocates and initializes a workspace for Monte Carlo integration in `dim` dimensions.

int **gsl_monte_plain_init**(*gsl_monte_plain_state* *s)

This function initializes a previously allocated integration state. This allows an existing workspace to be reused for different integrations.

int **gsl_monte_plain_integrate**(*gsl_monte_function* *f, const double xl[], const double xu[], size_t dim, size_t calls, *gsl_rng* *r, *gsl_monte_plain_state* *s, double *result, double *abserr)

This routines uses the plain Monte Carlo algorithm to integrate the function `f` over the `dim`-dimensional hypercubic region defined by the lower and upper limits in the arrays `xl` and `xu`, each of size `dim`. The integration uses a fixed number of function calls `calls`, and obtains random sampling points using the random number generator `r`. A previously allocated workspace `s` must be supplied. The result of the integration is returned in `result`, with an estimated absolute error `abserr`.

void **gsl_monte_plain_free**(*gsl_monte_plain_state* *s)

This function frees the memory associated with the integrator state `s`.

27.3 MISER

The MISER algorithm of Press and Farrar is based on recursive stratified sampling. This technique aims to reduce the overall integration error by concentrating integration points in the regions of highest variance.

The idea of stratified sampling begins with the observation that for two disjoint regions a and b with Monte Carlo estimates of the integral $E_a(f)$ and $E_b(f)$ and variances $\sigma_a^2(f)$ and $\sigma_b^2(f)$, the variance $\mathrm{Var}(f)$ of the combined estimate $E(f) = \frac{1}{2}(E_a(f) + E_b(f))$ is given by,

$$\mathrm{Var}(f) = \frac{\sigma_a^2(f)}{4N_a} + \frac{\sigma_b^2(f)}{4N_b}.$$

It can be shown that this variance is minimized by distributing the points such that,

$$\frac{N_a}{N_a + N_b} = \frac{\sigma_a}{\sigma_a + \sigma_b}.$$

Hence the smallest error estimate is obtained by allocating sample points in proportion to the standard deviation of the function in each sub-region.

The MISER algorithm proceeds by bisecting the integration region along one coordinate axis to give two sub-regions at each step. The direction is chosen by examining all d possible bisections and selecting the one which will minimize the combined variance of the two sub-regions. The variance in the sub-regions is estimated by sampling with a fraction of the total number of points available to the current step. The same procedure is then repeated recursively for each of the two half-spaces from the best bisection. The remaining sample points are allocated to the sub-regions using the formula for N_a and N_b. This recursive allocation of integration points continues down to a user-specified depth where each sub-region is integrated using a plain Monte Carlo estimate. These individual values and their error estimates are then combined upwards to give an overall result and an estimate of its error.

The functions described in this section are declared in the header file `gsl_monte_miser.h`.

type **gsl_monte_miser_state**

This workspace is used for MISER Monte Carlo integration

gsl_monte_miser_state ***gsl_monte_miser_alloc**(size_t dim)

This function allocates and initializes a workspace for Monte Carlo integration in `dim` dimensions. The workspace is used to maintain the state of the integration.

int **gsl_monte_miser_init**(*gsl_monte_miser_state* *s)

This function initializes a previously allocated integration state. This allows an existing workspace to be reused for different integrations.

int **gsl_monte_miser_integrate**(*gsl_monte_function* *f, const double xl[], const double xu[], size_t dim, size_t calls, *gsl_rng* *r, *gsl_monte_miser_state* *s, double *result, double *abserr)

This routines uses the MISER Monte Carlo algorithm to integrate the function `f` over the `dim`-dimensional hypercubic region defined by the lower and upper limits in the arrays `xl` and `xu`, each of size `dim`. The integration uses a fixed number of function calls `calls`, and obtains random sampling points using the random number generator `r`. A previously allocated workspace `s` must be supplied. The result of the integration is returned in `result`, with an estimated absolute error `abserr`.

void **gsl_monte_miser_free**(*gsl_monte_miser_state* *s)

This function frees the memory associated with the integrator state `s`.

The MISER algorithm has several configurable parameters which can be changed using the following two functions[1].

void **gsl_monte_miser_params_get**(const *gsl_monte_miser_state* *s, *gsl_monte_miser_params* *params)

This function copies the parameters of the integrator state into the user-supplied `params` structure.

void **gsl_monte_miser_params_set**(*gsl_monte_miser_state* *s, const *gsl_monte_miser_params* *params)

This function sets the integrator parameters based on values provided in the `params` structure.

Typically the values of the parameters are first read using `gsl_monte_miser_params_get()`, the necessary changes are made to the fields of the `params` structure, and the values are copied back into the integrator state using `gsl_monte_miser_params_set()`. The functions use the `gsl_monte_miser_params` structure which contains the following fields:

type **gsl_monte_miser_params**

double **estimate_frac**

This parameter specifies the fraction of the currently available number of function calls which are allocated to estimating the variance at each recursive step. The default value is 0.1.

size_t **min_calls**

This parameter specifies the minimum number of function calls required for each estimate of the variance. If the number of function calls allocated to the estimate using `estimate_frac` falls below `min_calls` then `min_calls` are used instead. This ensures that each estimate maintains a reasonable level of accuracy. The default value of `min_calls` is `16 * dim`.

size_t **min_calls_per_bisection**

This parameter specifies the minimum number of function calls required to proceed with a bisection step. When a recursive step has fewer calls available than `min_calls_per_bisection` it performs a plain Monte Carlo estimate of the current sub-region and terminates its branch of the recursion. The default value of this parameter is `32 * min_calls`.

double **alpha**

This parameter controls how the estimated variances for the two sub-regions of a bisection are combined when allocating points. With recursive sampling the overall variance should scale better than $1/N$, since the values from the sub-regions will be obtained using a procedure which explicitly minimizes their variance. To accommodate this behavior the MISER algorithm allows the total variance to depend on a scaling parameter α,

$$\mathrm{Var}(f) = \frac{\sigma_a}{N_a^\alpha} + \frac{\sigma_b}{N_b^\alpha}.$$

The authors of the original paper describing MISER recommend the value $\alpha = 2$ as a good choice, obtained from numerical experiments, and this is used as the default value in this implementation.

double **dither**

This parameter introduces a random fractional variation of size `dither` into each bisection, which can be used to break the symmetry of integrands which are concentrated near the exact center of the hypercubic

[1] The previous method of accessing these fields directly through the `gsl_monte_miser_state` struct is now deprecated.

integration region. The default value of dither is zero, so no variation is introduced. If needed, a typical value of `dither` is 0.1.

27.4 VEGAS

The VEGAS algorithm of Lepage is based on importance sampling. It samples points from the probability distribution described by the function $|f|$, so that the points are concentrated in the regions that make the largest contribution to the integral.

In general, if the Monte Carlo integral of f is sampled with points distributed according to a probability distribution described by the function g, we obtain an estimate $E_g(f; N)$,

$$E_g(f; N) = E(f/g; N)$$

with a corresponding variance,

$$\mathrm{Var}_g(f; N) = \mathrm{Var}(f/g; N)$$

If the probability distribution is chosen as $g = |f|/I(|f|)$ then it can be shown that the variance $V_g(f; N)$ vanishes, and the error in the estimate will be zero. In practice it is not possible to sample from the exact distribution g for an arbitrary function, so importance sampling algorithms aim to produce efficient approximations to the desired distribution.

The VEGAS algorithm approximates the exact distribution by making a number of passes over the integration region while histogramming the function f. Each histogram is used to define a sampling distribution for the next pass. Asymptotically this procedure converges to the desired distribution. In order to avoid the number of histogram bins growing like K^d the probability distribution is approximated by a separable function: $g(x_1, x_2, \ldots) = g_1(x_1)g_2(x_2)\ldots$ so that the number of bins required is only Kd. This is equivalent to locating the peaks of the function from the projections of the integrand onto the coordinate axes. The efficiency of VEGAS depends on the validity of this assumption. It is most efficient when the peaks of the integrand are well-localized. If an integrand can be rewritten in a form which is approximately separable this will increase the efficiency of integration with VEGAS.

VEGAS incorporates a number of additional features, and combines both stratified sampling and importance sampling. The integration region is divided into a number of "boxes", with each box getting a fixed number of points (the goal is 2). Each box can then have a fractional number of bins, but if the ratio of bins-per-box is less than two, Vegas switches to a kind variance reduction (rather than importance sampling).

type **`gsl_monte_vegas_state`**

This workspace is used for VEGAS Monte Carlo integration

gsl_monte_vegas_state ***`gsl_monte_vegas_alloc`**(size_t dim)

This function allocates and initializes a workspace for Monte Carlo integration in `dim` dimensions. The workspace is used to maintain the state of the integration.

int **`gsl_monte_vegas_init`**(*gsl_monte_vegas_state* *s)

This function initializes a previously allocated integration state. This allows an existing workspace to be reused for different integrations.

int **`gsl_monte_vegas_integrate`**(*gsl_monte_function* *f, double xl[], double xu[], size_t dim, size_t calls, *gsl_rng* *r, *gsl_monte_vegas_state* *s, double *result, double *abserr)

This routines uses the VEGAS Monte Carlo algorithm to integrate the function `f` over the `dim`-dimensional hypercubic region defined by the lower and upper limits in the arrays `xl` and `xu`, each of size `dim`. The integration uses a fixed number of function calls `calls`, and obtains random sampling points using the random number generator `r`. A previously allocated workspace `s` must be supplied. The result of the integration is returned in `result`, with an estimated absolute error `abserr`. The result and its error estimate are based on a weighted average of independent samples. The chi-squared per degree of freedom for the weighted average is returned via the state struct component, `s->chisq`, and must be consistent with 1 for the weighted average to be reliable.

void **gsl_monte_vegas_free**(*gsl_monte_vegas_state* *s)

This function frees the memory associated with the integrator state `s`.

The VEGAS algorithm computes a number of independent estimates of the integral internally, according to the `iterations` parameter described below, and returns their weighted average. Random sampling of the integrand can occasionally produce an estimate where the error is zero, particularly if the function is constant in some regions. An estimate with zero error causes the weighted average to break down and must be handled separately. In the original Fortran implementations of VEGAS the error estimate is made non-zero by substituting a small value (typically `1e-30`). The implementation in GSL differs from this and avoids the use of an arbitrary constant—it either assigns the value a weight which is the average weight of the preceding estimates or discards it according to the following procedure,

- current estimate has zero error, weighted average has finite error

  The current estimate is assigned a weight which is the average weight of the preceding estimates.

- current estimate has finite error, previous estimates had zero error

  The previous estimates are discarded and the weighted averaging procedure begins with the current estimate.

- current estimate has zero error, previous estimates had zero error

  The estimates are averaged using the arithmetic mean, but no error is computed.

The convergence of the algorithm can be tested using the overall chi-squared value of the results, which is available from the following function:

double **gsl_monte_vegas_chisq**(const *gsl_monte_vegas_state* *s)

This function returns the chi-squared per degree of freedom for the weighted estimate of the integral. The returned value should be close to 1. A value which differs significantly from 1 indicates that the values from different iterations are inconsistent. In this case the weighted error will be under-estimated, and further iterations of the algorithm are needed to obtain reliable results.

void **gsl_monte_vegas_runval**(const *gsl_monte_vegas_state* *s, double *result, double *sigma)

This function returns the raw (unaveraged) values of the integral `result` and its error `sigma` from the most recent iteration of the algorithm.

The VEGAS algorithm is highly configurable. Several parameters can be changed using the following two functions.

void **gsl_monte_vegas_params_get**(const *gsl_monte_vegas_state* *s, *gsl_monte_vegas_params* *params)

This function copies the parameters of the integrator state into the user-supplied `params` structure.

void **gsl_monte_vegas_params_set**(*gsl_monte_vegas_state* *s, const *gsl_monte_vegas_params* *params)

This function sets the integrator parameters based on values provided in the `params` structure.

Typically the values of the parameters are first read using `gsl_monte_vegas_params_get()`, the necessary changes are made to the fields of the `params` structure, and the values are copied back into the integrator state using `gsl_monte_vegas_params_set()`. The functions use the `gsl_monte_vegas_params` structure which contains the following fields:

type **gsl_monte_vegas_params**

double **alpha**

The parameter `alpha` controls the stiffness of the rebinning algorithm. It is typically set between one and two. A value of zero prevents rebinning of the grid. The default value is 1.5.

size_t **iterations**

The number of iterations to perform for each call to the routine. The default value is 5 iterations.

int **stage**

Setting this determines the *stage* of the calculation. Normally, `stage = 0` which begins with a new uniform grid and empty weighted average. Calling VEGAS with `stage = 1` retains the grid from the previous run but discards the weighted average, so that one can "tune" the grid using a relatively small number of points and then do a large run with `stage = 1` on the optimized grid. Setting `stage = 2` keeps the grid and the weighted average from the previous run, but may increase (or decrease) the number of histogram bins in the grid depending on the number of calls available. Choosing `stage = 3` enters at the main loop, so that nothing is changed, and is equivalent to performing additional iterations in a previous call.

int **mode**

The possible choices are `GSL_VEGAS_MODE_IMPORTANCE`, `GSL_VEGAS_MODE_STRATIFIED`, `GSL_VEGAS_MODE_IMPORTANCE_ONLY`. This determines whether VEGAS will use importance sampling or stratified sampling, or whether it can pick on its own. In low dimensions VEGAS uses strict stratified sampling (more precisely, stratified sampling is chosen if there are fewer than 2 bins per box).

int **verbose**

FILE ***ostream**

These parameters set the level of information printed by VEGAS. All information is written to the stream *ostream*. The default setting of *verbose* is `-1`, which turns off all output. A *verbose* value of `0` prints summary information about the weighted average and final result, while a value of `1` also displays the grid coordinates. A value of `2` prints information from the rebinning procedure for each iteration.

The above fields and the `chisq` value can also be accessed directly in the *gsl_monte_vegas_state* but such use is deprecated.

27.5 Examples

The example program below uses the Monte Carlo routines to estimate the value of the following 3-dimensional integral from the theory of random walks,

$$I = \int_{-\pi}^{+\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{+\pi} \frac{dk_y}{2\pi} \int_{-\pi}^{+\pi} \frac{dk_z}{2\pi} \frac{1}{(1 - \cos(k_x)\cos(k_y)\cos(k_z))}.$$

The analytic value of this integral can be shown to be $I = \Gamma(1/4)^4/(4\pi^3) = 1.393203929685676859...$. The integral gives the mean time spent at the origin by a random walk on a body-centered cubic lattice in three dimensions.

For simplicity we will compute the integral over the region $(0, 0, 0)$ to (π, π, π) and multiply by 8 to obtain the full result. The integral is slowly varying in the middle of the region but has integrable singularities at the corners $(0, 0, 0)$, $(0, \pi, \pi)$, $(\pi, 0, \pi)$ and $(\pi, \pi, 0)$. The Monte Carlo routines only select points which are strictly within the integration region and so no special measures are needed to avoid these singularities.

```
#include <stdlib.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_monte.h>
#include <gsl/gsl_monte_plain.h>
#include <gsl/gsl_monte_miser.h>
#include <gsl/gsl_monte_vegas.h>

/* Computation of the integral,

      I = int (dx dy dz)/(2pi)^3  1/(1-cos(x)cos(y)cos(z))

   over (-pi,-pi,-pi) to (+pi, +pi, +pi).  The exact answer
   is Gamma(1/4)^4/(4 pi^3).  This example is taken from
   C.Itzykson, J.M.Drouffe, "Statistical Field Theory -
   Volume 1", Section 1.1, p21, which cites the original
   paper M.L.Glasser, I.J.Zucker, Proc.Natl.Acad.Sci.USA 74
   1800 (1977) */
```

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```
/* For simplicity we compute the integral over the region
   (0,0,0) -> (pi,pi,pi) and multiply by 8 */

double exact = 1.3932039296856768591842462603255;

double
g (double *k, size_t dim, void *params)
{
  (void)(dim); /* avoid unused parameter warnings */
  (void)(params);
  double A = 1.0 / (M_PI * M_PI * M_PI);
  return A / (1.0 - cos (k[0]) * cos (k[1]) * cos (k[2]));
}

void
display_results (char *title, double result, double error)
{
  printf ("%s ==================\n", title);
  printf ("result = % .6f\n", result);
  printf ("sigma  = % .6f\n", error);
  printf ("exact  = % .6f\n", exact);
  printf ("error  = % .6f = %.2g sigma\n", result - exact,
          fabs (result - exact) / error);
}

int
main (void)
{
  double res, err;

  double xl[3] = { 0, 0, 0 };
  double xu[3] = { M_PI, M_PI, M_PI };

  const gsl_rng_type *T;
  gsl_rng *r;

  gsl_monte_function G = { &g, 3, 0 };

  size_t calls = 500000;

  gsl_rng_env_setup ();

  T = gsl_rng_default;
  r = gsl_rng_alloc (T);

  {
    gsl_monte_plain_state *s = gsl_monte_plain_alloc (3);
    gsl_monte_plain_integrate (&G, xl, xu, 3, calls, r, s,
                               &res, &err);
    gsl_monte_plain_free (s);
```

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```
    display_results ("plain", res, err);
  }

  {
    gsl_monte_miser_state *s = gsl_monte_miser_alloc (3);
    gsl_monte_miser_integrate (&G, xl, xu, 3, calls, r, s,
                               &res, &err);
    gsl_monte_miser_free (s);

    display_results ("miser", res, err);
  }

  {
    gsl_monte_vegas_state *s = gsl_monte_vegas_alloc (3);

    gsl_monte_vegas_integrate (&G, xl, xu, 3, 10000, r, s,
                               &res, &err);
    display_results ("vegas warm-up", res, err);

    printf ("converging...\n");

    do
      {
        gsl_monte_vegas_integrate (&G, xl, xu, 3, calls/5, r, s,
                                   &res, &err);
        printf ("result = % .6f sigma = % .6f "
                "chisq/dof = %.1f\n", res, err, gsl_monte_vegas_chisq (s));
      }
    while (fabs (gsl_monte_vegas_chisq (s) - 1.0) > 0.5);

    display_results ("vegas final", res, err);

    gsl_monte_vegas_free (s);
  }

  gsl_rng_free (r);

  return 0;
}
```

With 500,000 function calls the plain Monte Carlo algorithm achieves a fractional error of 1%. The estimated error `sigma` is roughly consistent with the actual error–the computed result differs from the true result by about 1.4 standard deviations:

```
plain ==================
result =  1.412209
sigma  =  0.013436
exact  =  1.393204
error  =  0.019005 = 1.4 sigma
```

The MISER algorithm reduces the error by a factor of four, and also correctly estimates the error:

```
miser ==================
result =  1.391322
sigma  =  0.003461
exact  =  1.393204
error  = -0.001882 = 0.54 sigma
```

In the case of the VEGAS algorithm the program uses an initial warm-up run of 10,000 function calls to prepare, or "warm up", the grid. This is followed by a main run with five iterations of 100,000 function calls. The chi-squared per degree of freedom for the five iterations are checked for consistency with 1, and the run is repeated if the results have not converged. In this case the estimates are consistent on the first pass:

```
vegas warm-up ==================
result =  1.392673
sigma  =  0.003410
exact  =  1.393204
error  = -0.000531 = 0.16 sigma
converging...
result =  1.393281 sigma =  0.000362 chisq/dof = 1.5
vegas final ==================
result =  1.393281
sigma  =  0.000362
exact  =  1.393204
error  =  0.000077 = 0.21 sigma
```

If the value of `chisq` had differed significantly from 1 it would indicate inconsistent results, with a correspondingly underestimated error. The final estimate from VEGAS (using a similar number of function calls) is significantly more accurate than the other two algorithms.

27.6 References and Further Reading

The MISER algorithm is described in the following article by Press and Farrar,

- W.H. Press, G.R. Farrar, *Recursive Stratified Sampling for Multidimensional Monte Carlo Integration*, Computers in Physics, v4 (1990), pp190–195.

The VEGAS algorithm is described in the following papers,

- G.P. Lepage, *A New Algorithm for Adaptive Multidimensional Integration*, Journal of Computational Physics 27, 192–203, (1978)
- G.P. Lepage, *VEGAS: An Adaptive Multi-dimensional Integration Program*, Cornell preprint CLNS 80-447, March 1980

CHAPTER

TWENTYEIGHT

SIMULATED ANNEALING

Stochastic search techniques are used when the structure of a space is not well understood or is not smooth, so that techniques like Newton's method (which requires calculating Jacobian derivative matrices) cannot be used. In particular, these techniques are frequently used to solve combinatorial optimization problems, such as the traveling salesman problem.

The goal is to find a point in the space at which a real valued *energy function* (or *cost function*) is minimized. Simulated annealing is a minimization technique which has given good results in avoiding local minima; it is based on the idea of taking a random walk through the space at successively lower temperatures, where the probability of taking a step is given by a Boltzmann distribution.

The functions described in this chapter are declared in the header file `gsl_siman.h`.

28.1 Simulated Annealing algorithm

The simulated annealing algorithm takes random walks through the problem space, looking for points with low energies; in these random walks, the probability of taking a step is determined by the Boltzmann distribution,

$$p = e^{-(E_{i+1}-E_i)/(kT)}$$

if $E_{i+1} > E_i$, and $p = 1$ when $E_{i+1} \leq E_i$.

In other words, a step will occur if the new energy is lower. If the new energy is higher, the transition can still occur, and its likelihood is proportional to the temperature T and inversely proportional to the energy difference $E_{i+1} - E_i$.

The temperature T is initially set to a high value, and a random walk is carried out at that temperature. Then the temperature is lowered very slightly according to a *cooling schedule*, for example: $T \to T/\mu_T$ where μ_T is slightly greater than 1.

The slight probability of taking a step that gives higher energy is what allows simulated annealing to frequently get out of local minima.

28.2 Simulated Annealing functions

void **gsl_siman_solve**(const *gsl_rng* *r, void *x0_p, *gsl_siman_Efunc_t* Ef, *gsl_siman_step_t* take_step, *gsl_siman_metric_t* distance, *gsl_siman_print_t* print_position, *gsl_siman_copy_t* copyfunc, *gsl_siman_copy_construct_t* copy_constructor, *gsl_siman_destroy_t* destructor, size_t element_size, *gsl_siman_params_t* params)

This function performs a simulated annealing search through a given space. The space is specified by providing the functions `Ef` and `distance`. The simulated annealing steps are generated using the random number generator `r` and the function `take_step`.

The starting configuration of the system should be given by *x0_p*. The routine offers two modes for updating configurations, a fixed-size mode and a variable-size mode. In the fixed-size mode the configuration is stored as a single block of memory of size *element_size*. Copies of this configuration are created, copied and destroyed internally using the standard library functions `malloc()`, `memcpy()` and `free()`. The function pointers *copyfunc*, *copy_constructor* and *destructor* should be null pointers in fixed-size mode. In the variable-size mode the functions *copyfunc*, *copy_constructor* and *destructor* are used to create, copy and destroy configurations internally. The variable *element_size* should be zero in the variable-size mode.

The *params* structure (described below) controls the run by providing the temperature schedule and other tunable parameters to the algorithm.

On exit the best result achieved during the search is placed in *x0_p*. If the annealing process has been successful this should be a good approximation to the optimal point in the space.

If the function pointer *print_position* is not null, a debugging log will be printed to `stdout` with the following columns:

```
#-iter  #-evals  temperature  position  energy  best_energy
```

and the output of the function *print_position* itself. If *print_position* is null then no information is printed.

The simulated annealing routines require several user-specified functions to define the configuration space and energy function. The prototypes for these functions are given below.

type **gsl_siman_Efunc_t**

This function type should return the energy of a configuration `xp`:

```
double (*gsl_siman_Efunc_t) (void *xp)
```

type **gsl_siman_step_t**

This function type should modify the configuration `xp` using a random step taken from the generator `r`, up to a maximum distance of `step_size`:

```
void (*gsl_siman_step_t) (const gsl_rng *r, void *xp,
                          double step_size)
```

type **gsl_siman_metric_t**

This function type should return the distance between two configurations `xp` and `yp`:

```
double (*gsl_siman_metric_t) (void *xp, void *yp)
```

type **gsl_siman_print_t**

This function type should print the contents of the configuration `xp`:

```
void (*gsl_siman_print_t) (void *xp)
```

type **gsl_siman_copy_t**

This function type should copy the configuration `source` into `dest`:

```
void (*gsl_siman_copy_t) (void *source, void *dest)
```

type **gsl_siman_copy_construct_t**

This function type should create a new copy of the configuration `xp`:

```
void * (*gsl_siman_copy_construct_t) (void *xp)
```

type **gsl_siman_destroy_t**

This function type should destroy the configuration `xp`, freeing its memory:

```
void (*gsl_siman_destroy_t) (void *xp)
```

type **gsl_siman_params_t**

These are the parameters that control a run of *gsl_siman_solve()*. This structure contains all the information needed to control the search, beyond the energy function, the step function and the initial guess.

`int n_tries`	The number of points to try for each step.
`int iters_fixed_T`	The number of iterations at each temperature.
`double step_size`	The maximum step size in the random walk.
`double k, t_initial, mu_t, t_min`	The parameters of the Boltzmann distribution and cooling schedule.

28.3 Examples

The simulated annealing package is clumsy, and it has to be because it is written in C, for C callers, and tries to be polymorphic at the same time. But here we provide some examples which can be pasted into your application with little change and should make things easier.

28.3.1 Trivial example

The first example, in one dimensional Cartesian space, sets up an energy function which is a damped sine wave; this has many local minima, but only one global minimum, somewhere between 1.0 and 1.5. The initial guess given is 15.5, which is several local minima away from the global minimum.

```
#include <math.h>
#include <stdlib.h>
#include <string.h>
#include <gsl/gsl_siman.h>

/* set up parameters for this simulated annealing run */

/* how many points do we try before stepping */
#define N_TRIES 200

/* how many iterations for each T? */
#define ITERS_FIXED_T 1000

/* max step size in random walk */
#define STEP_SIZE 1.0

/* Boltzmann constant */
#define K 1.0

/* initial temperature */
#define T_INITIAL 0.008

/* damping factor for temperature */
```

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```
#define MU_T 1.003
#define T_MIN 2.0e-6

gsl_siman_params_t params
  = {N_TRIES, ITERS_FIXED_T, STEP_SIZE,
     K, T_INITIAL, MU_T, T_MIN};

/* now some functions to test in one dimension */
double E1(void *xp)
{
  double x = * ((double *) xp);

  return exp(-pow((x-1.0),2.0))*sin(8*x);
}

double M1(void *xp, void *yp)
{
  double x = *((double *) xp);
  double y = *((double *) yp);

  return fabs(x - y);
}

void S1(const gsl_rng * r, void *xp, double step_size)
{
  double old_x = *((double *) xp);
  double new_x;

  double u = gsl_rng_uniform(r);
  new_x = u * 2 * step_size - step_size + old_x;

  memcpy(xp, &new_x, sizeof(new_x));
}

void P1(void *xp)
{
  printf ("%12g", *((double *) xp));
}

int
main(void)
{
  const gsl_rng_type * T;
  gsl_rng * r;

  double x_initial = 15.5;

  gsl_rng_env_setup();

  T = gsl_rng_default;
  r = gsl_rng_alloc(T);
```

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```
  gsl_siman_solve(r, &x_initial, E1, S1, M1, P1,
                  NULL, NULL, NULL,
                  sizeof(double), params);

  gsl_rng_free (r);
  return 0;
}
```

Fig. 28.1 is generated by running `siman_test` in the following way:

```
$ ./siman_test | awk '!/^#/ {print $1, $4}'
 | graph -y 1.34 1.4 -W0 -X generation -Y position
 | plot -Tps > siman-test.eps
```

Fig. 28.2 is generated by running `siman_test` in the following way:

```
$ ./siman_test | awk '!/^#/ {print $1, $5}'
 | graph -y -0.88 -0.83 -W0 -X generation -Y energy
 | plot -Tps > siman-energy.eps
```

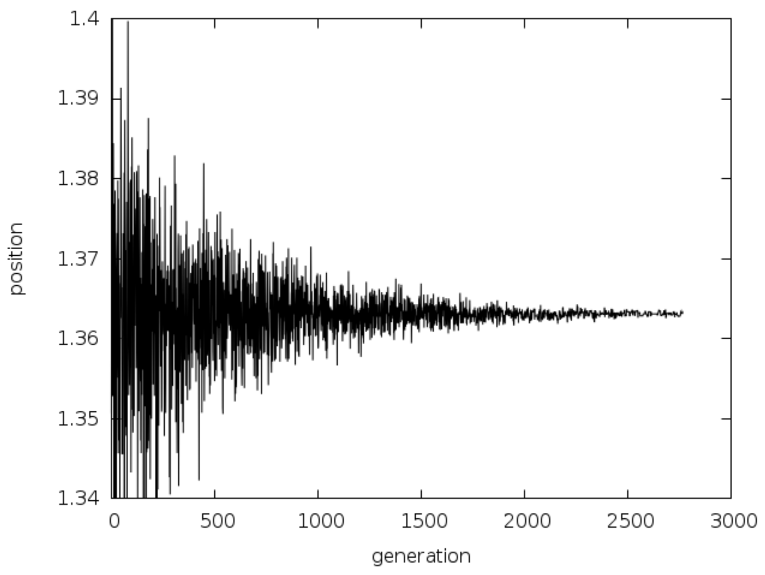

Fig. 28.1: Example of a simulated annealing run: at higher temperatures (early in the plot) you see that the solution can fluctuate, but at lower temperatures it converges.

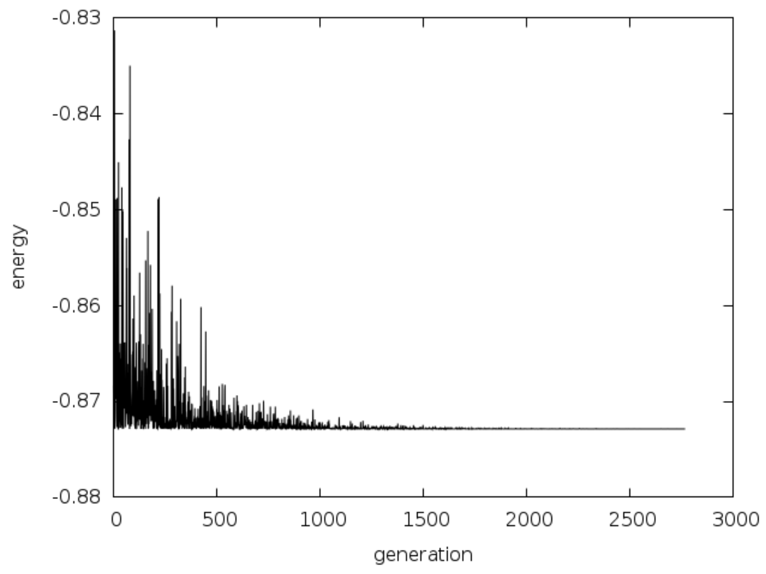

Fig. 28.2: Simulated annealing energy vs generation

28.3.2 Traveling Salesman Problem

The TSP (*Traveling Salesman Problem*) is the classic combinatorial optimization problem. I have provided a very simple version of it, based on the coordinates of twelve cities in the southwestern United States. This should maybe be called the *Flying Salesman Problem*, since I am using the great-circle distance between cities, rather than the driving distance. Also: I assume the earth is a sphere, so I don't use geoid distances.

The `gsl_siman_solve()` routine finds a route which is 3490.62 Kilometers long; this is confirmed by an exhaustive search of all possible routes with the same initial city.

The full code is given below.

```
/* siman/siman_tsp.c
 *
 * Copyright (C) 1996, 1997, 1998, 1999, 2000 Mark Galassi
 *
 * This program is free software; you can redistribute it and/or modify
 * it under the terms of the GNU General Public License as published by
 * the Free Software Foundation; either version 3 of the License, or (at
 * your option) any later version.
 *
 * This program is distributed in the hope that it will be useful, but
 * WITHOUT ANY WARRANTY; without even the implied warranty of
 * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the GNU
 * General Public License for more details.
 *
 * You should have received a copy of the GNU General Public License
 * along with this program; if not, write to the Free Software
 * Foundation, Inc., 51 Franklin Street, Fifth Floor, Boston, MA 02110-1301, USA.
 */

#include <config.h>
#include <math.h>
```

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```
#include <string.h>
#include <stdio.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_siman.h>
#include <gsl/gsl_ieee_utils.h>

/* set up parameters for this simulated annealing run */

#define N_TRIES 200             /* how many points do we try before stepping */
#define ITERS_FIXED_T 2000      /* how many iterations for each T? */
#define STEP_SIZE 1.0           /* max step size in random walk */
#define K 1.0                   /* Boltzmann constant */
#define T_INITIAL 5000.0        /* initial temperature */
#define MU_T 1.002              /* damping factor for temperature */
#define T_MIN 5.0e-1

gsl_siman_params_t params = {N_TRIES, ITERS_FIXED_T, STEP_SIZE,
                             K, T_INITIAL, MU_T, T_MIN};

struct s_tsp_city {
  const char * name;
  double lat, longitude;        /* coordinates */
};
typedef struct s_tsp_city Stsp_city;

void prepare_distance_matrix(void);
void exhaustive_search(void);
void print_distance_matrix(void);
double city_distance(Stsp_city c1, Stsp_city c2);
double Etsp(void *xp);
double Mtsp(void *xp, void *yp);
void Stsp(const gsl_rng * r, void *xp, double step_size);
void Ptsp(void *xp);

/* in this table, latitude and longitude are obtained from the US
   Census Bureau, at http://www.census.gov/cgi-bin/gazetteer */

Stsp_city cities[] = {{"Santa Fe",    35.68,   105.95},
                      {"Phoenix",     33.54,   112.07},
                      {"Albuquerque", 35.12,   106.62},
                      {"Clovis",      34.41,   103.20},
                      {"Durango",     37.29,   107.87},
                      {"Dallas",      32.79,    96.77},
                      {"Tesuque",     35.77,   105.92},
                      {"Grants",      35.15,   107.84},
                      {"Los Alamos",  35.89,   106.28},
                      {"Las Cruces",  32.34,   106.76},
                      {"Cortez",      37.35,   108.58},
                      {"Gallup",      35.52,   108.74}};

#define N_CITIES (sizeof(cities)/sizeof(Stsp_city))
```

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```
double distance_matrix[N_CITIES][N_CITIES];

/* distance between two cities */
double city_distance(Stsp_city c1, Stsp_city c2)
{
  const double earth_radius = 6375.000; /* 6000KM approximately */
  /* sin and cos of lat and long; must convert to radians */
  double sla1 = sin(c1.lat*M_PI/180), cla1 = cos(c1.lat*M_PI/180),
    slo1 = sin(c1.longitude*M_PI/180), clo1 = cos(c1.longitude*M_PI/180);
  double sla2 = sin(c2.lat*M_PI/180), cla2 = cos(c2.lat*M_PI/180),
    slo2 = sin(c2.longitude*M_PI/180), clo2 = cos(c2.longitude*M_PI/180);

  double x1 = cla1*clo1;
  double x2 = cla2*clo2;

  double y1 = cla1*slo1;
  double y2 = cla2*slo2;

  double z1 = sla1;
  double z2 = sla2;

  double dot_product = x1*x2 + y1*y2 + z1*z2;

  double angle = acos(dot_product);

  /* distance is the angle (in radians) times the earth radius */
  return angle*earth_radius;
}

/* energy for the travelling salesman problem */
double Etsp(void *xp)
{
  /* an array of N_CITIES integers describing the order */
  int *route = (int *) xp;
  double E = 0;
  unsigned int i;

  for (i = 0; i < N_CITIES; ++i) {
    /* use the distance_matrix to optimize this calculation; it had
       better be allocated!! */
    E += distance_matrix[route[i]][route[(i + 1) % N_CITIES]];
  }

  return E;
}

double Mtsp(void *xp, void *yp)
{
  int *route1 = (int *) xp, *route2 = (int *) yp;
  double distance = 0;
  unsigned int i;
```

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```
  for (i = 0; i < N_CITIES; ++i) {
    distance += ((route1[i] == route2[i]) ? 0 : 1);
  }

  return distance;
}

/* take a step through the TSP space */
void Stsp(const gsl_rng * r, void *xp, double step_size)
{
  int x1, x2, dummy;
  int *route = (int *) xp;

  step_size = 0 ; /* prevent warnings about unused parameter */

  /* pick the two cities to swap in the matrix; we leave the first
     city fixed */
  x1 = (gsl_rng_get (r) % (N_CITIES-1)) + 1;
  do {
    x2 = (gsl_rng_get (r) % (N_CITIES-1)) + 1;
  } while (x2 == x1);

  dummy = route[x1];
  route[x1] = route[x2];
  route[x2] = dummy;
}

void Ptsp(void *xp)
{
  unsigned int i;
  int *route = (int *) xp;
  printf("  [");
  for (i = 0; i < N_CITIES; ++i) {
    printf(" %d ", route[i]);
  }
  printf("]  ");
}

int main(void)
{
  int x_initial[N_CITIES];
  unsigned int i;

  const gsl_rng * r = gsl_rng_alloc (gsl_rng_env_setup()) ;

  gsl_ieee_env_setup ();

  prepare_distance_matrix();

  /* set up a trivial initial route */
  printf("# initial order of cities:\n");
```

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```
  for (i = 0; i < N_CITIES; ++i) {
    printf("# \"%s\"\n", cities[i].name);
    x_initial[i] = i;
  }

  printf("# distance matrix is:\n");
  print_distance_matrix();

  printf("# initial coordinates of cities (longitude and latitude)\n");
  /* this can be plotted with */
  /* ./siman_tsp > hhh ; grep city_coord hhh | awk '{print $2 "   " $3}' | xyplot -ps -d
↪"xy" > c.eps */
  for (i = 0; i < N_CITIES+1; ++i) {
    printf("###initial_city_coord: %g %g \"%s\"\n",
           -cities[x_initial[i % N_CITIES]].longitude,
           cities[x_initial[i % N_CITIES]].lat,
           cities[x_initial[i % N_CITIES]].name);
  }

/*   exhaustive_search(); */

  gsl_siman_solve(r, x_initial, Etsp, Stsp, Mtsp, Ptsp, NULL, NULL, NULL,
                  N_CITIES*sizeof(int), params);

  printf("# final order of cities:\n");
  for (i = 0; i < N_CITIES; ++i) {
    printf("# \"%s\"\n", cities[x_initial[i]].name);
  }

  printf("# final coordinates of cities (longitude and latitude)\n");
  /* this can be plotted with */
  /* ./siman_tsp > hhh ; grep city_coord hhh | awk '{print $2 "   " $3}' | xyplot -ps -d
↪"xy" > c.eps */
  for (i = 0; i < N_CITIES+1; ++i) {
    printf("###final_city_coord: %g %g %s\n",
           -cities[x_initial[i % N_CITIES]].longitude,
           cities[x_initial[i % N_CITIES]].lat,
           cities[x_initial[i % N_CITIES]].name);
  }

  printf("# ");
  fflush(stdout);
#if 0
  system("date");
#endif /* 0 */
  fflush(stdout);

  return 0;
}

void prepare_distance_matrix()
{
```

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```
  unsigned int i, j;
  double dist;

  for (i = 0; i < N_CITIES; ++i) {
    for (j = 0; j < N_CITIES; ++j) {
      if (i == j) {
        dist = 0;
      } else {
        dist = city_distance(cities[i], cities[j]);
      }
      distance_matrix[i][j] = dist;
    }
  }
}

void print_distance_matrix()
{
  unsigned int i, j;

  for (i = 0; i < N_CITIES; ++i) {
    printf("# ");
    for (j = 0; j < N_CITIES; ++j) {
      printf("%15.8f   ", distance_matrix[i][j]);
    }
    printf("\n");
  }
}

/* [only works for 12] search the entire space for solutions */
static double best_E = 1.0e100, second_E = 1.0e100, third_E = 1.0e100;
static int best_route[N_CITIES];
static int second_route[N_CITIES];
static int third_route[N_CITIES];
static void do_all_perms(int *route, int n);

void exhaustive_search()
{
  static int initial_route[N_CITIES] = {0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11};
  printf("\n# ");
  fflush(stdout);
#if 0
  system("date");
#endif
  fflush(stdout);
  do_all_perms(initial_route, 1);
  printf("\n# ");
  fflush(stdout);
#if 0
  system("date");
#endif /* 0 */
  fflush(stdout);
```

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```
  printf("# exhaustive best route: ");
  Ptsp(best_route);
  printf("\n# its energy is: %g\n", best_E);

  printf("# exhaustive second_best route: ");
  Ptsp(second_route);
  printf("\n# its energy is: %g\n", second_E);

  printf("# exhaustive third_best route: ");
  Ptsp(third_route);
  printf("\n# its energy is: %g\n", third_E);
}

/* James Theiler's recursive algorithm for generating all routes */
static void do_all_perms(int *route, int n)
{
  if (n == (N_CITIES-1)) {
    /* do it! calculate the energy/cost for that route */
    double E;
    E = Etsp(route);            /* TSP energy function */
    /* now save the best 3 energies and routes */
    if (E < best_E) {
      third_E = second_E;
      memcpy(third_route, second_route, N_CITIES*sizeof(*route));
      second_E = best_E;
      memcpy(second_route, best_route, N_CITIES*sizeof(*route));
      best_E = E;
      memcpy(best_route, route, N_CITIES*sizeof(*route));
    } else if (E < second_E) {
      third_E = second_E;
      memcpy(third_route, second_route, N_CITIES*sizeof(*route));
      second_E = E;
      memcpy(second_route, route, N_CITIES*sizeof(*route));
    } else if (E < third_E) {
      third_E = E;
      memcpy(route, third_route, N_CITIES*sizeof(*route));
    }
  } else {
    int new_route[N_CITIES];
    unsigned int j;
    int swap_tmp;
    memcpy(new_route, route, N_CITIES*sizeof(*route));
    for (j = n; j < N_CITIES; ++j) {
      swap_tmp = new_route[j];
      new_route[j] = new_route[n];
      new_route[n] = swap_tmp;
      do_all_perms(new_route, n+1);
    }
  }
}
```

Below are some plots generated in the following way:

```
$ ./siman_tsp > tsp.output
$ grep -v "^#" tsp.output
 | awk '{print $1, $NF}'
 | graph -y 3300 6500 -W0 -X generation -Y distance
    -L "TSP - 12 southwest cities"
 | plot -Tps > 12-cities.eps
$ grep initial_city_coord tsp.output
  | awk '{print $2, $3}'
  | graph -X "longitude (- means west)" -Y "latitude"
     -L "TSP - initial-order" -f 0.03 -S 1 0.1
  | plot -Tps > initial-route.eps
$ grep final_city_coord tsp.output
  | awk '{print $2, $3}'
  | graph -X "longitude (- means west)" -Y "latitude"
     -L "TSP - final-order" -f 0.03 -S 1 0.1
  | plot -Tps > final-route.eps
```

This is the output showing the initial order of the cities; longitude is negative, since it is west and I want the plot to look like a map:

```
# initial coordinates of cities (longitude and latitude)
###initial_city_coord: -105.95 35.68 Santa Fe
###initial_city_coord: -112.07 33.54 Phoenix
###initial_city_coord: -106.62 35.12 Albuquerque
###initial_city_coord: -103.2 34.41 Clovis
###initial_city_coord: -107.87 37.29 Durango
###initial_city_coord: -96.77 32.79 Dallas
###initial_city_coord: -105.92 35.77 Tesuque
###initial_city_coord: -107.84 35.15 Grants
###initial_city_coord: -106.28 35.89 Los Alamos
###initial_city_coord: -106.76 32.34 Las Cruces
###initial_city_coord: -108.58 37.35 Cortez
###initial_city_coord: -108.74 35.52 Gallup
###initial_city_coord: -105.95 35.68 Santa Fe
```

The optimal route turns out to be:

```
# final coordinates of cities (longitude and latitude)
###final_city_coord: -105.95 35.68 Santa Fe
###final_city_coord: -103.2 34.41 Clovis
###final_city_coord: -96.77 32.79 Dallas
###final_city_coord: -106.76 32.34 Las Cruces
###final_city_coord: -112.07 33.54 Phoenix
###final_city_coord: -108.74 35.52 Gallup
###final_city_coord: -108.58 37.35 Cortez
###final_city_coord: -107.87 37.29 Durango
###final_city_coord: -107.84 35.15 Grants
###final_city_coord: -106.62 35.12 Albuquerque
###final_city_coord: -106.28 35.89 Los Alamos
###final_city_coord: -105.92 35.77 Tesuque
###final_city_coord: -105.95 35.68 Santa Fe
```

Here's a plot of the cost function (energy) versus generation (point in the calculation at which a new temperature is set) for this problem:

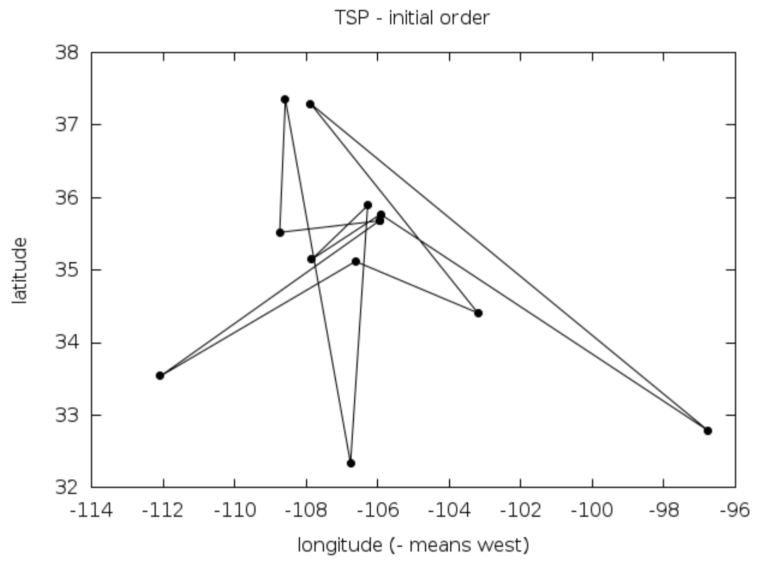

Fig. 28.3: Initial route for the 12 southwestern cities Flying Salesman Problem.

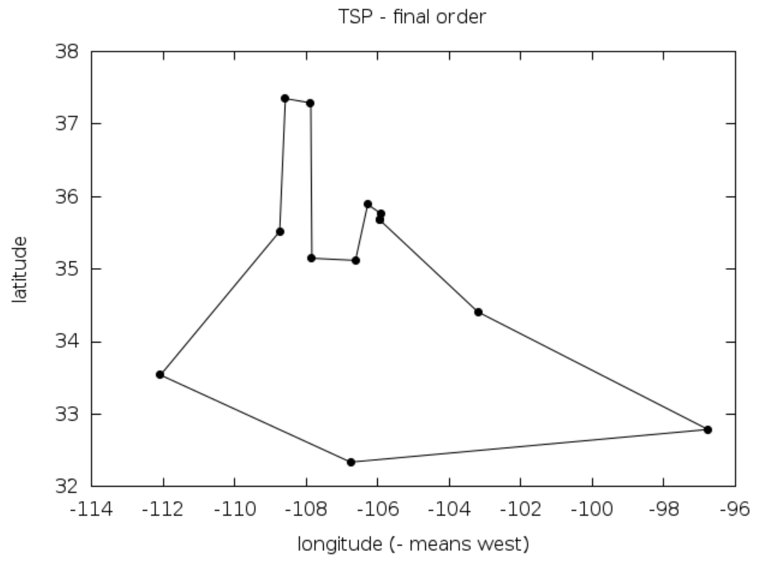

Fig. 28.4: Final (optimal) route for the 12 southwestern cities Flying Salesman Problem.

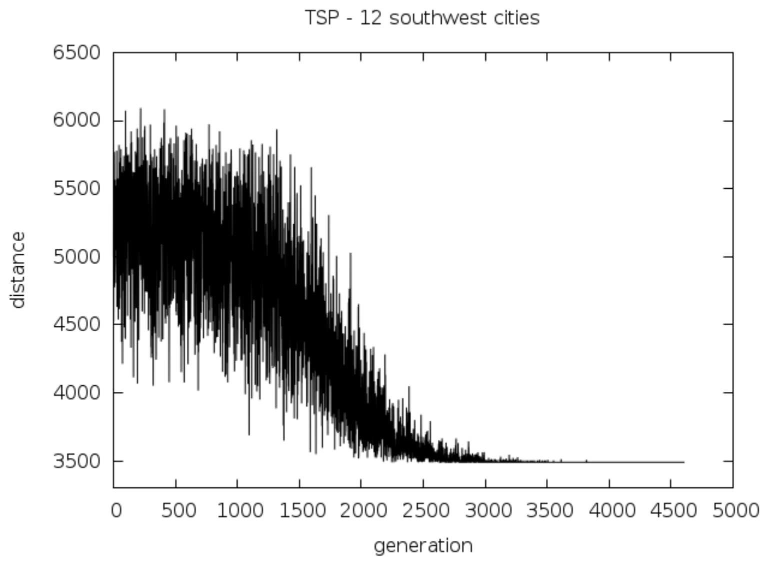

Fig. 28.5: Example of a simulated annealing run for the 12 southwestern cities Flying Salesman Problem.

28.4 References and Further Reading

Further information is available in the following book,

- *Modern Heuristic Techniques for Combinatorial Problems*, Colin R. Reeves (ed.), McGraw-Hill, 1995 (ISBN 0-07-709239-2).

CHAPTER

TWENTYNINE

ORDINARY DIFFERENTIAL EQUATIONS

This chapter describes functions for solving ordinary differential equation (ODE) initial value problems. The library provides a variety of low-level methods, such as Runge-Kutta and Bulirsch-Stoer routines, and higher-level components for adaptive step-size control. The components can be combined by the user to achieve the desired solution, with full access to any intermediate steps. A driver object can be used as a high level wrapper for easy use of low level functions.

These functions are declared in the header file `gsl_odeiv2.h`. This is a new interface in version 1.15 and uses the prefix `gsl_odeiv2` for all functions. It is recommended over the previous `gsl_odeiv` implementation defined in `gsl_odeiv.h` The old interface has been retained under the original name for backwards compatibility.

29.1 Defining the ODE System

The routines solve the general n-dimensional first-order system,

$$\frac{dy_i(t)}{dt} = f_i(t, y_1(t), \dots y_n(t))$$

for $i = 1, \dots, n$. The stepping functions rely on the vector of derivatives f_i and the Jacobian matrix,

$$J_{ij} = \partial f_i(t, y(t)) / \partial y_j$$

A system of equations is defined using the *`gsl_odeiv2_system`* datatype.

type **`gsl_odeiv2_system`**

This data type defines a general ODE system with arbitrary parameters.

`int (* function) (double t, const double y[], double dydt[], void * params)`

This function should store the vector elements $f_i(t, y, params)$ in the array `dydt`, for arguments (`t`, `y`) and parameters `params`.

The function should return `GSL_SUCCESS` if the calculation was completed successfully. Any other return value indicates an error. A special return value `GSL_EBADFUNC` causes `gsl_odeiv2` routines to immediately stop and return. If `function` is modified (for example contents of `params`), the user must call an appropriate reset function (*`gsl_odeiv2_driver_reset()`*, *`gsl_odeiv2_evolve_reset()`* or *`gsl_odeiv2_step_reset()`*) before continuing. Use return values distinct from standard GSL error codes to distinguish your function as the source of the error.

`int (* jacobian) (double t, const double y[], double * dfdy, double dfdt[], void * params)`

This function should store the vector of derivative elements

$$\partial f_i(t, y, params) / \partial t$$

in the array `dfdt` and the Jacobian matrix J_{ij} in the array `dfdy`, regarded as a row-ordered matrix `J(i,j) = dfdy[i * dimension + j]` where `dimension` is the dimension of the system.

Not all of the stepper algorithms of `gsl_odeiv2` make use of the Jacobian matrix, so it may not be necessary to provide this function (the `jacobian` element of the struct can be replaced by a null pointer for those algorithms).

The function should return `GSL_SUCCESS` if the calculation was completed successfully. Any other return value indicates an error. A special return value `GSL_EBADFUNC` causes `gsl_odeiv2` routines to immediately stop and return. If `jacobian` is modified (for example contents of `params`), the user must call an appropriate reset function (`gsl_odeiv2_driver_reset()`, `gsl_odeiv2_evolve_reset()` or `gsl_odeiv2_step_reset()`) before continuing. Use return values distinct from standard GSL error codes to distinguish your function as the source of the error.

`size_t dimension`

This is the dimension of the system of equations.

`void * params`

This is a pointer to the arbitrary parameters of the system.

29.2 Stepping Functions

The lowest level components are the *stepping functions* which advance a solution from time t to $t + h$ for a fixed step-size h and estimate the resulting local error.

type **gsl_odeiv2_step**

This contains internal parameters for a stepping function.

gsl_odeiv2_step ***gsl_odeiv2_step_alloc**(const *gsl_odeiv2_step_type* *T, size_t dim)

This function returns a pointer to a newly allocated instance of a stepping function of type `T` for a system of `dim` dimensions. Please note that if you use a stepper method that requires access to a driver object, it is advisable to use a driver allocation method, which automatically allocates a stepper, too.

int **gsl_odeiv2_step_reset**(*gsl_odeiv2_step* *s)

This function resets the stepping function `s`. It should be used whenever the next use of `s` will not be a continuation of a previous step.

void **gsl_odeiv2_step_free**(*gsl_odeiv2_step* *s)

This function frees all the memory associated with the stepping function `s`.

const char ***gsl_odeiv2_step_name**(const *gsl_odeiv2_step* *s)

This function returns a pointer to the name of the stepping function. For example:

```
printf ("step method is '%s'\n", gsl_odeiv2_step_name (s));
```

would print something like `step method is 'rkf45'`.

unsigned int **gsl_odeiv2_step_order**(const *gsl_odeiv2_step* *s)

This function returns the order of the stepping function on the previous step. The order can vary if the stepping function itself is adaptive.

int **gsl_odeiv2_step_set_driver**(*gsl_odeiv2_step* *s, const gsl_odeiv2_driver *d)

This function sets a pointer of the driver object `d` for stepper `s`, to allow the stepper to access control (and evolve) object through the driver object. This is a requirement for some steppers, to get the desired error level for internal iteration of stepper. Allocation of a driver object calls this function automatically.

int **gsl_odeiv2_step_apply**(*gsl_odeiv2_step* *s, double t, double h, double y[], double yerr[], const double dydt_in[], double dydt_out[], const *gsl_odeiv2_system* *sys)

This function applies the stepping function `s` to the system of equations defined by `sys`, using the step-size `h` to advance the system from time `t` and state `y` to time `t + h`. The new state of the system is stored in `y` on output, with an estimate of the absolute error in each component stored in `yerr`. If the argument `dydt_in` is not null it should point an array containing the derivatives for the system at time `t` on input. This is optional as the derivatives will be computed internally if they are not provided, but allows the reuse of existing derivative information. On output the new derivatives of the system at time `t + h` will be stored in `dydt_out` if it is not null.

The stepping function returns `GSL_FAILURE` if it is unable to compute the requested step. Also, if the user-supplied functions defined in the system `sys` return a status other than `GSL_SUCCESS` the step will be aborted. In that case, the elements of `y` will be restored to their pre-step values and the error code from the user-supplied function will be returned. Failure may be due to a singularity in the system or too large step-size `h`. In that case the step should be attempted again with a smaller step-size, e.g. `h / 2`.

If the driver object is not appropriately set via `gsl_odeiv2_step_set_driver()` for those steppers that need it, the stepping function returns `GSL_EFAULT`. If the user-supplied functions defined in the system `sys` returns `GSL_EBADFUNC`, the function returns immediately with the same return code. In this case the user must call `gsl_odeiv2_step_reset()` before calling this function again.

The following algorithms are available. Please note that algorithms which use step doubling for error estimation apply the more accurate values from two half steps instead of values from a single step for the new state `y`.

type **gsl_odeiv2_step_type**

gsl_odeiv2_step_type ***gsl_odeiv2_step_rk2***

Explicit embedded Runge-Kutta (2, 3) method.

gsl_odeiv2_step_type ***gsl_odeiv2_step_rk4***

Explicit 4th order (classical) Runge-Kutta. Error estimation is carried out by the step doubling method. For more efficient estimate of the error, use the embedded methods described below.

gsl_odeiv2_step_type ***gsl_odeiv2_step_rkf45***

Explicit embedded Runge-Kutta-Fehlberg (4, 5) method. This method is a good general-purpose integrator.

gsl_odeiv2_step_type ***gsl_odeiv2_step_rkck***

Explicit embedded Runge-Kutta Cash-Karp (4, 5) method.

gsl_odeiv2_step_type ***gsl_odeiv2_step_rk8pd***

Explicit embedded Runge-Kutta Prince-Dormand (8, 9) method.

gsl_odeiv2_step_type ***gsl_odeiv2_step_rk1imp***

Implicit Gaussian first order Runge-Kutta. Also known as implicit Euler or backward Euler method. Error estimation is carried out by the step doubling method. This algorithm requires the Jacobian and access to the driver object via `gsl_odeiv2_step_set_driver()`.

gsl_odeiv2_step_type ***gsl_odeiv2_step_rk2imp***

Implicit Gaussian second order Runge-Kutta. Also known as implicit mid-point rule. Error estimation is carried out by the step doubling method. This stepper requires the Jacobian and access to the driver object via `gsl_odeiv2_step_set_driver()`.

gsl_odeiv2_step_type ***gsl_odeiv2_step_rk4imp***

Implicit Gaussian 4th order Runge-Kutta. Error estimation is carried out by the step doubling method. This algorithm requires the Jacobian and access to the driver object via `gsl_odeiv2_step_set_driver()`.

gsl_odeiv2_step_type ***gsl_odeiv2_step_bsimp***

Implicit Bulirsch-Stoer method of Bader and Deuflhard. The method is generally suitable for stiff problems. This stepper requires the Jacobian.

gsl_odeiv2_step_type ***gsl_odeiv2_step_msadams***

A variable-coefficient linear multistep Adams method in Nordsieck form. This stepper uses explicit Adams-Bashforth (predictor) and implicit Adams-Moulton (corrector) methods in $P(EC)^m$ functional iteration mode. Method order varies dynamically between 1 and 12. This stepper requires the access to the driver object via `gsl_odeiv2_step_set_driver()`.

gsl_odeiv2_step_type ***gsl_odeiv2_step_msbdf***

A variable-coefficient linear multistep backward differentiation formula (BDF) method in Nordsieck form. This stepper uses the explicit BDF formula as predictor and implicit BDF formula as corrector. A modified Newton iteration method is used to solve the system of non-linear equations. Method order varies dynamically between 1 and 5. The method is generally suitable for stiff problems. This stepper requires the Jacobian and the access to the driver object via `gsl_odeiv2_step_set_driver()`.

29.3 Adaptive Step-size Control

The control function examines the proposed change to the solution produced by a stepping function and attempts to determine the optimal step-size for a user-specified level of error.

type **gsl_odeiv2_control**

This is a workspace for controlling step size.

type **gsl_odeiv2_control_type**

This specifies the control type.

gsl_odeiv2_control ***gsl_odeiv2_control_standard_new***(double eps_abs, double eps_rel, double a_y, double a_dydt)

The standard control object is a four parameter heuristic based on absolute and relative errors `eps_abs` and `eps_rel`, and scaling factors `a_y` and `a_dydt` for the system state $y(t)$ and derivatives $y'(t)$ respectively.

The step-size adjustment procedure for this method begins by computing the desired error level D_i for each component,

$$D_i = \epsilon_{abs} + \epsilon_{rel} * (a_y |y_i| + a_{dydt} h |y\prime_i|)$$

and comparing it with the observed error $E_i = |yerr_i|$. If the observed error `E` exceeds the desired error level `D` by more than 10% for any component then the method reduces the step-size by an appropriate factor,

$$h_{new} = h_{old} * S * (E/D)^{-1/q}$$

where q is the consistency order of the method (e.g. $q = 4$ for 4(5) embedded RK), and S is a safety factor of 0.9. The ratio E/D is taken to be the maximum of the ratios E_i/D_i.

If the observed error E is less than 50% of the desired error level `D` for the maximum ratio E_i/D_i then the algorithm takes the opportunity to increase the step-size to bring the error in line with the desired level,

$$h_{new} = h_{old} * S * (E/D)^{-1/(q+1)}$$

This encompasses all the standard error scaling methods. To avoid uncontrolled changes in the stepsize, the overall scaling factor is limited to the range $1/5$ to 5.

gsl_odeiv2_control ***gsl_odeiv2_control_y_new***(double eps_abs, double eps_rel)

This function creates a new control object which will keep the local error on each step within an absolute error of `eps_abs` and relative error of `eps_rel` with respect to the solution $y_i(t)$. This is equivalent to the standard control object with `a_y` = 1 and `a_dydt` = 0.

gsl_odeiv2_control ***gsl_odeiv2_control_yp_new**(double eps_abs, double eps_rel)

This function creates a new control object which will keep the local error on each step within an absolute error of *eps_abs* and relative error of *eps_rel* with respect to the derivatives of the solution $y'_i(t)$. This is equivalent to the standard control object with `a_y` = 0 and `a_dydt` = 1.

gsl_odeiv2_control ***gsl_odeiv2_control_scaled_new**(double eps_abs, double eps_rel, double a_y, double a_dydt, const double scale_abs[], size_t dim)

This function creates a new control object which uses the same algorithm as *gsl_odeiv2_control_standard_new()* but with an absolute error which is scaled for each component by the array *scale_abs*. The formula for D_i for this control object is,

$$D_i = \epsilon_{abs} s_i + \epsilon_{rel} * (a_y |y_i| + a_{dydt} h |y\prime_i|)$$

where s_i is the i-th component of the array *scale_abs*. The same error control heuristic is used by the Matlab ODE suite.

gsl_odeiv2_control ***gsl_odeiv2_control_alloc**(const *gsl_odeiv2_control_type* *T)

This function returns a pointer to a newly allocated instance of a control function of type *T*. This function is only needed for defining new types of control functions. For most purposes the standard control functions described above should be sufficient.

int **gsl_odeiv2_control_init**(*gsl_odeiv2_control* *c, double eps_abs, double eps_rel, double a_y, double a_dydt)

This function initializes the control function *c* with the parameters *eps_abs* (absolute error), *eps_rel* (relative error), *a_y* (scaling factor for y) and *a_dydt* (scaling factor for derivatives).

void **gsl_odeiv2_control_free**(*gsl_odeiv2_control* *c)

This function frees all the memory associated with the control function *c*.

int **gsl_odeiv2_control_hadjust**(*gsl_odeiv2_control* *c, *gsl_odeiv2_step* *s, const double y[], const double yerr[], const double dydt[], double *h)

This function adjusts the step-size *h* using the control function *c*, and the current values of *y*, *yerr* and *dydt*. The stepping function `step` is also needed to determine the order of the method. If the error in the y-values *yerr* is found to be too large then the step-size *h* is reduced and the function returns `GSL_ODEIV_HADJ_DEC`. If the error is sufficiently small then *h* may be increased and `GSL_ODEIV_HADJ_INC` is returned. The function returns `GSL_ODEIV_HADJ_NIL` if the step-size is unchanged. The goal of the function is to estimate the largest step-size which satisfies the user-specified accuracy requirements for the current point.

const char ***gsl_odeiv2_control_name**(const *gsl_odeiv2_control* *c)

This function returns a pointer to the name of the control function. For example:

```
printf ("control method is '%s'\n", gsl_odeiv2_control_name (c));
```

would print something like `control method is 'standard'`

int **gsl_odeiv2_control_errlevel**(*gsl_odeiv2_control* *c, const double y, const double dydt, const double h, const size_t ind, double *errlev)

This function calculates the desired error level of the *ind*-th component to *errlev*. It requires the value (*y*) and value of the derivative (*dydt*) of the component, and the current step size *h*.

int **gsl_odeiv2_control_set_driver**(*gsl_odeiv2_control* *c, const gsl_odeiv2_driver *d)

This function sets a pointer of the driver object *d* for control object *c*.

29.4 Evolution

The evolution function combines the results of a stepping function and control function to reliably advance the solution forward one step using an acceptable step-size.

type **gsl_odeiv2_evolve**

This workspace contains parameters for controlling the evolution function

gsl_odeiv2_evolve ***gsl_odeiv2_evolve_alloc**(size_t dim)

This function returns a pointer to a newly allocated instance of an evolution function for a system of `dim` dimensions.

int **gsl_odeiv2_evolve_apply**(*gsl_odeiv2_evolve* *e, *gsl_odeiv2_control* *con, *gsl_odeiv2_step* *step, const *gsl_odeiv2_system* *sys, double *t, double t1, double *h, double y[])

This function advances the system (`e`, `sys`) from time `t` and position `y` using the stepping function `step`. The new time and position are stored in `t` and `y` on output.

The initial step-size is taken as `h`. The control function `con` is applied to check whether the local error estimated by the stepping function `step` using step-size `h` exceeds the required error tolerance. If the error is too high, the step is retried by calling `step` with a decreased step-size. This process is continued until an acceptable step-size is found. An estimate of the local error for the step can be obtained from the components of the array `e->yerr[]`.

If the user-supplied functions defined in the system `sys` returns `GSL_EBADFUNC`, the function returns immediately with the same return code. In this case the user must call `gsl_odeiv2_step_reset()` and `gsl_odeiv2_evolve_reset()` before calling this function again.

Otherwise, if the user-supplied functions defined in the system `sys` or the stepping function `step` return a status other than `GSL_SUCCESS`, the step is retried with a decreased step-size. If the step-size decreases below machine precision, a status of `GSL_FAILURE` is returned if the user functions returned `GSL_SUCCESS`. Otherwise the value returned by user function is returned. If no acceptable step can be made, `t` and `y` will be restored to their pre-step values and `h` contains the final attempted step-size.

If the step is successful the function returns a suggested step-size for the next step in `h`. The maximum time `t1` is guaranteed not to be exceeded by the time-step. On the final time-step the value of `t` will be set to `t1` exactly.

int **gsl_odeiv2_evolve_apply_fixed_step**(*gsl_odeiv2_evolve* *e, *gsl_odeiv2_control* *con, *gsl_odeiv2_step* *step, const *gsl_odeiv2_system* *sys, double *t, const double h, double y[])

This function advances the ODE-system (`e`, `sys`, `con`) from time `t` and position `y` using the stepping function `step` by a specified step size `h`. If the local error estimated by the stepping function exceeds the desired error level, the step is not taken and the function returns `GSL_FAILURE`. Otherwise the value returned by user function is returned.

int **gsl_odeiv2_evolve_reset**(*gsl_odeiv2_evolve* *e)

This function resets the evolution function `e`. It should be used whenever the next use of `e` will not be a continuation of a previous step.

void **gsl_odeiv2_evolve_free**(*gsl_odeiv2_evolve* *e)

This function frees all the memory associated with the evolution function `e`.

int **gsl_odeiv2_evolve_set_driver**(*gsl_odeiv2_evolve* *e, const gsl_odeiv2_driver *d)

This function sets a pointer of the driver object `d` for evolve object `e`.

If a system has discontinuous changes in the derivatives at known points, it is advisable to evolve the system between each discontinuity in sequence. For example, if a step-change in an external driving force occurs at times t_a, t_b and t_c then evolution should be carried out over the ranges (t_0, t_a), (t_a, t_b), (t_b, t_c), and (t_c, t_1) separately and not directly over the range (t_0, t_1).

29.5 Driver

The driver object is a high level wrapper that combines the evolution, control and stepper objects for easy use.

gsl_odeiv2_driver ***gsl_odeiv2_driver_alloc_y_new**(const *gsl_odeiv2_system* *sys, const *gsl_odeiv2_step_type* *T, const double hstart, const double epsabs, const double epsrel)

gsl_odeiv2_driver ***gsl_odeiv2_driver_alloc_yp_new**(const *gsl_odeiv2_system* *sys, const *gsl_odeiv2_step_type* *T, const double hstart, const double epsabs, const double epsrel)

gsl_odeiv2_driver ***gsl_odeiv2_driver_alloc_standard_new**(const *gsl_odeiv2_system* *sys, const *gsl_odeiv2_step_type* *T, const double hstart, const double epsabs, const double epsrel, const double a_y, const double a_dydt)

gsl_odeiv2_driver ***gsl_odeiv2_driver_alloc_scaled_new**(const *gsl_odeiv2_system* *sys, const *gsl_odeiv2_step_type* *T, const double hstart, const double epsabs, const double epsrel, const double a_y, const double a_dydt, const double scale_abs[])

These functions return a pointer to a newly allocated instance of a driver object. The functions automatically allocate and initialise the evolve, control and stepper objects for ODE system `sys` using stepper type `T`. The initial step size is given in `hstart`. The rest of the arguments follow the syntax and semantics of the control functions with same name (`gsl_odeiv2_control_*_new`).

int **gsl_odeiv2_driver_set_hmin**(gsl_odeiv2_driver *d, const double hmin)

The function sets a minimum for allowed step size `hmin` for driver `d`. Default value is 0.

int **gsl_odeiv2_driver_set_hmax**(gsl_odeiv2_driver *d, const double hmax)

The function sets a maximum for allowed step size `hmax` for driver `d`. Default value is `GSL_DBL_MAX`.

int **gsl_odeiv2_driver_set_nmax**(gsl_odeiv2_driver *d, const unsigned long int nmax)

The function sets a maximum for allowed number of steps `nmax` for driver `d`. Default value of 0 sets no limit for steps.

int **gsl_odeiv2_driver_apply**(gsl_odeiv2_driver *d, double *t, const double t1, double y[])

This function evolves the driver system `d` from `t` to `t1`. Initially vector `y` should contain the values of dependent variables at point `t`. If the function is unable to complete the calculation, an error code from `gsl_odeiv2_evolve_apply()` is returned, and `t` and `y` contain the values from last successful step.

If maximum number of steps is reached, a value of `GSL_EMAXITER` is returned. If the step size drops below minimum value, the function returns with `GSL_ENOPROG`. If the user-supplied functions defined in the system `sys` returns `GSL_EBADFUNC`, the function returns immediately with the same return code. In this case the user must call `gsl_odeiv2_driver_reset()` before calling this function again.

int **gsl_odeiv2_driver_apply_fixed_step**(gsl_odeiv2_driver *d, double *t, const double h, const unsigned long int n, double y[])

This function evolves the driver system `d` from `t` with `n` steps of size `h`. If the function is unable to complete the calculation, an error code from `gsl_odeiv2_evolve_apply_fixed_step()` is returned, and `t` and `y` contain the values from last successful step.

int **gsl_odeiv2_driver_reset**(gsl_odeiv2_driver *d)

This function resets the evolution and stepper objects.

int **gsl_odeiv2_driver_reset_hstart**(gsl_odeiv2_driver *d, const double hstart)
The routine resets the evolution and stepper objects and sets new initial step size to `hstart`. This function can be used e.g. to change the direction of integration.

int **gsl_odeiv2_driver_free**(gsl_odeiv2_driver *d)
This function frees the driver object, and the related evolution, stepper and control objects.

29.6 Examples

The following program solves the second-order nonlinear Van der Pol oscillator equation,

$$u''(t) + \mu u'(t)(u(t)^2 - 1) + u(t) = 0$$

This can be converted into a first order system suitable for use with the routines described in this chapter by introducing a separate variable for the velocity, $v = u'(t)$,

$$\begin{aligned} u' &= v \\ v' &= -u + \mu v(1 - u^2) \end{aligned}$$

The program begins by defining functions for these derivatives and their Jacobian. The main function uses driver level functions to solve the problem. The program evolves the solution from $(u, v) = (1, 0)$ at $t = 0$ to $t = 100$. The step-size h is automatically adjusted by the controller to maintain an absolute accuracy of 10^{-6} in the function values (u, v). The loop in the example prints the solution at the points $t_i = 1, 2, \dots, 100$.

```
#include <stdio.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_odeiv2.h>

int
func (double t, const double y[], double f[],
      void *params)
{
  (void)(t); /* avoid unused parameter warning */
  double mu = *(double *)params;
  f[0] = y[1];
  f[1] = -y[0] - mu*y[1]*(y[0]*y[0] - 1);
  return GSL_SUCCESS;
}

int
jac (double t, const double y[], double *dfdy,
     double dfdt[], void *params)
{
  (void)(t); /* avoid unused parameter warning */
  double mu = *(double *)params;
  gsl_matrix_view dfdy_mat
    = gsl_matrix_view_array (dfdy, 2, 2);
  gsl_matrix * m = &dfdy_mat.matrix;
  gsl_matrix_set (m, 0, 0, 0.0);
  gsl_matrix_set (m, 0, 1, 1.0);
  gsl_matrix_set (m, 1, 0, -2.0*mu*y[0]*y[1] - 1.0);
  gsl_matrix_set (m, 1, 1, -mu*(y[0]*y[0] - 1.0));
```

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```
  dfdt[0] = 0.0;
  dfdt[1] = 0.0;
  return GSL_SUCCESS;
}

int
main (void)
{
  double mu = 10;
  gsl_odeiv2_system sys = {func, jac, 2, &mu};

  gsl_odeiv2_driver * d =
    gsl_odeiv2_driver_alloc_y_new (&sys, gsl_odeiv2_step_rk8pd,
                                  1e-6, 1e-6, 0.0);
  int i;
  double t = 0.0, t1 = 100.0;
  double y[2] = { 1.0, 0.0 };

  for (i = 1; i <= 100; i++)
    {
      double ti = i * t1 / 100.0;
      int status = gsl_odeiv2_driver_apply (d, &t, ti, y);

      if (status != GSL_SUCCESS)
        {
          printf ("error, return value=%d\n", status);
          break;
        }

      printf ("%.5e %.5e %.5e\n", t, y[0], y[1]);
    }

  gsl_odeiv2_driver_free (d);
  return 0;
}
```

The user can work with the lower level functions directly, as in the following example. In this case an intermediate result is printed after each successful step instead of equidistant time points.

```
int
main (void)
{
  const gsl_odeiv2_step_type * T
    = gsl_odeiv2_step_rk8pd;

  gsl_odeiv2_step * s
    = gsl_odeiv2_step_alloc (T, 2);
  gsl_odeiv2_control * c
    = gsl_odeiv2_control_y_new (1e-6, 0.0);
  gsl_odeiv2_evolve * e
    = gsl_odeiv2_evolve_alloc (2);
```

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```
  double mu = 10;
  gsl_odeiv2_system sys = {func, jac, 2, &mu};

  double t = 0.0, t1 = 100.0;
  double h = 1e-6;
  double y[2] = { 1.0, 0.0 };

  while (t < t1)
    {
      int status = gsl_odeiv2_evolve_apply (e, c, s,
                                            &sys,
                                            &t, t1,
                                            &h, y);

      if (status != GSL_SUCCESS)
          break;

      printf ("%.5e %.5e %.5e\n", t, y[0], y[1]);
    }

  gsl_odeiv2_evolve_free (e);
  gsl_odeiv2_control_free (c);
  gsl_odeiv2_step_free (s);
  return 0;
}
```

For functions with multiple parameters, the appropriate information can be passed in through the `params` argument in *gsl_odeiv2_system* definition (`mu` in this example) by using a pointer to a struct.

It is also possible to work with a non-adaptive integrator, using only the stepping function itself, *gsl_odeiv2_driver_apply_fixed_step()* or *gsl_odeiv2_evolve_apply_fixed_step()*. The following program uses the driver level function, with fourth-order Runge-Kutta stepping function with a fixed stepsize of 0.001.

```
int
main (void)
{
  double mu = 10;
  gsl_odeiv2_system sys = { func, jac, 2, &mu };

  gsl_odeiv2_driver *d =
    gsl_odeiv2_driver_alloc_y_new (&sys, gsl_odeiv2_step_rk4,
                                   1e-3, 1e-8, 1e-8);

  double t = 0.0;
  double y[2] = { 1.0, 0.0 };
  int i, s;

  for (i = 0; i < 100; i++)
    {
      s = gsl_odeiv2_driver_apply_fixed_step (d, &t, 1e-3, 1000, y);

      if (s != GSL_SUCCESS)
```

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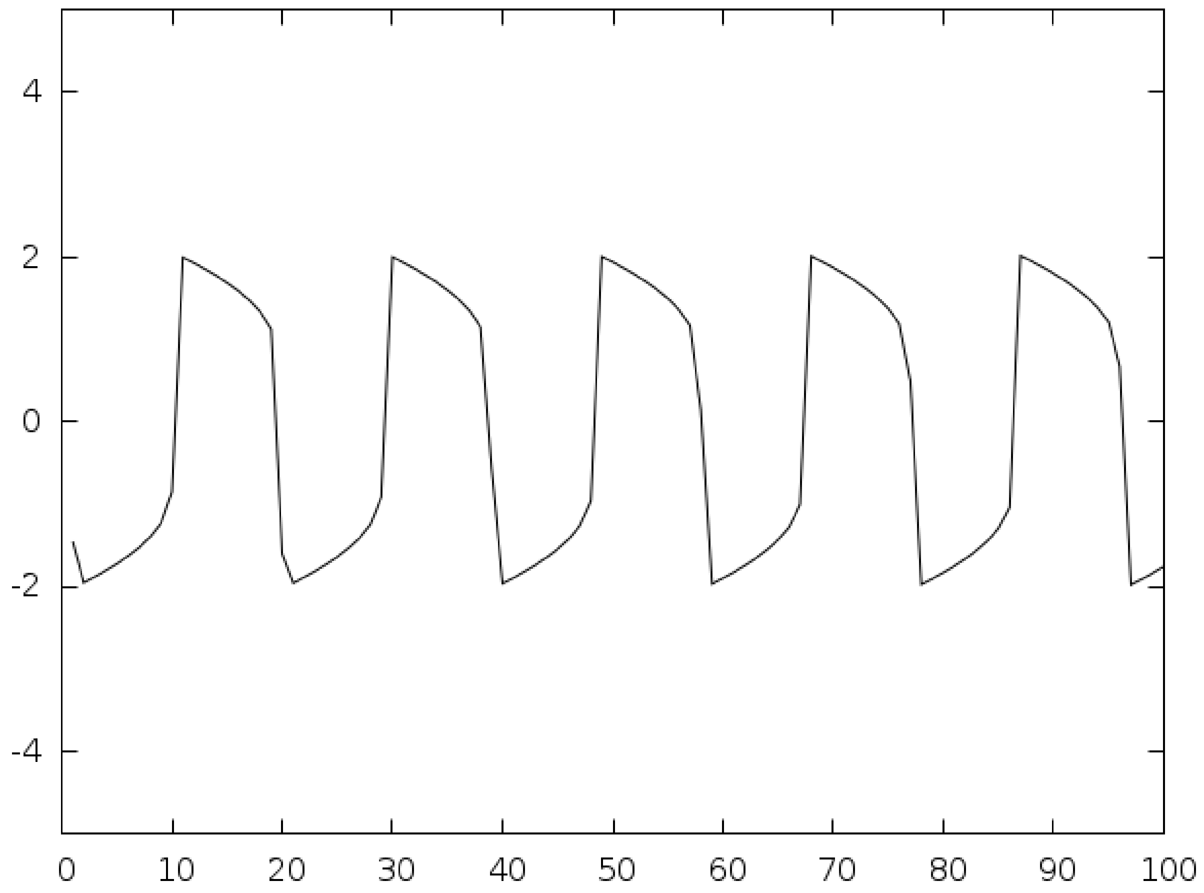

Fig. 29.1: Numerical solution of the Van der Pol oscillator equation using Prince-Dormand 8th order Runge-Kutta.

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```
        {
          printf ("error: driver returned %d\n", s);
          break;
        }

      printf ("%.5e %.5e %.5e\n", t, y[0], y[1]);
    }

  gsl_odeiv2_driver_free (d);
  return s;
}
```

29.7 References and Further Reading

- Ascher, U.M., Petzold, L.R., *Computer Methods for Ordinary Differential and Differential-Algebraic Equations*, SIAM, Philadelphia, 1998.
- Hairer, E., Norsett, S. P., Wanner, G., *Solving Ordinary Differential Equations I: Nonstiff Problems*, Springer, Berlin, 1993.
- Hairer, E., Wanner, G., *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*, Springer, Berlin, 1996.

Many of the basic Runge-Kutta formulas can be found in the Handbook of Mathematical Functions,

- Abramowitz & Stegun (eds.), *Handbook of Mathematical Functions*, Section 25.5.

The implicit Bulirsch-Stoer algorithm `bsimp` is described in the following paper,

- G. Bader and P. Deuflhard, "A Semi-Implicit Mid-Point Rule for Stiff Systems of Ordinary Differential Equations.", Numer.: Math.: 41, 373–398, 1983.

The Adams and BDF multistep methods `msadams` and `msbdf` are based on the following articles,

- G. D. Byrne and A. C. Hindmarsh, "A Polyalgorithm for the Numerical Solution of Ordinary Differential Equations.", ACM Trans. Math. Software, 1, 71–96, 1975.
- P. N. Brown, G. D. Byrne and A. C. Hindmarsh, "VODE: A Variable-coefficient ODE Solver.", SIAM J. Sci. Stat. Comput. 10, 1038–1051, 1989.
- A. C. Hindmarsh, P. N. Brown, K. E. Grant, S. L. Lee, R. Serban, D. E. Shumaker and C. S. Woodward, "SUNDIALS: Suite of Nonlinear and Differential/Algebraic Equation Solvers.", ACM Trans. Math. Software 31, 363–396, 2005.

CHAPTER

THIRTY

INTERPOLATION

This chapter describes functions for performing interpolation. The library provides a variety of interpolation methods, including Cubic, Akima, and Steffen splines. The interpolation types are interchangeable, allowing different methods to be used without recompiling. Interpolations can be defined for both normal and periodic boundary conditions. Additional functions are available for computing derivatives and integrals of interpolating functions. Routines are provided for interpolating both one and two dimensional datasets.

These interpolation methods produce curves that pass through each datapoint. To interpolate noisy data with a smoothing curve see *Basis Splines*.

The functions described in this section are declared in the header files `gsl_interp.h` and `gsl_spline.h`.

30.1 Introduction to 1D Interpolation

Given a set of data points $(x_1, y_1) \dots (x_n, y_n)$ the routines described in this section compute a continuous interpolating function $y(x)$ such that $y(x_i) = y_i$. The interpolation is piecewise smooth, and its behavior at the end-points is determined by the type of interpolation used.

30.2 1D Interpolation Functions

The interpolation function for a given dataset is stored in a `gsl_interp` object. These are created by the following functions.

type **`gsl_interp`**

Workspace for 1D interpolation

gsl_interp ***`gsl_interp_alloc`**(const *gsl_interp_type* *T, size_t size)

This function returns a pointer to a newly allocated interpolation object of type `T` for `size` data-points.

int **`gsl_interp_init`**(*gsl_interp* *interp, const double xa[], const double ya[], size_t size)

This function initializes the interpolation object `interp` for the data (`xa`, `ya`) where `xa` and `ya` are arrays of size `size`. The interpolation object (`gsl_interp`) does not save the data arrays `xa` and `ya` and only stores the static state computed from the data. The `xa` data array is always assumed to be strictly ordered, with increasing x values; the behavior for other arrangements is not defined.

void **`gsl_interp_free`**(*gsl_interp* *interp)

This function frees the interpolation object `interp`.

30.3 1D Interpolation Types

The interpolation library provides the following interpolation types:

type **gsl_interp_type**

gsl_interp_type ***gsl_interp_linear***
Linear interpolation. This interpolation method does not require any additional memory.

gsl_interp_type ***gsl_interp_polynomial***
Polynomial interpolation. This method should only be used for interpolating small numbers of points because polynomial interpolation introduces large oscillations, even for well-behaved datasets. The number of terms in the interpolating polynomial is equal to the number of points.

gsl_interp_type ***gsl_interp_cspline***
Cubic spline with natural boundary conditions. The resulting curve is piecewise cubic on each interval, with matching first and second derivatives at the supplied data-points. The second derivative is chosen to be zero at the first point and last point.

gsl_interp_type ***gsl_interp_cspline_periodic***
Cubic spline with periodic boundary conditions. The resulting curve is piecewise cubic on each interval, with matching first and second derivatives at the supplied data-points. The derivatives at the first and last points are also matched. Note that the last point in the data must have the same y-value as the first point, otherwise the resulting periodic interpolation will have a discontinuity at the boundary.

gsl_interp_type ***gsl_interp_akima***
Non-rounded Akima spline with natural boundary conditions. This method uses the non-rounded corner algorithm of Wodicka.

gsl_interp_type ***gsl_interp_akima_periodic***
Non-rounded Akima spline with periodic boundary conditions. This method uses the non-rounded corner algorithm of Wodicka.

gsl_interp_type ***gsl_interp_steffen***
Steffen's method guarantees the monotonicity of the interpolating function between the given data points. Therefore, minima and maxima can only occur exactly at the data points, and there can never be spurious oscillations between data points. The interpolated function is piecewise cubic in each interval. The resulting curve and its first derivative are guaranteed to be continuous, but the second derivative may be discontinuous.

The following related functions are available:

const char ***gsl_interp_name**(const *gsl_interp* *interp)
This function returns the name of the interpolation type used by *interp*. For example:

```
printf ("interp uses '%s' interpolation.\n", gsl_interp_name (interp));
```

would print something like:

```
interp uses 'cspline' interpolation.
```

unsigned int **gsl_interp_min_size**(const *gsl_interp* *interp)

unsigned int **gsl_interp_type_min_size**(const *gsl_interp_type* *T)
These functions return the minimum number of points required by the interpolation object `interp` or interpolation type *T*. For example, Akima spline interpolation requires a minimum of 5 points.

30.4 1D Index Look-up and Acceleration

The state of searches can be stored in a *gsl_interp_accel* object, which is a kind of iterator for interpolation lookups.

type **gsl_interp_accel**

This workspace stores state variables for interpolation lookups. It caches the previous value of an index lookup. When the subsequent interpolation point falls in the same interval its index value can be returned immediately.

size_t **gsl_interp_bsearch**(const double x_array[], double x, size_t index_lo, size_t index_hi)

This function returns the index i of the array *x_array* such that `x_array[i] <= x < x_array[i+1]`. The index is searched for in the range [*index_lo*, *index_hi*]. An inline version of this function is used when `HAVE_INLINE` is defined.

gsl_interp_accel ***gsl_interp_accel_alloc**(void)

This function returns a pointer to an accelerator object, which is a kind of iterator for interpolation lookups. It tracks the state of lookups, thus allowing for application of various acceleration strategies. When multiple interpolants are in use, the same accelerator object may be used for all datasets with the same domain (`x_array`), but different accelerators should be used for data defined on different domains.

size_t **gsl_interp_accel_find**(*gsl_interp_accel* *a, const double x_array[], size_t size, double x)

This function performs a lookup action on the data array *x_array* of size *size*, using the given accelerator *a*. This is how lookups are performed during evaluation of an interpolation. The function returns an index i such that `x_array[i] <= x < x_array[i+1]`. An inline version of this function is used when `HAVE_INLINE` is defined.

int **gsl_interp_accel_reset**(*gsl_interp_accel* *acc);

This function reinitializes the accelerator object *acc*. It should be used when the cached information is no longer applicable—for example, when switching to a new dataset.

void **gsl_interp_accel_free**(*gsl_interp_accel* *acc)

This function frees the accelerator object *acc*.

30.5 1D Evaluation of Interpolating Functions

double **gsl_interp_eval**(const *gsl_interp* *interp, const double xa[], const double ya[], double x, *gsl_interp_accel* *acc)

int **gsl_interp_eval_e**(const *gsl_interp* *interp, const double xa[], const double ya[], double x, *gsl_interp_accel* *acc, double *y)

These functions return the interpolated value of *y* for a given point *x*, using the interpolation object *interp*, data arrays *xa* and *ya* and the accelerator *acc*. When *x* is outside the range of *xa*, the error code *GSL_EDOM* is returned with a value of *GSL_NAN* for *y*.

double **gsl_interp_eval_deriv**(const *gsl_interp* *interp, const double xa[], const double ya[], double x, *gsl_interp_accel* *acc)

int **gsl_interp_eval_deriv_e**(const *gsl_interp* *interp, const double xa[], const double ya[], double x, *gsl_interp_accel* *acc, double *d)

These functions return the derivative *d* of an interpolated function for a given point *x*, using the interpolation object *interp*, data arrays *xa* and *ya* and the accelerator *acc*.

double **gsl_interp_eval_deriv2**(const *gsl_interp* *interp, const double xa[], const double ya[], double x, *gsl_interp_accel* *acc) int **gsl_interp_eval_deriv2_e**(const *gsl_interp* *interp, const double xa[], const double ya[], double x, *gsl_interp_accel* *acc, double *d2)

These functions return the second derivative `d2` of an interpolated function for a given point `x`, using the interpolation object `interp`, data arrays `xa` and `ya` and the accelerator `acc`.

double **gsl_interp_eval_integ**(const *gsl_interp* *interp, const double xa[], const double ya[], double a, double b, *gsl_interp_accel* *acc)

int **gsl_interp_eval_integ_e**(const *gsl_interp* *interp, const double xa[], const double ya[], double a, double b, *gsl_interp_accel* *acc, double *result)

These functions return the numerical integral `result` of an interpolated function over the range [`a`, `b`], using the interpolation object `interp`, data arrays `xa` and `ya` and the accelerator `acc`.

30.6 1D Higher-level Interface

The functions described in the previous sections required the user to supply pointers to the x and y arrays on each call. The following functions are equivalent to the corresponding `gsl_interp` functions but maintain a copy of this data in the `gsl_spline` object. This removes the need to pass both `xa` and `ya` as arguments on each evaluation. These functions are defined in the header file `gsl_spline.h`.

type **gsl_spline**

This workspace provides a higher level interface for the `gsl_interp` object

gsl_spline ***gsl_spline_alloc**(const *gsl_interp_type* *T, size_t size)

int **gsl_spline_init**(*gsl_spline* *spline, const double xa[], const double ya[], size_t size)

void **gsl_spline_free**(*gsl_spline* *spline)

const char ***gsl_spline_name**(const *gsl_spline* *spline)

unsigned int **gsl_spline_min_size**(const *gsl_spline* *spline)

double **gsl_spline_eval**(const *gsl_spline* *spline, double x, *gsl_interp_accel* *acc)

int **gsl_spline_eval_e**(const *gsl_spline* *spline, double x, *gsl_interp_accel* *acc, double *y)

double **gsl_spline_eval_deriv**(const *gsl_spline* *spline, double x, *gsl_interp_accel* *acc)

int **gsl_spline_eval_deriv_e**(const *gsl_spline* *spline, double x, *gsl_interp_accel* *acc, double *d)

double **gsl_spline_eval_deriv2**(const *gsl_spline* *spline, double x, *gsl_interp_accel* *acc)

int **gsl_spline_eval_deriv2_e**(const *gsl_spline* *spline, double x, *gsl_interp_accel* *acc, double *d2)

double **gsl_spline_eval_integ**(const *gsl_spline* *spline, double a, double b, *gsl_interp_accel* *acc) int **gsl_spline_eval_integ_e**(const *gsl_spline* *spline, double a, double b, *gsl_interp_accel* *acc, double *result)

30.7 1D Interpolation Example Programs

The following program demonstrates the use of the interpolation and spline functions. It computes a cubic spline interpolation of the 10-point dataset (x_i, y_i) where $x_i = i + \sin(i)/2$ and $y_i = i + \cos(i^2)$ for $i = 0 \ldots 9$.

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_spline.h>

int
main (void)
{
  int i;
  double xi, yi, x[10], y[10];

  printf ("#m=0,S=17\n");

  for (i = 0; i < 10; i++)
    {
      x[i] = i + 0.5 * sin (i);
      y[i] = i + cos (i * i);
      printf ("%g %g\n", x[i], y[i]);
    }

  printf ("#m=1,S=0\n");

  {
    gsl_interp_accel *acc
      = gsl_interp_accel_alloc ();
    gsl_spline *spline
      = gsl_spline_alloc (gsl_interp_cspline, 10);

    gsl_spline_init (spline, x, y, 10);

    for (xi = x[0]; xi < x[9]; xi += 0.01)
      {
        yi = gsl_spline_eval (spline, xi, acc);
        printf ("%g %g\n", xi, yi);
      }
    gsl_spline_free (spline);
    gsl_interp_accel_free (acc);
  }
  return 0;
}
```

The output is designed to be used with the GNU plotutils `graph` program:

```
$ ./a.out > interp.dat
$ graph -T ps < interp.dat > interp.ps
```

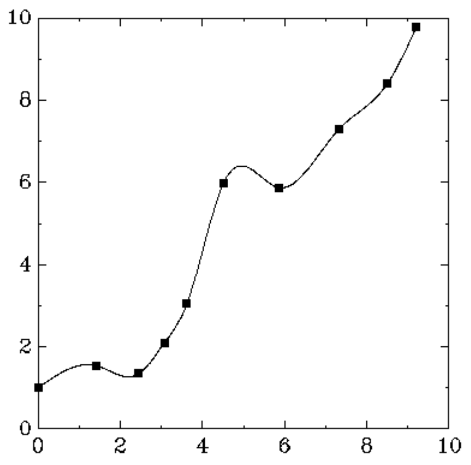

Fig. 30.1: Cubic spline interpolation

Fig. 30.1 shows a smooth interpolation of the original points. The interpolation method can be changed simply by varying the first argument of *gsl_spline_alloc()*.

The next program demonstrates a periodic cubic spline with 4 data points. Note that the first and last points must be supplied with the same y-value for a periodic spline.

```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_spline.h>

int
main (void)
{
  int N = 4;
  double x[4] = {0.00, 0.10,  0.27,  0.30};
  double y[4] = {0.15, 0.70, -0.10,  0.15};
             /* Note: y[0] == y[3] for periodic data */

  gsl_interp_accel *acc = gsl_interp_accel_alloc ();
  const gsl_interp_type *t = gsl_interp_cspline_periodic;
  gsl_spline *spline = gsl_spline_alloc (t, N);

  int i; double xi, yi;
```

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```
  printf ("#m=0,S=5\n");
  for (i = 0; i < N; i++)
    {
      printf ("%g %g\n", x[i], y[i]);
    }

  printf ("#m=1,S=0\n");
  gsl_spline_init (spline, x, y, N);

  for (i = 0; i <= 100; i++)
    {
      xi = (1 - i / 100.0) * x[0] + (i / 100.0) * x[N-1];
      yi = gsl_spline_eval (spline, xi, acc);
      printf ("%g %g\n", xi, yi);
    }

  gsl_spline_free (spline);
  gsl_interp_accel_free (acc);
  return 0;
}
```

The output can be plotted with GNU graph:

```
$ ./a.out > interp.dat
$ graph -T ps < interp.dat > interp.ps
```

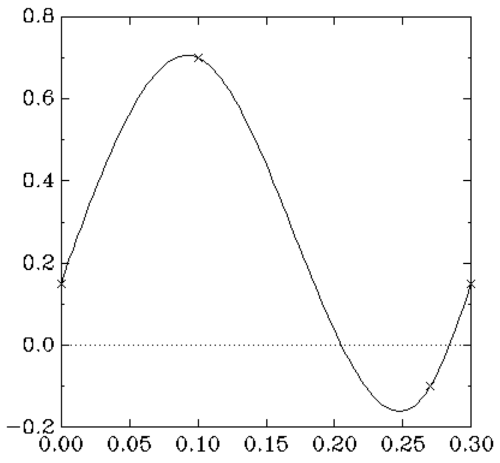

Fig. 30.2: Periodic cubic spline interpolation

Fig. 30.2 shows a periodic interpolation of the original points. The slope of the fitted curve is the same at the beginning and end of the data, and the second derivative is also.

The next program illustrates the difference between the cubic spline, Akima, and Steffen interpolation types on a difficult dataset.

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_spline.h>

int
main(void)
{
  size_t i;
  const size_t N = 9;

  /* this dataset is taken from
   * J. M. Hyman, Accurate Monotonicity preserving cubic interpolation,
   * SIAM J. Sci. Stat. Comput. 4, 4, 1983. */
  const double x[] = { 7.99, 8.09, 8.19, 8.7, 9.2,
                       10.0, 12.0, 15.0, 20.0 };
  const double y[] = { 0.0, 2.76429e-5, 4.37498e-2,
                       0.169183, 0.469428, 0.943740,
                       0.998636, 0.999919, 0.999994 };

  gsl_interp_accel *acc = gsl_interp_accel_alloc();
  gsl_spline *spline_cubic = gsl_spline_alloc(gsl_interp_cspline, N);
  gsl_spline *spline_akima = gsl_spline_alloc(gsl_interp_akima, N);
  gsl_spline *spline_steffen = gsl_spline_alloc(gsl_interp_steffen, N);

  gsl_spline_init(spline_cubic, x, y, N);
  gsl_spline_init(spline_akima, x, y, N);
  gsl_spline_init(spline_steffen, x, y, N);

  for (i = 0; i < N; ++i)
    printf("%g %g\n", x[i], y[i]);

  printf("\n\n");

  for (i = 0; i <= 100; ++i)
    {
      double xi = (1 - i / 100.0) * x[0] + (i / 100.0) * x[N-1];
      double yi_cubic = gsl_spline_eval(spline_cubic, xi, acc);
      double yi_akima = gsl_spline_eval(spline_akima, xi, acc);
      double yi_steffen = gsl_spline_eval(spline_steffen, xi, acc);

      printf("%g %g %g %g\n", xi, yi_cubic, yi_akima, yi_steffen);
    }

  gsl_spline_free(spline_cubic);
  gsl_spline_free(spline_akima);
  gsl_spline_free(spline_steffen);
  gsl_interp_accel_free(acc);
```

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```
  return 0;
}
```

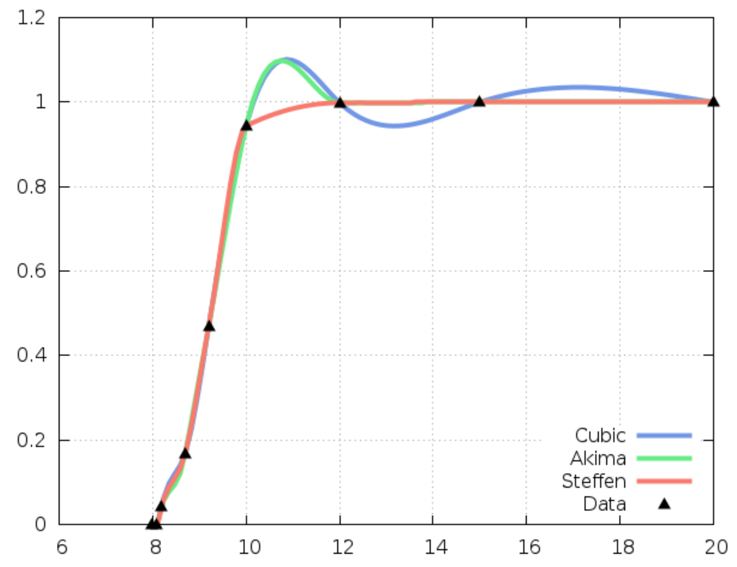

Fig. 30.3: Comparison of different 1D interpolation methods

The output is shown in Fig. 30.3. The cubic method exhibits a local maxima between the 6th and 7th data points and continues oscillating for the rest of the data. Akima also shows a local maxima but recovers and follows the data well after the 7th grid point. Steffen preserves monotonicity in all intervals and does not exhibit oscillations, at the expense of having a discontinuous second derivative.

30.8 Introduction to 2D Interpolation

Given a set of x coordinates $x_1, ..., x_m$ and a set of y coordinates $y_1, ..., y_n$, each in increasing order, plus a set of function values z_{ij} for each grid point (x_i, y_j), the routines described in this section compute a continuous interpolation function $z(x, y)$ such that $z(x_i, y_j) = z_{ij}$.

30.9 2D Interpolation Functions

The interpolation function for a given dataset is stored in a `gsl_interp2d` object. These are created by the following functions.

type **`gsl_interp2d`**

  Workspace for 2D interpolation

gsl_interp2d ***`gsl_interp2d_alloc`**(const *gsl_interp2d_type* *T, const size_t xsize, const size_t ysize)

  This function returns a pointer to a newly allocated interpolation object of type `T` for `xsize` grid points in the x direction and `ysize` grid points in the y direction.

int **`gsl_interp2d_init`**(*gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const size_t xsize, const size_t ysize)

  This function initializes the interpolation object `interp` for the data (`xa`, `ya`, `za`) where `xa` and `ya` are arrays of the x and y grid points of size `xsize` and `ysize` respectively, and `za` is an array of function values of size `xsize` * `ysize`. The interpolation object (`gsl_interp2d`) does not save the data arrays `xa`, `ya`, and `za` and only stores the static state computed from the data. The `xa` and `ya` data arrays are always assumed to be strictly ordered, with increasing x, y values; the behavior for other arrangements is not defined.

void **gsl_interp2d_free**(*gsl_interp2d* *interp)

This function frees the interpolation object `interp`.

30.10 2D Interpolation Grids

The 2D interpolation routines access the function values z_{ij} with the following ordering:

$$z_{ij} = za[j * xsize + i]$$

with $i = 0, ..., xsize - 1$ and $j = 0, ..., ysize - 1$. However, for ease of use, the following functions are provided to add and retrieve elements from the function grid without requiring knowledge of the internal ordering.

int **gsl_interp2d_set**(const *gsl_interp2d* *interp, double za[], const size_t i, const size_t j, const double z)

This function sets the value z_{ij} for grid point (`i`, `j`) of the array `za` to `z`.

double **gsl_interp2d_get**(const *gsl_interp2d* *interp, const double za[], const size_t i, const size_t j)

This function returns the value z_{ij} for grid point (`i`, `j`) stored in the array `za`.

size_t **gsl_interp2d_idx**(const *gsl_interp2d* *interp, const size_t i, const size_t j)

This function returns the index corresponding to the grid point (`i`, `j`). The index is given by $j * xsize + i$.

30.11 2D Interpolation Types

type **gsl_interp2d_type**

The interpolation library provides the following 2D interpolation types:

gsl_interp2d_type ***gsl_interp2d_bilinear***

Bilinear interpolation. This interpolation method does not require any additional memory.

gsl_interp2d_type ***gsl_interp2d_bicubic***

Bicubic interpolation.

const char ***gsl_interp2d_name**(const *gsl_interp2d* *interp)

This function returns the name of the interpolation type used by `interp`. For example:

```
printf ("interp uses '%s' interpolation.\n", gsl_interp2d_name (interp));
```

would print something like:

```
interp uses 'bilinear' interpolation.
```

unsigned int **gsl_interp2d_min_size**(const *gsl_interp2d* *interp)

unsigned int **gsl_interp2d_type_min_size**(const *gsl_interp2d_type* *T)

These functions return the minimum number of points required by the interpolation object `interp` or interpolation type `T`. For example, bicubic interpolation requires a minimum of 4 points.

30.12 2D Evaluation of Interpolating Functions

double **gsl_interp2d_eval**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_interp2d_eval_e**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *z)

These functions return the interpolated value of `z` for a given point (`x`, `y`), using the interpolation object `interp`, data arrays `xa`, `ya`, and `za` and the accelerators `xacc` and `yacc`. When `x` is outside the range of `xa` or `y` is outside the range of `ya`, the error code `GSL_EDOM` is returned.

double **gsl_interp2d_eval_extrap**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_interp2d_eval_extrap_e**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *z)

These functions return the interpolated value of `z` for a given point (`x`, `y`), using the interpolation object `interp`, data arrays `xa`, `ya`, and `za` and the accelerators `xacc` and `yacc`. The functions perform no bounds checking, so when `x` is outside the range of `xa` or `y` is outside the range of `ya`, extrapolation is performed.

double **gsl_interp2d_eval_deriv_x**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_interp2d_eval_deriv_x_e**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

These functions return the interpolated value `d` $= \partial z/\partial x$ for a given point (`x`, `y`), using the interpolation object `interp`, data arrays `xa`, `ya`, and `za` and the accelerators `xacc` and `yacc`. When `x` is outside the range of `xa` or `y` is outside the range of `ya`, the error code `GSL_EDOM` is returned.

double **gsl_interp2d_eval_deriv_y**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_interp2d_eval_deriv_y_e**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

These functions return the interpolated value `d` $= \partial z/\partial y$ for a given point (`x`, `y`), using the interpolation object `interp`, data arrays `xa`, `ya`, and `za` and the accelerators `xacc` and `yacc`. When `x` is outside the range of `xa` or `y` is outside the range of `ya`, the error code `GSL_EDOM` is returned.

double **gsl_interp2d_eval_deriv_xx**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_interp2d_eval_deriv_xx_e**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

These functions return the interpolated value `d` $= \partial^2 z/\partial x^2$ for a given point (`x`, `y`), using the interpolation object `interp`, data arrays `xa`, `ya`, and `za` and the accelerators `xacc` and `yacc`. When `x` is outside the range of `xa` or `y` is outside the range of `ya`, the error code `GSL_EDOM` is returned.

double **gsl_interp2d_eval_deriv_yy**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_interp2d_eval_deriv_yy_e**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

These functions return the interpolated value $d = \partial^2 z/\partial y^2$ for a given point (`x`, `y`), using the interpolation object `interp`, data arrays `xa`, `ya`, and `za` and the accelerators `xacc` and `yacc`. When `x` is outside the range of `xa` or `y` is outside the range of `ya`, the error code `GSL_EDOM` is returned.

double **gsl_interp2d_eval_deriv_xy**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_interp2d_eval_deriv_xy_e**(const *gsl_interp2d* *interp, const double xa[], const double ya[], const double za[], const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

These functions return the interpolated value $d = \partial^2 z/\partial x \partial y$ for a given point (`x`, `y`), using the interpolation object `interp`, data arrays `xa`, `ya`, and `za` and the accelerators `xacc` and `yacc`. When `x` is outside the range of `xa` or `y` is outside the range of `ya`, the error code `GSL_EDOM` is returned.

30.13 2D Higher-level Interface

The functions described in the previous sections required the user to supply pointers to the x, y, and z arrays on each call. The following functions are equivalent to the corresponding `gsl_interp2d` functions but maintain a copy of this data in the `gsl_spline2d` object. This removes the need to pass `xa`, `ya`, and `za` as arguments on each evaluation. These functions are defined in the header file `gsl_spline2d.h`.

type **gsl_spline2d**

This workspace provides a higher level interface for the `gsl_interp2d` object

gsl_spline2d ***gsl_spline2d_alloc**(const *gsl_interp2d_type* *T, size_t xsize, size_t ysize)

int **gsl_spline2d_init**(*gsl_spline2d* *spline, const double xa[], const double ya[], const double za[], size_t xsize, size_t ysize)

void **gsl_spline2d_free**(*gsl_spline2d* *spline)

const char ***gsl_spline2d_name**(const *gsl_spline2d* *spline)

unsigned int **gsl_spline2d_min_size**(const *gsl_spline2d* *spline)

double **gsl_spline2d_eval**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_spline2d_eval_e**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *z) double **gsl_spline2d_eval_extrap**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_spline2d_eval_extrap_e**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *z)

double **gsl_spline2d_eval_deriv_x**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_spline2d_eval_deriv_x_e**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

double **gsl_spline2d_eval_deriv_y**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_spline2d_eval_deriv_y_e**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

double **gsl_spline2d_eval_deriv_xx**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_spline2d_eval_deriv_xx_e**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

double **gsl_spline2d_eval_deriv_yy**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_spline2d_eval_deriv_yy_e**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

double **gsl_spline2d_eval_deriv_xy**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc)

int **gsl_spline2d_eval_deriv_xy_e**(const *gsl_spline2d* *spline, const double x, const double y, *gsl_interp_accel* *xacc, *gsl_interp_accel* *yacc, double *d)

int **gsl_spline2d_set**(const *gsl_spline2d* *spline, double za[], const size_t i, const size_t j, const double z)

double **gsl_spline2d_get**(const *gsl_spline2d* *spline, const double za[], const size_t i, const size_t j)

This function returns the value z_{ij} for grid point (`i`, `j`) stored in the array `za`.

30.14 2D Interpolation Example programs

The following example performs bilinear interpolation on the unit square, using z values of $(0, 1, 0.5, 1)$ going clockwise around the square.

```
#include <stdio.h>
#include <stdlib.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_interp2d.h>
#include <gsl/gsl_spline2d.h>

int
main()
{
  const gsl_interp2d_type *T = gsl_interp2d_bilinear;
  const size_t N = 100;             /* number of points to interpolate */
  const double xa[] = { 0.0, 1.0 }; /* define unit square */
  const double ya[] = { 0.0, 1.0 };
  const size_t nx = sizeof(xa) / sizeof(double); /* x grid points */
  const size_t ny = sizeof(ya) / sizeof(double); /* y grid points */
  double *za = malloc(nx * ny * sizeof(double));
  gsl_spline2d *spline = gsl_spline2d_alloc(T, nx, ny);
  gsl_interp_accel *xacc = gsl_interp_accel_alloc();
  gsl_interp_accel *yacc = gsl_interp_accel_alloc();
  size_t i, j;

  /* set z grid values */
  gsl_spline2d_set(spline, za, 0, 0, 0.0);
  gsl_spline2d_set(spline, za, 0, 1, 1.0);
  gsl_spline2d_set(spline, za, 1, 1, 0.5);
  gsl_spline2d_set(spline, za, 1, 0, 1.0);

  /* initialize interpolation */
  gsl_spline2d_init(spline, xa, ya, za, nx, ny);

  /* interpolate N values in x and y and print out grid for plotting */
  for (i = 0; i < N; ++i)
    {
      double xi = i / (N - 1.0);

      for (j = 0; j < N; ++j)
        {
          double yj = j / (N - 1.0);
          double zij = gsl_spline2d_eval(spline, xi, yj, xacc, yacc);

          printf("%f %f %f\n", xi, yj, zij);
        }
      printf("\n");
    }

  gsl_spline2d_free(spline);
  gsl_interp_accel_free(xacc);
```

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```
  gsl_interp_accel_free(yacc);
  free(za);

  return 0;
}
```

The results of the interpolation are shown in Fig. 30.4, where the corners are labeled with their fixed z values.

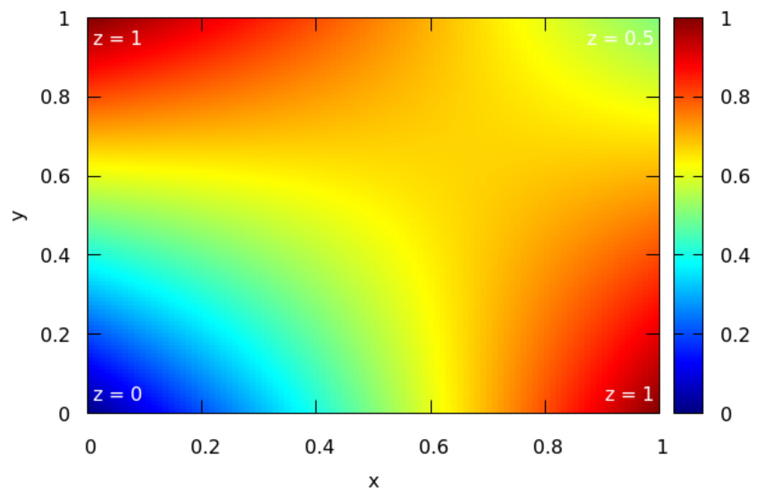

Fig. 30.4: 2D interpolation example

30.15 References and Further Reading

Descriptions of the interpolation algorithms and further references can be found in the following publications:

- C.W. Ueberhuber, *Numerical Computation (Volume 1), Chapter 9 "Interpolation"*, Springer (1997), ISBN 3-540-62058-3.
- D.M. Young, R.T. Gregory, *A Survey of Numerical Mathematics (Volume 1), Chapter 6.8*, Dover (1988), ISBN 0-486-65691-8.
- M. Steffen, *A simple method for monotonic interpolation in one dimension*, Astron. Astrophys. 239, 443-450, 1990.

CHAPTER

THIRTYONE

NUMERICAL DIFFERENTIATION

The functions described in this chapter compute numerical derivatives by finite differencing. An adaptive algorithm is used to find the best choice of finite difference and to estimate the error in the derivative. These functions are declared in the header file `gsl_deriv.h`.

31.1 Functions

int **gsl_deriv_central**(const *gsl_function* *f, double x, double h, double *result, double *abserr)

This function computes the numerical derivative of the function `f` at the point `x` using an adaptive central difference algorithm with a step-size of `h`. The derivative is returned in `result` and an estimate of its absolute error is returned in `abserr`.

The initial value of `h` is used to estimate an optimal step-size, based on the scaling of the truncation error and round-off error in the derivative calculation. The derivative is computed using a 5-point rule for equally spaced abscissae at $x - h$, $x - h/2$, x, $x + h/2$, $x + h$, with an error estimate taken from the difference between the 5-point rule and the corresponding 3-point rule $x - h$, x, $x + h$. Note that the value of the function at x does not contribute to the derivative calculation, so only 4-points are actually used.

int **gsl_deriv_forward**(const *gsl_function* *f, double x, double h, double *result, double *abserr)

This function computes the numerical derivative of the function `f` at the point `x` using an adaptive forward difference algorithm with a step-size of `h`. The function is evaluated only at points greater than `x`, and never at `x` itself. The derivative is returned in `result` and an estimate of its absolute error is returned in `abserr`. This function should be used if $f(x)$ has a discontinuity at `x`, or is undefined for values less than `x`.

The initial value of `h` is used to estimate an optimal step-size, based on the scaling of the truncation error and round-off error in the derivative calculation. The derivative at x is computed using an "open" 4-point rule for equally spaced abscissae at $x + h/4$, $x + h/2$, $x + 3h/4$, $x + h$, with an error estimate taken from the difference between the 4-point rule and the corresponding 2-point rule $x + h/2$, $x + h$.

int **gsl_deriv_backward**(const *gsl_function* *f, double x, double h, double *result, double *abserr)

This function computes the numerical derivative of the function `f` at the point `x` using an adaptive backward difference algorithm with a step-size of `h`. The function is evaluated only at points less than `x`, and never at `x` itself. The derivative is returned in `result` and an estimate of its absolute error is returned in `abserr`. This function should be used if $f(x)$ has a discontinuity at `x`, or is undefined for values greater than `x`.

This function is equivalent to calling `gsl_deriv_forward()` with a negative step-size.

31.2 Examples

The following code estimates the derivative of the function $f(x) = x^{3/2}$ at $x = 2$ and at $x = 0$. The function $f(x)$ is undefined for $x < 0$ so the derivative at $x = 0$ is computed using *gsl_deriv_forward()*.

```
#include <stdio.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_deriv.h>

double f (double x, void * params)
{
  (void)(params); /* avoid unused parameter warning */
  return pow (x, 1.5);
}

int
main (void)
{
  gsl_function F;
  double result, abserr;

  F.function = &f;
  F.params = 0;

  printf ("f(x) = x^(3/2)\n");

  gsl_deriv_central (&F, 2.0, 1e-8, &result, &abserr);
  printf ("x = 2.0\n");
  printf ("f'(x) = %.10f +/- %.10f\n", result, abserr);
  printf ("exact = %.10f\n\n", 1.5 * sqrt(2.0));

  gsl_deriv_forward (&F, 0.0, 1e-8, &result, &abserr);
  printf ("x = 0.0\n");
  printf ("f'(x) = %.10f +/- %.10f\n", result, abserr);
  printf ("exact = %.10f\n", 0.0);

  return 0;
}
```

Here is the output of the program,

```
f(x) = x^(3/2)
x = 2.0
f'(x) = 2.1213203120 +/- 0.0000005006
exact = 2.1213203436

x = 0.0
f'(x) = 0.0000000160 +/- 0.0000000339
exact = 0.0000000000
```

31.3 References and Further Reading

The algorithms used by these functions are described in the following sources:

- Abramowitz and Stegun, *Handbook of Mathematical Functions*, Section 25.3.4, and Table 25.5 (Coefficients for Differentiation).
- S.D. Conte and Carl de Boor, *Elementary Numerical Analysis: An Algorithmic Approach*, McGraw-Hill, 1972.

CHAPTER

THIRTYTWO

CHEBYSHEV APPROXIMATIONS

This chapter describes routines for computing Chebyshev approximations to univariate functions. A Chebyshev approximation is a truncation of the series $f(x) = \sum c_n T_n(x)$, where the Chebyshev polynomials $T_n(x) = \cos(n \arccos x)$ provide an orthogonal basis of polynomials on the interval $[-1, 1]$ with the weight function $1/\sqrt{1-x^2}$. The first few Chebyshev polynomials are, $T_0(x) = 1$, $T_1(x) = x$, $T_2(x) = 2x^2 - 1$. For further information see Abramowitz & Stegun, Chapter 22.

The functions described in this chapter are declared in the header file `gsl_chebyshev.h`.

32.1 Definitions

type **gsl_cheb_series**

A Chebyshev series is stored using the following structure:

```
typedef struct
{
  double * c;   /* coefficients  c[0] .. c[order] */
  int order;    /* order of expansion             */
  double a;     /* lower interval point           */
  double b;     /* upper interval point           */
  ...
} gsl_cheb_series
```

The approximation is made over the range $[a, b]$ using `order` + 1 terms, including the coefficient $c[0]$. The series is computed using the following convention,

$$f(x) = \frac{c_0}{2} + \sum_{n=1} c_n T_n(x)$$

which is needed when accessing the coefficients directly.

32.2 Creation and Calculation of Chebyshev Series

gsl_cheb_series ***gsl_cheb_alloc**(const size_t n)

This function allocates space for a Chebyshev series of order `n` and returns a pointer to a new `gsl_cheb_series` struct.

void **gsl_cheb_free**(*gsl_cheb_series* *cs)

This function frees a previously allocated Chebyshev series `cs`.

int **gsl_cheb_init**(*gsl_cheb_series* *cs, const *gsl_function* *f, const double a, const double b)

This function computes the Chebyshev approximation `cs` for the function `f` over the range (a, b) to the previously specified order. The computation of the Chebyshev approximation is an $O(n^2)$ process, and requires n function evaluations.

32.3 Auxiliary Functions

The following functions provide information about an existing Chebyshev series.

size_t **gsl_cheb_order**(const *gsl_cheb_series* *cs)

This function returns the order of Chebyshev series `cs`.

size_t **gsl_cheb_size**(const *gsl_cheb_series* *cs)

double ***gsl_cheb_coeffs**(const *gsl_cheb_series* *cs)

These functions return the size of the Chebyshev coefficient array `c[]` and a pointer to its location in memory for the Chebyshev series `cs`.

32.4 Chebyshev Series Evaluation

double **gsl_cheb_eval**(const *gsl_cheb_series* *cs, double x)

This function evaluates the Chebyshev series `cs` at a given point `x`.

int **gsl_cheb_eval_err**(const *gsl_cheb_series* *cs, const double x, double *result, double *abserr)

This function computes the Chebyshev series `cs` at a given point `x`, estimating both the series `result` and its absolute error `abserr`. The error estimate is made from the first neglected term in the series.

double **gsl_cheb_eval_n**(const *gsl_cheb_series* *cs, size_t order, double x)

This function evaluates the Chebyshev series `cs` at a given point `x`, to (at most) the given order `order`.

int **gsl_cheb_eval_n_err**(const *gsl_cheb_series* *cs, const size_t order, const double x, double *result, double *abserr)

This function evaluates a Chebyshev series `cs` at a given point `x`, estimating both the series `result` and its absolute error `abserr`, to (at most) the given order `order`. The error estimate is made from the first neglected term in the series.

32.5 Derivatives and Integrals

The following functions allow a Chebyshev series to be differentiated or integrated, producing a new Chebyshev series. Note that the error estimate produced by evaluating the derivative series will be underestimated due to the contribution of higher order terms being neglected.

int **gsl_cheb_calc_deriv**(*gsl_cheb_series* *deriv, const *gsl_cheb_series* *cs)

This function computes the derivative of the series `cs`, storing the derivative coefficients in the previously allocated `deriv`. The two series `cs` and `deriv` must have been allocated with the same order.

int **gsl_cheb_calc_integ**(*gsl_cheb_series* *integ, const *gsl_cheb_series* *cs)

This function computes the integral of the series `cs`, storing the integral coefficients in the previously allocated `integ`. The two series `cs` and `integ` must have been allocated with the same order. The lower limit of the integration is taken to be the left hand end of the range `a`.

32.6 Examples

The following example program computes Chebyshev approximations to a step function. This is an extremely difficult approximation to make, due to the discontinuity, and was chosen as an example where approximation error is visible. For smooth functions the Chebyshev approximation converges extremely rapidly and errors would not be visible.

```
#include <stdio.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_chebyshev.h>

double
f (double x, void *p)
{
  (void)(p); /* avoid unused parameter warning */

  if (x < 0.5)
    return 0.25;
  else
    return 0.75;
}

int
main (void)
{
  int i, n = 10000;

  gsl_cheb_series *cs = gsl_cheb_alloc (40);

  gsl_function F;

  F.function = f;
  F.params = 0;

  gsl_cheb_init (cs, &F, 0.0, 1.0);

  for (i = 0; i < n; i++)
    {
      double x = i / (double)n;
      double r10 = gsl_cheb_eval_n (cs, 10, x);
      double r40 = gsl_cheb_eval (cs, x);
      printf ("%g %g %g %g\n",
              x, GSL_FN_EVAL (&F, x), r10, r40);
    }

  gsl_cheb_free (cs);

  return 0;
}
```

Fig. 32.1 shows output from the program with the original function, 10-th order approximation and 40-th order approximation, all sampled at intervals of 0.001 in x.

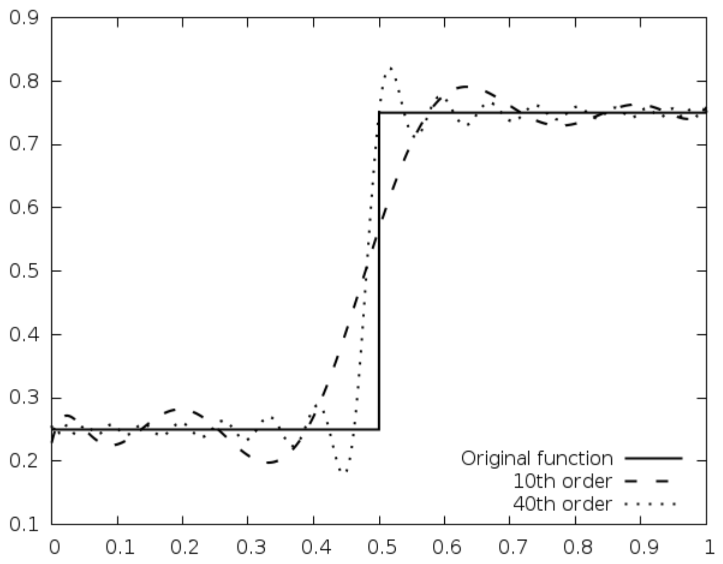

Fig. 32.1: Chebyshev approximations to a step function

32.7 References and Further Reading

The following paper describes the use of Chebyshev series,

- R. Broucke, "Ten Subroutines for the Manipulation of Chebyshev Series [C1] (Algorithm 446)". *Communications of the ACM* 16(4), 254–256 (1973)

CHAPTER

THIRTYTHREE

SERIES ACCELERATION

The functions described in this chapter accelerate the convergence of a series using the Levin u-transform. This method takes a small number of terms from the start of a series and uses a systematic approximation to compute an extrapolated value and an estimate of its error. The u-transform works for both convergent and divergent series, including asymptotic series.

These functions are declared in the header file `gsl_sum.h`.

33.1 Acceleration functions

The following functions compute the full Levin u-transform of a series with its error estimate. The error estimate is computed by propagating rounding errors from each term through to the final extrapolation.

These functions are intended for summing analytic series where each term is known to high accuracy, and the rounding errors are assumed to originate from finite precision. They are taken to be relative errors of order `GSL_DBL_EPSILON` for each term.

The calculation of the error in the extrapolated value is an $O(N^2)$ process, which is expensive in time and memory. A faster but less reliable method which estimates the error from the convergence of the extrapolated value is described in the next section. For the method described here a full table of intermediate values and derivatives through to $O(N)$ must be computed and stored, but this does give a reliable error estimate.

type **gsl_sum_levin_u_workspace**

Workspace for a Leven u-transform.

gsl_sum_levin_u_workspace ***gsl_sum_levin_u_alloc**(size_t n)

This function allocates a workspace for a Levin u-transform of `n` terms. The size of the workspace is $O(2n^2+3n)$.

void **gsl_sum_levin_u_free**(*gsl_sum_levin_u_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **gsl_sum_levin_u_accel**(const double *array, size_t array_size, *gsl_sum_levin_u_workspace* *w, double *sum_accel, double *abserr)

This function takes the terms of a series in `array` of size `array_size` and computes the extrapolated limit of the series using a Levin u-transform. Additional working space must be provided in `w`. The extrapolated sum is stored in `sum_accel`, with an estimate of the absolute error stored in `abserr`. The actual term-by-term sum is returned in `w->sum_plain`. The algorithm calculates the truncation error (the difference between two successive extrapolations) and round-off error (propagated from the individual terms) to choose an optimal number of terms for the extrapolation. All the terms of the series passed in through `array` should be non-zero.

33.2 Acceleration functions without error estimation

The functions described in this section compute the Levin u-transform of series and attempt to estimate the error from the "truncation error" in the extrapolation, the difference between the final two approximations. Using this method avoids the need to compute an intermediate table of derivatives because the error is estimated from the behavior of the extrapolated value itself. Consequently this algorithm is an $O(N)$ process and only requires $O(N)$ terms of storage. If the series converges sufficiently fast then this procedure can be acceptable. It is appropriate to use this method when there is a need to compute many extrapolations of series with similar convergence properties at high-speed. For example, when numerically integrating a function defined by a parameterized series where the parameter varies only slightly. A reliable error estimate should be computed first using the full algorithm described above in order to verify the consistency of the results.

type **`gsl_sum_levin_utrunc_workspace`**

Workspace for a Levin u-transform without error estimation

gsl_sum_levin_utrunc_workspace ***`gsl_sum_levin_utrunc_alloc`**(size_t n)

This function allocates a workspace for a Levin u-transform of `n` terms, without error estimation. The size of the workspace is $O(3n)$.

void **`gsl_sum_levin_utrunc_free`**(*gsl_sum_levin_utrunc_workspace* *w)

This function frees the memory associated with the workspace `w`.

int **`gsl_sum_levin_utrunc_accel`**(const double *array, size_t array_size, *gsl_sum_levin_utrunc_workspace* *w, double *sum_accel, double *abserr_trunc)

This function takes the terms of a series in `array` of size `array_size` and computes the extrapolated limit of the series using a Levin u-transform. Additional working space must be provided in `w`. The extrapolated sum is stored in `sum_accel`. The actual term-by-term sum is returned in `w->sum_plain`. The algorithm terminates when the difference between two successive extrapolations reaches a minimum or is sufficiently small. The difference between these two values is used as estimate of the error and is stored in `abserr_trunc`. To improve the reliability of the algorithm the extrapolated values are replaced by moving averages when calculating the truncation error, smoothing out any fluctuations.

33.3 Examples

The following code calculates an estimate of $\zeta(2) = \pi^2/6$ using the series,

$$\zeta(2) = 1 + 1/2^2 + 1/3^2 + 1/4^2 + \dots$$

After `N` terms the error in the sum is $O(1/N)$, making direct summation of the series converge slowly.

```
#include <stdio.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_sum.h>

#define N 20

int
main (void)
{
  double t[N];
  double sum_accel, err;
  double sum = 0;
  int n;
```

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```
  gsl_sum_levin_u_workspace * w
    = gsl_sum_levin_u_alloc (N);

  const double zeta_2 = M_PI * M_PI / 6.0;

  /* terms for zeta(2) = \sum_{n=1}^{\infty} 1/n^2 */

  for (n = 0; n < N; n++)
    {
      double np1 = n + 1.0;
      t[n] = 1.0 / (np1 * np1);
      sum += t[n];
    }

  gsl_sum_levin_u_accel (t, N, w, &sum_accel, &err);

  printf ("term-by-term sum = % .16f using %d terms\n",
          sum, N);

  printf ("term-by-term sum = % .16f using %zu terms\n",
          w->sum_plain, w->terms_used);

  printf ("exact value      = % .16f\n", zeta_2);
  printf ("accelerated sum  = % .16f using %zu terms\n",
          sum_accel, w->terms_used);

  printf ("estimated error  = % .16f\n", err);
  printf ("actual error     = % .16f\n",
          sum_accel - zeta_2);

  gsl_sum_levin_u_free (w);
  return 0;
}
```

The output below shows that the Levin u-transform is able to obtain an estimate of the sum to 1 part in 10^{10} using the first eleven terms of the series. The error estimate returned by the function is also accurate, giving the correct number of significant digits.

```
term-by-term sum =  1.5961632439130233 using 20 terms
term-by-term sum =  1.5759958390005426 using 13 terms
exact value      =  1.6449340668482264
accelerated sum  =  1.6449340669228176 using 13 terms
estimated error  =  0.0000000000888360
actual error     =  0.0000000000745912
```

Note that a direct summation of this series would require 10^{10} terms to achieve the same precision as the accelerated sum does in 13 terms.

33.4 References and Further Reading

The algorithms used by these functions are described in the following papers,

- T. Fessler, W.F. Ford, D.A. Smith, HURRY: An acceleration algorithm for scalar sequences and series *ACM Transactions on Mathematical Software*, 9(3):346–354, 1983. and Algorithm 602 9(3):355–357, 1983.

The theory of the u-transform was presented by Levin,

- D. Levin, Development of Non-Linear Transformations for Improving Convergence of Sequences, *Intern.: J.: Computer Math.* B3:371–388, 1973.

A review paper on the Levin Transform is available online,

- Herbert H. H. Homeier, Scalar Levin-Type Sequence Transformations, http://arxiv.org/abs/math/0005209

CHAPTER

THIRTYFOUR

WAVELET TRANSFORMS

This chapter describes functions for performing Discrete Wavelet Transforms (DWTs). The library includes wavelets for real data in both one and two dimensions. The wavelet functions are declared in the header files `gsl_wavelet.h` and `gsl_wavelet2d.h`.

34.1 Definitions

The continuous wavelet transform and its inverse are defined by the relations,

$$w(s,\tau) = \int_{-\infty}^{\infty} f(t) * \psi^*_{s,\tau}(t) dt$$

and,

$$f(t) = \int_0^{\infty} ds \int_{-\infty}^{\infty} w(s,\tau) * \psi_{s,\tau}(t) d\tau$$

where the basis functions $\psi_{s,\tau}$ are obtained by scaling and translation from a single function, referred to as the *mother wavelet*.

The discrete version of the wavelet transform acts on equally-spaced samples, with fixed scaling and translation steps (s, τ). The frequency and time axes are sampled *dyadically* on scales of 2^j through a level parameter j.

The resulting family of functions $\{\psi_{j,n}\}$ constitutes an orthonormal basis for square-integrable signals. The discrete wavelet transform is an $O(N)$ algorithm, and is also referred to as the *fast wavelet transform*.

34.2 Initialization

type **`gsl_wavelet`**

This structure contains the filter coefficients defining the wavelet and any associated offset parameters.

gsl_wavelet ***`gsl_wavelet_alloc`**(const *gsl_wavelet_type* *T, size_t k)

This function allocates and initializes a wavelet object of type *`T`*. The parameter *`k`* selects the specific member of the wavelet family. A null pointer is returned if insufficient memory is available or if a unsupported member is selected.

The following wavelet types are implemented:

type **`gsl_wavelet_type`**

gsl_wavelet_type ***`gsl_wavelet_daubechies`**

gsl_wavelet_type ***gsl_wavelet_daubechies_centered***
: This is the Daubechies wavelet family of maximum phase with $k/2$ vanishing moments. The implemented wavelets are $k = 4, 6, \ldots, 20$, with k even.

gsl_wavelet_type ***gsl_wavelet_haar***

gsl_wavelet_type ***gsl_wavelet_haar_centered***
: This is the Haar wavelet. The only valid choice of k for the Haar wavelet is $k = 2$.

gsl_wavelet_type ***gsl_wavelet_bspline***

gsl_wavelet_type ***gsl_wavelet_bspline_centered***
: This is the biorthogonal B-spline wavelet family of order (i, j). The implemented values of $k = 100 * i + j$ are 103, 105, 202, 204, 206, 208, 301, 303, 305 307, 309.

The centered forms of the wavelets align the coefficients of the various sub-bands on edges. Thus the resulting visualization of the coefficients of the wavelet transform in the phase plane is easier to understand.

const char ***gsl_wavelet_name**(const *gsl_wavelet* *w)
: This function returns a pointer to the name of the wavelet family for *w*.

void **gsl_wavelet_free**(*gsl_wavelet* *w)
: This function frees the wavelet object *w*.

type **gsl_wavelet_workspace**
: This structure contains scratch space of the same size as the input data and is used to hold intermediate results during the transform.

gsl_wavelet_workspace ***gsl_wavelet_workspace_alloc**(size_t n)
: This function allocates a workspace for the discrete wavelet transform. To perform a one-dimensional transform on *n* elements, a workspace of size *n* must be provided. For two-dimensional transforms of *n*-by-*n* matrices it is sufficient to allocate a workspace of size *n*, since the transform operates on individual rows and columns. A null pointer is returned if insufficient memory is available.

void **gsl_wavelet_workspace_free**(*gsl_wavelet_workspace* *work)
: This function frees the allocated workspace *work*.

34.3 Transform Functions

This sections describes the actual functions performing the discrete wavelet transform. Note that the transforms use periodic boundary conditions. If the signal is not periodic in the sample length then spurious coefficients will appear at the beginning and end of each level of the transform.

34.3.1 Wavelet transforms in one dimension

int **gsl_wavelet_transform**(const *gsl_wavelet* *w, double *data, size_t stride, size_t n, gsl_wavelet_direction dir, *gsl_wavelet_workspace* *work)

int **gsl_wavelet_transform_forward**(const *gsl_wavelet* *w, double *data, size_t stride, size_t n, *gsl_wavelet_workspace* *work)

int **gsl_wavelet_transform_inverse**(const *gsl_wavelet* *w, double *data, size_t stride, size_t n, *gsl_wavelet_workspace* *work)
: These functions compute in-place forward and inverse discrete wavelet transforms of length *n* with stride *stride* on the array *data*. The length of the transform *n* is restricted to powers of two. For the `transform` version of the function the argument `dir` can be either `forward` $(+1)$ or `backward` (-1). A workspace *work* of length *n* must be provided.

For the forward transform, the elements of the original array are replaced by the discrete wavelet transform $f_i \rightarrow w_{j,k}$ in a packed triangular storage layout, where `j` is the index of the level $j = 0 \dots J-1$ and `k` is the index of the coefficient within each level, $k = 0 \dots 2^j - 1$. The total number of levels is $J = \log_2(n)$. The output data has the following form,

$$(s_{-1,0}, d_{0,0}, d_{1,0}, d_{1,1}, d_{2,0}, \cdots, d_{j,k}, \cdots, d_{J-1,2^{J-1}-1})$$

where the first element is the smoothing coefficient $s_{-1,0}$, followed by the detail coefficients $d_{j,k}$ for each level j. The backward transform inverts these coefficients to obtain the original data.

These functions return a status of `GSL_SUCCESS` upon successful completion. *`GSL_EINVAL`* is returned if *`n`* is not an integer power of 2 or if insufficient workspace is provided.

34.3.2 Wavelet transforms in two dimension

The library provides functions to perform two-dimensional discrete wavelet transforms on square matrices. The matrix dimensions must be an integer power of two. There are two possible orderings of the rows and columns in the two-dimensional wavelet transform, referred to as the "standard" and "non-standard" forms.

The "standard" transform performs a complete discrete wavelet transform on the rows of the matrix, followed by a separate complete discrete wavelet transform on the columns of the resulting row-transformed matrix. This procedure uses the same ordering as a two-dimensional Fourier transform.

The "non-standard" transform is performed in interleaved passes on the rows and columns of the matrix for each level of the transform. The first level of the transform is applied to the matrix rows, and then to the matrix columns. This procedure is then repeated across the rows and columns of the data for the subsequent levels of the transform, until the full discrete wavelet transform is complete. The non-standard form of the discrete wavelet transform is typically used in image analysis.

The functions described in this section are declared in the header file `gsl_wavelet2d.h`.

int **`gsl_wavelet2d_transform`**(const *gsl_wavelet* *w, double *data, size_t tda, size_t size1, size_t size2, gsl_wavelet_direction dir, *gsl_wavelet_workspace* *work)

int **`gsl_wavelet2d_transform_forward`**(const *gsl_wavelet* *w, double *data, size_t tda, size_t size1, size_t size2, *gsl_wavelet_workspace* *work)

int **`gsl_wavelet2d_transform_inverse`**(const *gsl_wavelet* *w, double *data, size_t tda, size_t size1, size_t size2, *gsl_wavelet_workspace* *work)

These functions compute two-dimensional in-place forward and inverse discrete wavelet transforms in standard form on the array *`data`* stored in row-major form with dimensions *`size1`* and *`size2`* and physical row length *`tda`*. The dimensions must be equal (square matrix) and are restricted to powers of two. For the `transform` version of the function the argument `dir` can be either `forward` ($+1$) or `backward` (-1). A workspace *`work`* of the appropriate size must be provided. On exit, the appropriate elements of the array *`data`* are replaced by their two-dimensional wavelet transform.

The functions return a status of `GSL_SUCCESS` upon successful completion. *`GSL_EINVAL`* is returned if *`size1`* and *`size2`* are not equal and integer powers of 2, or if insufficient workspace is provided.

int **`gsl_wavelet2d_transform_matrix`**(const *gsl_wavelet* *w, *gsl_matrix* *m, gsl_wavelet_direction dir, *gsl_wavelet_workspace* *work)

int **`gsl_wavelet2d_transform_matrix_forward`**(const *gsl_wavelet* *w, *gsl_matrix* *m, *gsl_wavelet_workspace* *work) int **gsl_wavelet2d_transform_matrix_inverse**(const *gsl_wavelet* *w, *gsl_matrix* *m, *gsl_wavelet_workspace* *work)

These functions compute the two-dimensional in-place wavelet transform on a matrix `m`.

int **gsl_wavelet2d_nstransform**(const *gsl_wavelet* *w, double *data, size_t tda, size_t size1, size_t size2, gsl_wavelet_direction dir, *gsl_wavelet_workspace* *work)

int **gsl_wavelet2d_nstransform_forward**(const *gsl_wavelet* *w, double *data, size_t tda, size_t size1, size_t size2, *gsl_wavelet_workspace* *work)

int **gsl_wavelet2d_nstransform_inverse**(const *gsl_wavelet* *w, double *data, size_t tda, size_t size1, size_t size2, *gsl_wavelet_workspace* *work)

These functions compute the two-dimensional wavelet transform in non-standard form.

int **gsl_wavelet2d_nstransform_matrix**(const *gsl_wavelet* *w, *gsl_matrix* *m, gsl_wavelet_direction dir, *gsl_wavelet_workspace* *work)

int **gsl_wavelet2d_nstransform_matrix_forward**(const *gsl_wavelet* *w, *gsl_matrix* *m, *gsl_wavelet_workspace* *work)

int **gsl_wavelet2d_nstransform_matrix_inverse**(const *gsl_wavelet* *w, *gsl_matrix* *m, *gsl_wavelet_workspace* *work)

These functions compute the non-standard form of the two-dimensional in-place wavelet transform on a matrix `m`.

34.4 Examples

The following program demonstrates the use of the one-dimensional wavelet transform functions. It computes an approximation to an input signal (of length 256) using the 20 largest components of the wavelet transform, while setting the others to zero.

```
#include <stdio.h>
#include <math.h>
#include <gsl/gsl_sort.h>
#include <gsl/gsl_wavelet.h>

int
main (int argc, char **argv)
{
  (void)(argc); /* avoid unused parameter warning */
  int i, n = 256, nc = 20;
  double *orig_data = malloc (n * sizeof (double));
  double *data = malloc (n * sizeof (double));
  double *abscoeff = malloc (n * sizeof (double));
  size_t *p = malloc (n * sizeof (size_t));

  FILE * f;
  gsl_wavelet *w;
  gsl_wavelet_workspace *work;

  w = gsl_wavelet_alloc (gsl_wavelet_daubechies, 4);
  work = gsl_wavelet_workspace_alloc (n);
```

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```
  f = fopen (argv[1], "r");
  for (i = 0; i < n; i++)
    {
      fscanf (f, "%lg", &orig_data[i]);
      data[i] = orig_data[i];
    }
  fclose (f);

  gsl_wavelet_transform_forward (w, data, 1, n, work);

  for (i = 0; i < n; i++)
    {
      abscoeff[i] = fabs (data[i]);
    }

  gsl_sort_index (p, abscoeff, 1, n);

  for (i = 0; (i + nc) < n; i++)
    data[p[i]] = 0;

  gsl_wavelet_transform_inverse (w, data, 1, n, work);

  for (i = 0; i < n; i++)
    {
      printf ("%g %g\n", orig_data[i], data[i]);
    }

  gsl_wavelet_free (w);
  gsl_wavelet_workspace_free (work);

  free (data);
  free (orig_data);
  free (abscoeff);
  free (p);
  return 0;
}
```

The output can be used with the GNU plotutils `graph` program:

```
$ ./a.out ecg.dat > dwt.txt
$ graph -T ps -x 0 256 32 -h 0.3 -a dwt.txt > dwt.ps
```

Fig. 34.1 shows an original and compressed version of a sample ECG recording from the MIT-BIH Arrhythmia Database, part of the PhysioNet archive of public-domain of medical datasets.

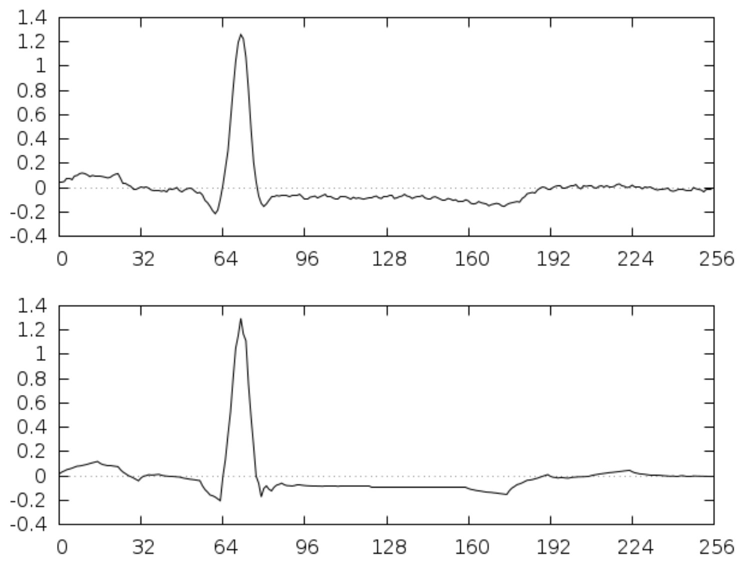

Fig. 34.1: Original (upper) and wavelet-compressed (lower) ECG signals, using the 20 largest components of the Daubechies(4) discrete wavelet transform.

34.5 References and Further Reading

The mathematical background to wavelet transforms is covered in the original lectures by Daubechies,

- Ingrid Daubechies. Ten Lectures on Wavelets. *CBMS-NSF Regional Conference Series in Applied Mathematics* (1992), SIAM, ISBN 0898712742.

An easy to read introduction to the subject with an emphasis on the application of the wavelet transform in various branches of science is,

- Paul S. Addison. *The Illustrated Wavelet Transform Handbook*. Institute of Physics Publishing (2002), ISBN 0750306920.

For extensive coverage of signal analysis by wavelets, wavelet packets and local cosine bases see,

- S. G. Mallat. *A wavelet tour of signal processing* (Second edition). Academic Press (1999), ISBN 012466606X.

The concept of multiresolution analysis underlying the wavelet transform is described in,

- S. G. Mallat. Multiresolution Approximations and Wavelet Orthonormal Bases of L^2(R). *Transactions of the American Mathematical Society*, 315(1), 1989, 69–87.
- S. G. Mallat. A Theory for Multiresolution Signal Decomposition—The Wavelet Representation. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 11, 1989, 674–693.

The coefficients for the individual wavelet families implemented by the library can be found in the following papers,

- I. Daubechies. Orthonormal Bases of Compactly Supported Wavelets. *Communications on Pure and Applied Mathematics*, 41 (1988) 909–996.
- A. Cohen, I. Daubechies, and J.-C. Feauveau. Biorthogonal Bases of Compactly Supported Wavelets. *Communications on Pure and Applied Mathematics*, 45 (1992) 485–560.

The PhysioNet archive of physiological datasets can be found online at http://www.physionet.org/ and is described in the following paper,

- Goldberger et al. PhysioBank, PhysioToolkit, and PhysioNet: Components of a New Research Resource for Complex Physiologic Signals. *Circulation* 101(23):e215-e220 2000.

CHAPTER

THIRTYFIVE

DISCRETE HANKEL TRANSFORMS

This chapter describes functions for performing Discrete Hankel Transforms (DHTs). The functions are declared in the header file `gsl_dht.h`.

35.1 Definitions

The discrete Hankel transform acts on a vector of sampled data, where the samples are assumed to have been taken at points related to the zeros of a Bessel function of fixed order; compare this to the case of the discrete Fourier transform, where samples are taken at points related to the zeroes of the sine or cosine function.

Starting with its definition, the Hankel transform (or Bessel transform) of order ν of a function f with $\nu > -1/2$ is defined as (see Johnson, 1987 and Lemoine, 1994)

$$F_\nu(u) = \int_0^\infty f(t) J_\nu(ut) t dt$$

If the integral exists, F_ν is called the Hankel transformation of f. The reverse transform is given by

$$f(t) = \int_0^\infty F_\nu(u) J_\nu(ut) u du$$

where $\int_0^\infty f(t) t^{1/2} dt$ must exist and be absolutely convergent, and where $f(t)$ satisfies Dirichlet's conditions (of limited total fluctuations) in the interval $[0, \infty]$.

Now the discrete Hankel transform works on a discrete function f, which is sampled on points $n = 1...M$ located at positions $t_n = (j_{\nu,n}/j_{\nu,M}) X$ in real space and at $u_n = j_{\nu,n}/X$ in reciprocal space. Here, $j_{\nu,m}$ are the m-th zeros of the Bessel function $J_\nu(x)$ arranged in ascending order. Moreover, the discrete functions are assumed to be band limited, so $f(t_n) = 0$ and $F(u_n) = 0$ for $n > M$. Accordingly, the function f is defined on the interval $[0, X]$.

Following the work of Johnson, 1987 and Lemoine, 1994, the discrete Hankel transform is given by

$$F_\nu(u_m) = \frac{2X^2}{j_{\nu,M}^2} \sum_{k=1}^{M-1} f\left(\frac{j_{\nu,k} X}{j_{\nu,M}}\right) \frac{J_\nu(j_{\nu,m} j_{\nu,k}/j_{\nu,M})}{J_{\nu+1}(j_{\nu,k})^2}.$$

It is this discrete expression which defines the discrete Hankel transform calculated by GSL. In GSL, forward and backward transforms are defined equally and calculate $F_\nu(u_m)$. Following Johnson, the backward transform reads

$$f(t_k) = \frac{2}{X^2} \sum_{m=1}^{M-1} F\left(\frac{j_{\nu,m}}{X}\right) \frac{J_\nu(j_{\nu,m} j_{\nu,k}/j_{\nu,M})}{J_{\nu+1}(j_{\nu,m})^2}.$$

Obviously, using the forward transform instead of the backward transform gives an additional factor $X^4/j_{\nu,M}^2 = t_m^2/u_m^2$.

The kernel in the summation above defines the matrix of the ν-Hankel transform of size $M-1$. The coefficients of this matrix, being dependent on ν and M, must be precomputed and stored; the `gsl_dht` object encapsulates this data. The allocation function `gsl_dht_alloc()` returns a `gsl_dht` object which must be properly initialized with `gsl_dht_init()` before it can be used to perform transforms on data sample vectors, for fixed ν and M, using the `gsl_dht_apply()` function. The implementation allows to define the length X of the fundamental interval, for convenience, while discrete Hankel transforms are often defined on the unit interval instead of $[0, X]$.

Notice that by assumption $f(t)$ vanishes at the endpoints of the interval, consistent with the inversion formula and the sampling formula given above. Therefore, this transform corresponds to an orthogonal expansion in eigenfunctions of the Dirichlet problem for the Bessel differential equation.

35.2 Functions

type **`gsl_dht`**

Workspace for computing discrete Hankel transforms

gsl_dht ***`gsl_dht_alloc`**(size_t size)

This function allocates a Discrete Hankel transform object of size `size`.

int **`gsl_dht_init`**(*gsl_dht* *t, double nu, double xmax)

This function initializes the transform `t` for the given values of `nu` and `xmax`.

gsl_dht ***`gsl_dht_new`**(size_t size, double nu, double xmax)

This function allocates a Discrete Hankel transform object of size `size` and initializes it for the given values of `nu` and `xmax`.

void **`gsl_dht_free`**(*gsl_dht* *t)

This function frees the transform `t`.

int **`gsl_dht_apply`**(const *gsl_dht* *t, double *f_in, double *f_out)

This function applies the transform `t` to the array `f_in` whose size is equal to the size of the transform. The result is stored in the array `f_out` which must be of the same length.

Applying this function to its output gives the original data multiplied by $(X^2/j_{\nu,M})^2$, up to numerical errors.

double **`gsl_dht_x_sample`**(const *gsl_dht* *t, int n)

This function returns the value of the `n`-th sample point in the unit interval, $(j_{\nu,n+1}/j_{\nu,M})X$. These are the points where the function $f(t)$ is assumed to be sampled.

double **`gsl_dht_k_sample`**(const *gsl_dht* *t, int n)

This function returns the value of the `n`-th sample point in “k-space”, $j_{\nu,n+1}/X$.

35.3 References and Further Reading

The algorithms used by these functions are described in the following papers,

- H. Fisk Johnson, Comp.: Phys.: Comm.: 43, 181 (1987).
- D. Lemoine, J. Chem.: Phys.: 101, 3936 (1994).

CHAPTER

THIRTYSIX

ONE DIMENSIONAL ROOT-FINDING

This chapter describes routines for finding roots of arbitrary one-dimensional functions. The library provides low level components for a variety of iterative solvers and convergence tests. These can be combined by the user to achieve the desired solution, with full access to the intermediate steps of the iteration. Each class of methods uses the same framework, so that you can switch between solvers at runtime without needing to recompile your program. Each instance of a solver keeps track of its own state, allowing the solvers to be used in multi-threaded programs.

The header file `gsl_roots.h` contains prototypes for the root finding functions and related declarations.

36.1 Overview

One-dimensional root finding algorithms can be divided into two classes, *root bracketing* and *root polishing*. Algorithms which proceed by bracketing a root are guaranteed to converge. Bracketing algorithms begin with a bounded region known to contain a root. The size of this bounded region is reduced, iteratively, until it encloses the root to a desired tolerance. This provides a rigorous error estimate for the location of the root.

The technique of *root polishing* attempts to improve an initial guess to the root. These algorithms converge only if started "close enough" to a root, and sacrifice a rigorous error bound for speed. By approximating the behavior of a function in the vicinity of a root they attempt to find a higher order improvement of an initial guess. When the behavior of the function is compatible with the algorithm and a good initial guess is available a polishing algorithm can provide rapid convergence.

In GSL both types of algorithm are available in similar frameworks. The user provides a high-level driver for the algorithms, and the library provides the individual functions necessary for each of the steps. There are three main phases of the iteration. The steps are,

- initialize solver state, `s`, for algorithm `T`
- update `s` using the iteration `T`
- test `s` for convergence, and repeat iteration if necessary

The state for bracketing solvers is held in a *`gsl_root_fsolver`* struct. The updating procedure uses only function evaluations (not derivatives). The state for root polishing solvers is held in a *`gsl_root_fdfsolver`* struct. The updates require both the function and its derivative (hence the name `fdf`) to be supplied by the user.

36.2 Caveats

Note that root finding functions can only search for one root at a time. When there are several roots in the search area, the first root to be found will be returned; however it is difficult to predict which of the roots this will be. *In most cases, no error will be reported if you try to find a root in an area where there is more than one.*

Care must be taken when a function may have a multiple root (such as $f(x) = (x - x_0)^2$ or $f(x) = (x - x_0)^3$. It is not possible to use root-bracketing algorithms on even-multiplicity roots. For these algorithms the initial interval must contain a zero-crossing, where the function is negative at one end of the interval and positive at the other end. Roots with even-multiplicity do not cross zero, but only touch it instantaneously. Algorithms based on root bracketing will still work for odd-multiplicity roots (e.g. cubic, quintic, …). Root polishing algorithms generally work with higher multiplicity roots, but at a reduced rate of convergence. In these cases the *Steffenson algorithm* can be used to accelerate the convergence of multiple roots.

While it is not absolutely required that f have a root within the search region, numerical root finding functions should not be used haphazardly to check for the *existence* of roots. There are better ways to do this. Because it is easy to create situations where numerical root finders can fail, it is a bad idea to throw a root finder at a function you do not know much about. In general it is best to examine the function visually by plotting before searching for a root.

36.3 Initializing the Solver

type **gsl_root_fsolver**

This is a workspace for finding roots using methods which do not require derivatives.

type **gsl_root_fdfsolver**

This is a workspace for finding roots using methods which require derivatives.

gsl_root_fsolver ***gsl_root_fsolver_alloc**(const *gsl_root_fsolver_type* *T)

This function returns a pointer to a newly allocated instance of a solver of type *T*. For example, the following code creates an instance of a bisection solver:

```
const gsl_root_fsolver_type * T = gsl_root_fsolver_bisection;
gsl_root_fsolver * s = gsl_root_fsolver_alloc (T);
```

If there is insufficient memory to create the solver then the function returns a null pointer and the error handler is invoked with an error code of *GSL_ENOMEM*.

gsl_root_fdfsolver ***gsl_root_fdfsolver_alloc**(const *gsl_root_fdfsolver_type* *T)

This function returns a pointer to a newly allocated instance of a derivative-based solver of type *T*. For example, the following code creates an instance of a Newton-Raphson solver:

```
const gsl_root_fdfsolver_type * T = gsl_root_fdfsolver_newton;
gsl_root_fdfsolver * s = gsl_root_fdfsolver_alloc (T);
```

If there is insufficient memory to create the solver then the function returns a null pointer and the error handler is invoked with an error code of *GSL_ENOMEM*.

int **gsl_root_fsolver_set**(*gsl_root_fsolver* *s, *gsl_function* *f, double x_lower, double x_upper)

This function initializes, or reinitializes, an existing solver *s* to use the function *f* and the initial search interval [*x_lower*, *x_upper*].

int **gsl_root_fdfsolver_set**(*gsl_root_fdfsolver* *s, *gsl_function_fdf* *fdf, double root)

This function initializes, or reinitializes, an existing solver *s* to use the function and derivative *fdf* and the initial guess *root*.

void **gsl_root_fsolver_free**(*gsl_root_fsolver* *s)

void **gsl_root_fdfsolver_free**(*gsl_root_fdfsolver* *s)

These functions free all the memory associated with the solver `s`.

const char ***gsl_root_fsolver_name**(const *gsl_root_fsolver* *s)

const char ***gsl_root_fdfsolver_name**(const *gsl_root_fdfsolver* *s)

These functions return a pointer to the name of the solver. For example:

```
printf ("s is a '%s' solver\n", gsl_root_fsolver_name (s));
```

would print something like `s is a 'bisection' solver`.

36.4 Providing the function to solve

You must provide a continuous function of one variable for the root finders to operate on, and, sometimes, its first derivative. In order to allow for general parameters the functions are defined by the following data types:

type **gsl_function**

This data type defines a general function with parameters.

`double (* function) (double x, void * params)`

this function should return the value $f(x, params)$ for argument `x` and parameters `params`

`void * params`

a pointer to the parameters of the function

Here is an example for the general quadratic function,

$$f(x) = ax^2 + bx + c$$

with $a = 3$, $b = 2$, $c = 1$. The following code defines a `gsl_function` `F` which you could pass to a root finder as a function pointer:

```
struct my_f_params { double a; double b; double c; };

double
my_f (double x, void * p)
  {
    struct my_f_params * params = (struct my_f_params *)p;
    double a = (params->a);
    double b = (params->b);
    double c = (params->c);

    return  (a * x + b) * x + c;
  }

gsl_function F;
struct my_f_params params = { 3.0, 2.0, 1.0 };

F.function = &my_f;
F.params = &params;
```

The function $f(x)$ can be evaluated using the macro `GSL_FN_EVAL(&F,x)` defined in `gsl_math.h`.

type **`gsl_function_fdf`**

This data type defines a general function with parameters and its first derivative.

`double (* f) (double x, void * params)`

this function should return the value of $f(x, params)$ for argument `x` and parameters `params`

`double (* df) (double x, void * params)`

this function should return the value of the derivative of `f` with respect to `x`, $f'(x, params)$, for argument `x` and parameters `params`

`void (* fdf) (double x, void * params, double * f, double * df)`

this function should set the values of the function `f` to $f(x, params)$ and its derivative `df` to $f'(x, params)$ for argument `x` and parameters `params`. This function provides an optimization of the separate functions for $f(x)$ and $f'(x)$—it is always faster to compute the function and its derivative at the same time.

`void * params`

a pointer to the parameters of the function

Here is an example where $f(x) = \exp(2x)$:

```
double
my_f (double x, void * params)
{
   return exp (2 * x);
}

double
my_df (double x, void * params)
{
   return 2 * exp (2 * x);
}

void
my_fdf (double x, void * params,
        double * f, double * df)
{
   double t = exp (2 * x);

   *f = t;
   *df = 2 * t;   /* uses existing value */
}

gsl_function_fdf FDF;

FDF.f = &my_f;
FDF.df = &my_df;
FDF.fdf = &my_fdf;
FDF.params = 0;
```

The function $f(x)$ can be evaluated using the macro `GSL_FN_FDF_EVAL_F(&FDF,x)` and the derivative $f'(x)$ can be evaluated using the macro `GSL_FN_FDF_EVAL_DF(&FDF,x)`. Both the function $y = f(x)$ and its derivative $dy = f'(x)$

can be evaluated at the same time using the macro `GSL_FN_FDF_EVAL_F_DF(&FDF,x,y,dy)`. The macro stores $f(x)$ in its `y` argument and $f'(x)$ in its `dy` argument—both of these should be pointers to `double`.

36.5 Search Bounds and Guesses

You provide either search bounds or an initial guess; this section explains how search bounds and guesses work and how function arguments control them.

A guess is simply an x value which is iterated until it is within the desired precision of a root. It takes the form of a `double`.

Search bounds are the endpoints of an interval which is iterated until the length of the interval is smaller than the requested precision. The interval is defined by two values, the lower limit and the upper limit. Whether the endpoints are intended to be included in the interval or not depends on the context in which the interval is used.

36.6 Iteration

The following functions drive the iteration of each algorithm. Each function performs one iteration to update the state of any solver of the corresponding type. The same functions work for all solvers so that different methods can be substituted at runtime without modifications to the code.

int **gsl_root_fsolver_iterate**(*gsl_root_fsolver* *s)

int **gsl_root_fdfsolver_iterate**(*gsl_root_fdfsolver* *s)

These functions perform a single iteration of the solver `s`. If the iteration encounters an unexpected problem then an error code will be returned,

`GSL_EBADFUNC`

the iteration encountered a singular point where the function or its derivative evaluated to `Inf` or `NaN`.

`GSL_EZERODIV`

the derivative of the function vanished at the iteration point, preventing the algorithm from continuing without a division by zero.

The solver maintains a current best estimate of the root at all times. The bracketing solvers also keep track of the current best interval bounding the root. This information can be accessed with the following auxiliary functions,

double **gsl_root_fsolver_root**(const *gsl_root_fsolver* *s)

double **gsl_root_fdfsolver_root**(const *gsl_root_fdfsolver* *s)

These functions return the current estimate of the root for the solver `s`.

double **gsl_root_fsolver_x_lower**(const *gsl_root_fsolver* *s)

double **gsl_root_fsolver_x_upper**(const *gsl_root_fsolver* *s)

These functions return the current bracketing interval for the solver `s`.

36.7 Search Stopping Parameters

A root finding procedure should stop when one of the following conditions is true:

- A root has been found to within the user-specified precision.
- A user-specified maximum number of iterations has been reached.
- An error has occurred.

The handling of these conditions is under user control. The functions below allow the user to test the precision of the current result in several standard ways.

int **gsl_root_test_interval**(double x_lower, double x_upper, double epsabs, double epsrel)

This function tests for the convergence of the interval [*x_lower*, *x_upper*] with absolute error *epsabs* and relative error *epsrel*. The test returns `GSL_SUCCESS` if the following condition is achieved,

$$|a - b| < \mathit{epsabs} + \mathit{epsrel}\ \min(|a|, |b|)$$

when the interval $x = [a, b]$ does not include the origin. If the interval includes the origin then $\min(|a|, |b|)$ is replaced by zero (which is the minimum value of $|x|$ over the interval). This ensures that the relative error is accurately estimated for roots close to the origin.

This condition on the interval also implies that any estimate of the root r in the interval satisfies the same condition with respect to the true root r^*,

$$|r - r^*| < \mathit{epsabs} + \mathit{epsrel}\, r^*$$

assuming that the true root r^* is contained within the interval.

int **gsl_root_test_delta**(double x1, double x0, double epsabs, double epsrel)

This function tests for the convergence of the sequence *x0*, *x1* with absolute error *epsabs* and relative error *epsrel*. The test returns `GSL_SUCCESS` if the following condition is achieved,

$$|x_1 - x_0| < \mathit{epsabs} + \mathit{epsrel}\,|x_1|$$

and returns `GSL_CONTINUE` otherwise.

int **gsl_root_test_residual**(double f, double epsabs)

This function tests the residual value *f* against the absolute error bound *epsabs*. The test returns `GSL_SUCCESS` if the following condition is achieved,

$$|f| < \mathit{epsabs}$$

and returns `GSL_CONTINUE` otherwise. This criterion is suitable for situations where the precise location of the root, x, is unimportant provided a value can be found where the residual, $|f(x)|$, is small enough.

36.8 Root Bracketing Algorithms

The root bracketing algorithms described in this section require an initial interval which is guaranteed to contain a root—if a and b are the endpoints of the interval then $f(a)$ must differ in sign from $f(b)$. This ensures that the function crosses zero at least once in the interval. If a valid initial interval is used then these algorithm cannot fail, provided the function is well-behaved.

Note that a bracketing algorithm cannot find roots of even degree, since these do not cross the x-axis.

type **gsl_root_fsolver_type**

gsl_root_fsolver_type ***gsl_root_fsolver_bisection**

The *bisection algorithm* is the simplest method of bracketing the roots of a function. It is the slowest algorithm provided by the library, with linear convergence.

On each iteration, the interval is bisected and the value of the function at the midpoint is calculated. The sign of this value is used to determine which half of the interval does not contain a root. That half is discarded to give a new, smaller interval containing the root. This procedure can be continued indefinitely until the interval is sufficiently small.

At any time the current estimate of the root is taken as the midpoint of the interval.

gsl_root_fsolver_type ***gsl_root_fsolver_falsepos**

The *false position algorithm* is a method of finding roots based on linear interpolation. Its convergence is linear, but it is usually faster than bisection.

On each iteration a line is drawn between the endpoints $(a, f(a))$ and $(b, f(b))$ and the point where this line crosses the x-axis taken as a "midpoint". The value of the function at this point is calculated and its sign is used to determine which side of the interval does not contain a root. That side is discarded to give a new, smaller interval containing the root. This procedure can be continued indefinitely until the interval is sufficiently small.

The best estimate of the root is taken from the linear interpolation of the interval on the current iteration.

gsl_root_fsolver_type ***gsl_root_fsolver_brent**

The *Brent-Dekker method* (referred to here as *Brent's method*) combines an interpolation strategy with the bisection algorithm. This produces a fast algorithm which is still robust.

On each iteration Brent's method approximates the function using an interpolating curve. On the first iteration this is a linear interpolation of the two endpoints. For subsequent iterations the algorithm uses an inverse quadratic fit to the last three points, for higher accuracy. The intercept of the interpolating curve with the x-axis is taken as a guess for the root. If it lies within the bounds of the current interval then the interpolating point is accepted, and used to generate a smaller interval. If the interpolating point is not accepted then the algorithm falls back to an ordinary bisection step.

The best estimate of the root is taken from the most recent interpolation or bisection.

36.9 Root Finding Algorithms using Derivatives

The root polishing algorithms described in this section require an initial guess for the location of the root. There is no absolute guarantee of convergence—the function must be suitable for this technique and the initial guess must be sufficiently close to the root for it to work. When these conditions are satisfied then convergence is quadratic.

These algorithms make use of both the function and its derivative.

type **gsl_root_fdfsolver_type**

gsl_root_fdfsolver_type ***gsl_root_fdfsolver_newton**

Newton's Method is the standard root-polishing algorithm. The algorithm begins with an initial guess for the location of the root. On each iteration, a line tangent to the function f is drawn at that position. The point where this line crosses the x-axis becomes the new guess. The iteration is defined by the following sequence,

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Newton's method converges quadratically for single roots, and linearly for multiple roots.

gsl_root_fdfsolver_type ***gsl_root_fdfsolver_secant***

The *secant method* is a simplified version of Newton's method which does not require the computation of the derivative on every step.

On its first iteration the algorithm begins with Newton's method, using the derivative to compute a first step,

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

Subsequent iterations avoid the evaluation of the derivative by replacing it with a numerical estimate, the slope of the line through the previous two points,

$$x_{i+1} = x_i - \frac{f(x_i)}{f'_{est}} \text{ where } f'_{est} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

When the derivative does not change significantly in the vicinity of the root the secant method gives a useful saving. Asymptotically the secant method is faster than Newton's method whenever the cost of evaluating the derivative is more than 0.44 times the cost of evaluating the function itself. As with all methods of computing a numerical derivative the estimate can suffer from cancellation errors if the separation of the points becomes too small.

On single roots, the method has a convergence of order $(1 + \sqrt{5})/2$ (approximately 1.62). It converges linearly for multiple roots.

gsl_root_fdfsolver_type ***gsl_root_fdfsolver_steffenson***

The *Steffenson Method*[1] provides the fastest convergence of all the routines. It combines the basic Newton algorithm with an Aitken "delta-squared" acceleration. If the Newton iterates are x_i then the acceleration procedure generates a new sequence R_i,

$$R_i = x_i - \frac{(x_{i+1} - x_i)^2}{(x_{i+2} - 2x_{i+1} + x_i)}$$

which converges faster than the original sequence under reasonable conditions. The new sequence requires three terms before it can produce its first value so the method returns accelerated values on the second and subsequent iterations. On the first iteration it returns the ordinary Newton estimate. The Newton iterate is also returned if the denominator of the acceleration term ever becomes zero.

As with all acceleration procedures this method can become unstable if the function is not well-behaved.

36.10 Examples

For any root finding algorithm we need to prepare the function to be solved. For this example we will use the general quadratic equation described earlier. We first need a header file (`demo_fn.h`) to define the function parameters,

```
struct quadratic_params
  {
    double a, b, c;
  };

double quadratic (double x, void *params);
double quadratic_deriv (double x, void *params);
void quadratic_fdf (double x, void *params,
                    double *y, double *dy);
```

[1] J.F. Steffensen (1873–1961). The spelling used in the name of the function is slightly incorrect, but has been preserved to avoid incompatibility.

We place the function definitions in a separate file (demo_fn.c),

```
double
quadratic (double x, void *params)
{
  struct quadratic_params *p
    = (struct quadratic_params *) params;

  double a = p->a;
  double b = p->b;
  double c = p->c;

  return (a * x + b) * x + c;
}

double
quadratic_deriv (double x, void *params)
{
  struct quadratic_params *p
    = (struct quadratic_params *) params;

  double a = p->a;
  double b = p->b;

  return 2.0 * a * x + b;
}

void
quadratic_fdf (double x, void *params,
               double *y, double *dy)
{
  struct quadratic_params *p
    = (struct quadratic_params *) params;

  double a = p->a;
  double b = p->b;
  double c = p->c;

  *y = (a * x + b) * x + c;
  *dy = 2.0 * a * x + b;
}
```

The first program uses the function solver gsl_root_fsolver_brent for Brent's method and the general quadratic defined above to solve the following equation,

$$x^2 - 5 = 0$$

with solution $x = \sqrt{5} = 2.236068...$

```
#include <stdio.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_roots.h>

```

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```
#include "demo_fn.h"
#include "demo_fn.c"

int
main (void)
{
  int status;
  int iter = 0, max_iter = 100;
  const gsl_root_fsolver_type *T;
  gsl_root_fsolver *s;
  double r = 0, r_expected = sqrt (5.0);
  double x_lo = 0.0, x_hi = 5.0;
  gsl_function F;
  struct quadratic_params params = {1.0, 0.0, -5.0};

  F.function = &quadratic;
  F.params = &params;

  T = gsl_root_fsolver_brent;
  s = gsl_root_fsolver_alloc (T);
  gsl_root_fsolver_set (s, &F, x_lo, x_hi);

  printf ("using %s method\n",
          gsl_root_fsolver_name (s));

  printf ("%5s [%9s, %9s] %9s %10s %9s\n",
          "iter", "lower", "upper", "root",
          "err", "err(est)");

  do
    {
      iter++;
      status = gsl_root_fsolver_iterate (s);
      r = gsl_root_fsolver_root (s);
      x_lo = gsl_root_fsolver_x_lower (s);
      x_hi = gsl_root_fsolver_x_upper (s);
      status = gsl_root_test_interval (x_lo, x_hi,
                                       0, 0.001);

      if (status == GSL_SUCCESS)
        printf ("Converged:\n");

      printf ("%5d [%.7f, %.7f] %.7f %+.7f %.7f\n",
              iter, x_lo, x_hi,
              r, r - r_expected,
              x_hi - x_lo);
    }
  while (status == GSL_CONTINUE && iter < max_iter);

  gsl_root_fsolver_free (s);

  return status;
```

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```
}
```

Here are the results of the iterations:

```
$ ./a.out
using brent method
 iter [    lower,      upper]       root         err  err(est)
    1 [1.0000000, 5.0000000] 1.0000000 -1.2360680 4.0000000
    2 [1.0000000, 3.0000000] 3.0000000 +0.7639320 2.0000000
    3 [2.0000000, 3.0000000] 2.0000000 -0.2360680 1.0000000
    4 [2.2000000, 3.0000000] 2.2000000 -0.0360680 0.8000000
    5 [2.2000000, 2.2366300] 2.2366300 +0.0005621 0.0366300
Converged:
    6 [2.2360634, 2.2366300] 2.2360634 -0.0000046 0.0005666
```

If the program is modified to use the bisection solver instead of Brent's method, by changing `gsl_root_fsolver_brent` to `gsl_root_fsolver_bisection` the slower convergence of the Bisection method can be observed:

```
$ ./a.out
using bisection method
 iter [    lower,      upper]       root         err  err(est)
    1 [0.0000000, 2.5000000] 1.2500000 -0.9860680 2.5000000
    2 [1.2500000, 2.5000000] 1.8750000 -0.3610680 1.2500000
    3 [1.8750000, 2.5000000] 2.1875000 -0.0485680 0.6250000
    4 [2.1875000, 2.5000000] 2.3437500 +0.1076820 0.3125000
    5 [2.1875000, 2.3437500] 2.2656250 +0.0295570 0.1562500
    6 [2.1875000, 2.2656250] 2.2265625 -0.0095055 0.0781250
    7 [2.2265625, 2.2656250] 2.2460938 +0.0100258 0.0390625
    8 [2.2265625, 2.2460938] 2.2363281 +0.0002601 0.0195312
    9 [2.2265625, 2.2363281] 2.2314453 -0.0046227 0.0097656
   10 [2.2314453, 2.2363281] 2.2338867 -0.0021813 0.0048828
   11 [2.2338867, 2.2363281] 2.2351074 -0.0009606 0.0024414
Converged:
   12 [2.2351074, 2.2363281] 2.2357178 -0.0003502 0.0012207
```

The next program solves the same function using a derivative solver instead.

```
#include <stdio.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_roots.h>

#include "demo_fn.h"
#include "demo_fn.c"

int
main (void)
{
  int status;
  int iter = 0, max_iter = 100;
  const gsl_root_fdfsolver_type *T;
  gsl_root_fdfsolver *s;
```

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```
  double x0, x = 5.0, r_expected = sqrt (5.0);
  gsl_function_fdf FDF;
  struct quadratic_params params = {1.0, 0.0, -5.0};

  FDF.f = &quadratic;
  FDF.df = &quadratic_deriv;
  FDF.fdf = &quadratic_fdf;
  FDF.params = &params;

  T = gsl_root_fdfsolver_newton;
  s = gsl_root_fdfsolver_alloc (T);
  gsl_root_fdfsolver_set (s, &FDF, x);

  printf ("using %s method\n",
          gsl_root_fdfsolver_name (s));

  printf ("%-5s %10s %10s %10s\n",
          "iter", "root", "err", "err(est)");
  do
    {
      iter++;
      status = gsl_root_fdfsolver_iterate (s);
      x0 = x;
      x = gsl_root_fdfsolver_root (s);
      status = gsl_root_test_delta (x, x0, 0, 1e-3);

      if (status == GSL_SUCCESS)
        printf ("Converged:\n");

      printf ("%5d %10.7f %+10.7f %10.7f\n",
              iter, x, x - r_expected, x - x0);
    }
  while (status == GSL_CONTINUE && iter < max_iter);

  gsl_root_fdfsolver_free (s);
  return status;
}
```

Here are the results for Newton's method:

```
$ ./a.out
using newton method
iter        root        err   err(est)
    1  3.0000000 +0.7639320 -2.0000000
    2  2.3333333 +0.0972654 -0.6666667
    3  2.2380952 +0.0020273 -0.0952381
Converged:
    4  2.2360689 +0.0000009 -0.0020263
```

Note that the error can be estimated more accurately by taking the difference between the current iterate and next iterate rather than the previous iterate. The other derivative solvers can be investigated by changing `gsl_root_fdfsolver_newton` to `gsl_root_fdfsolver_secant` or `gsl_root_fdfsolver_steffenson`.

36.11 References and Further Reading

For information on the Brent-Dekker algorithm see the following two papers,

- R. P. Brent, “An algorithm with guaranteed convergence for finding a zero of a function”, *Computer Journal*, 14 (1971) 422–425
- J. C. P. Bus and T. J. Dekker, “Two Efficient Algorithms with Guaranteed Convergence for Finding a Zero of a Function”, *ACM Transactions of Mathematical Software*, Vol.: 1 No.: 4 (1975) 330–345

CHAPTER

THIRTYSEVEN

ONE DIMENSIONAL MINIMIZATION

This chapter describes routines for finding minima of arbitrary one-dimensional functions. The library provides low level components for a variety of iterative minimizers and convergence tests. These can be combined by the user to achieve the desired solution, with full access to the intermediate steps of the algorithms. Each class of methods uses the same framework, so that you can switch between minimizers at runtime without needing to recompile your program. Each instance of a minimizer keeps track of its own state, allowing the minimizers to be used in multi-threaded programs.

The header file `gsl_min.h` contains prototypes for the minimization functions and related declarations. To use the minimization algorithms to find the maximum of a function simply invert its sign.

37.1 Overview

The minimization algorithms begin with a bounded region known to contain a minimum. The region is described by a lower bound a and an upper bound b, with an estimate of the location of the minimum x, as shown in Fig. 37.1.

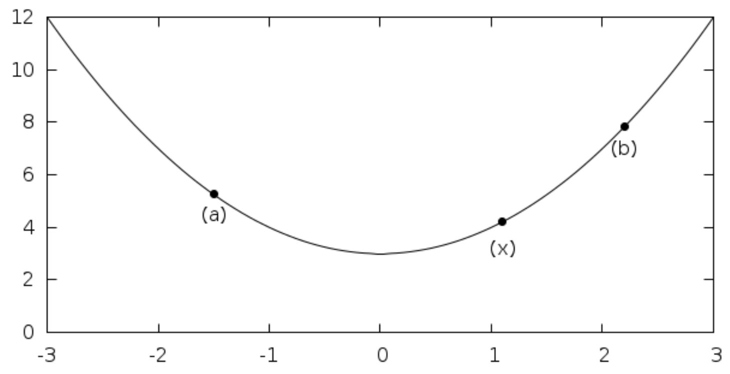

Fig. 37.1: Function with lower and upper bounds with an estimate of the minimum.

The value of the function at x must be less than the value of the function at the ends of the interval,

$$f(a) > f(x) < f(b)$$

This condition guarantees that a minimum is contained somewhere within the interval. On each iteration a new point x' is selected using one of the available algorithms. If the new point is a better estimate of the minimum, i.e.: where $f(x') < f(x)$, then the current estimate of the minimum x is updated. The new point also allows the size of the bounded interval to be reduced, by choosing the most compact set of points which satisfies the constraint $f(a) > f(x) < f(b)$. The interval is reduced until it encloses the true minimum to a desired tolerance. This provides a best estimate of the location of the minimum and a rigorous error estimate.

Several bracketing algorithms are available within a single framework. The user provides a high-level driver for the algorithm, and the library provides the individual functions necessary for each of the steps. There are three main phases of the iteration. The steps are,

- initialize minimizer state, `s`, for algorithm `T`
- update `s` using the iteration `T`
- test `s` for convergence, and repeat iteration if necessary

The state for the minimizers is held in a *gsl_min_fminimizer* struct. The updating procedure uses only function evaluations (not derivatives).

37.2 Caveats

Note that minimization functions can only search for one minimum at a time. When there are several minima in the search area, the first minimum to be found will be returned; however it is difficult to predict which of the minima this will be. *In most cases, no error will be reported if you try to find a minimum in an area where there is more than one.*

With all minimization algorithms it can be difficult to determine the location of the minimum to full numerical precision. The behavior of the function in the region of the minimum x^* can be approximated by a Taylor expansion,

$$y = f(x^*) + \frac{1}{2} f''(x^*)(x - x^*)^2$$

and the second term of this expansion can be lost when added to the first term at finite precision. This magnifies the error in locating x^*, making it proportional to $\sqrt{\epsilon}$ (where ϵ is the relative accuracy of the floating point numbers). For functions with higher order minima, such as x^4, the magnification of the error is correspondingly worse. The best that can be achieved is to converge to the limit of numerical accuracy in the function values, rather than the location of the minimum itself.

37.3 Initializing the Minimizer

type **gsl_min_fminimizer**

This is a workspace for minimizing functions.

gsl_min_fminimizer ***gsl_min_fminimizer_alloc**(const *gsl_min_fminimizer_type* *T)

This function returns a pointer to a newly allocated instance of a minimizer of type *T*. For example, the following code creates an instance of a golden section minimizer:

```
const gsl_min_fminimizer_type * T = gsl_min_fminimizer_goldensection;
gsl_min_fminimizer * s = gsl_min_fminimizer_alloc (T);
```

If there is insufficient memory to create the minimizer then the function returns a null pointer and the error handler is invoked with an error code of *GSL_ENOMEM*.

int **gsl_min_fminimizer_set**(*gsl_min_fminimizer* *s, *gsl_function* *f, double x_minimum, double x_lower, double x_upper)

This function sets, or resets, an existing minimizer *s* to use the function *f* and the initial search interval [*x_lower*, *x_upper*], with a guess for the location of the minimum *x_minimum*.

If the interval given does not contain a minimum, then the function returns an error code of *GSL_EINVAL*.

int **gsl_min_fminimizer_set_with_values**(*gsl_min_fminimizer* *s, *gsl_function* *f, double x_minimum, double f_minimum, double x_lower, double f_lower, double x_upper, double f_upper)

This function is equivalent to `gsl_min_fminimizer_set()` but uses the values *f_minimum*, *f_lower* and *f_upper* instead of computing `f(x_minimum)`, `f(x_lower)` and `f(x_upper)`.

void **gsl_min_fminimizer_free**(*gsl_min_fminimizer* *s)

This function frees all the memory associated with the minimizer *s*.

const char ***gsl_min_fminimizer_name**(const *gsl_min_fminimizer* *s)

This function returns a pointer to the name of the minimizer. For example:

```
printf ("s is a '%s' minimizer\n", gsl_min_fminimizer_name (s));
```

would print something like `s is a 'brent' minimizer`.

37.4 Providing the function to minimize

You must provide a continuous function of one variable for the minimizers to operate on. In order to allow for general parameters the functions are defined by a `gsl_function` data type (*Providing the function to solve*).

37.5 Iteration

The following functions drive the iteration of each algorithm. Each function performs one iteration to update the state of any minimizer of the corresponding type. The same functions work for all minimizers so that different methods can be substituted at runtime without modifications to the code.

int **gsl_min_fminimizer_iterate**(*gsl_min_fminimizer* *s)

This function performs a single iteration of the minimizer *s*. If the iteration encounters an unexpected problem then an error code will be returned,

`GSL_EBADFUNC`

the iteration encountered a singular point where the function evaluated to `Inf` or `NaN`.

`GSL_FAILURE`

the algorithm could not improve the current best approximation or bounding interval.

The minimizer maintains a current best estimate of the position of the minimum at all times, and the current interval bounding the minimum. This information can be accessed with the following auxiliary functions,

double **gsl_min_fminimizer_x_minimum**(const *gsl_min_fminimizer* *s)

This function returns the current estimate of the position of the minimum for the minimizer *s*.

double **gsl_min_fminimizer_x_upper**(const *gsl_min_fminimizer* *s)

double **gsl_min_fminimizer_x_lower**(const *gsl_min_fminimizer* *s)

These functions return the current upper and lower bound of the interval for the minimizer *s*.

double **gsl_min_fminimizer_f_minimum**(const *gsl_min_fminimizer* *s)

double **gsl_min_fminimizer_f_upper**(const *gsl_min_fminimizer* *s) double **gsl_min_fminimizer_f_lower**(const *gsl_min_fminimizer* *s)

These functions return the value of the function at the current estimate of the minimum and at the upper and lower bounds of the interval for the minimizer `s`.

37.6 Stopping Parameters

A minimization procedure should stop when one of the following conditions is true:

- A minimum has been found to within the user-specified precision.
- A user-specified maximum number of iterations has been reached.
- An error has occurred.

The handling of these conditions is under user control. The function below allows the user to test the precision of the current result.

int **gsl_min_test_interval**(double x_lower, double x_upper, double epsabs, double epsrel)

This function tests for the convergence of the interval [`x_lower`, `x_upper`] with absolute error `epsabs` and relative error `epsrel`. The test returns `GSL_SUCCESS` if the following condition is achieved,

$$|a - b| < \mathit{epsabs} + \mathit{epsrel}\,\min(|a|, |b|)$$

when the interval $x = [a, b]$ does not include the origin. If the interval includes the origin then $\min(|a|, |b|)$ is replaced by zero (which is the minimum value of $|x|$ over the interval). This ensures that the relative error is accurately estimated for minima close to the origin.

This condition on the interval also implies that any estimate of the minimum x_m in the interval satisfies the same condition with respect to the true minimum x_m^*,

$$|x_m - x_m^*| < \mathit{epsabs} + \mathit{epsrel}\, x_m^*$$

assuming that the true minimum x_m^* is contained within the interval.

37.7 Minimization Algorithms

The minimization algorithms described in this section require an initial interval which is guaranteed to contain a minimum—if a and b are the endpoints of the interval and x is an estimate of the minimum then $f(a) > f(x) < f(b)$. This ensures that the function has at least one minimum somewhere in the interval. If a valid initial interval is used then these algorithm cannot fail, provided the function is well-behaved.

type **gsl_min_fminimizer_type**

gsl_min_fminimizer_type ***gsl_min_fminimizer_goldensection**

The *golden section algorithm* is the simplest method of bracketing the minimum of a function. It is the slowest algorithm provided by the library, with linear convergence.

On each iteration, the algorithm first compares the subintervals from the endpoints to the current minimum. The larger subinterval is divided in a golden section (using the famous ratio $(3 - \sqrt{5})/2 \approx 0.3819660$ and the value of the function at this new point is calculated. The new value is used with the constraint $f(a') > f(x') < f(b')$ to a select new interval containing the minimum, by discarding the least useful point. This procedure can be continued indefinitely until the interval is sufficiently small. Choosing the golden section as the bisection ratio can be shown to provide the fastest convergence for this type of algorithm.

gsl_min_fminimizer_type ***gsl_min_fminimizer_brent***

The *Brent minimization algorithm* combines a parabolic interpolation with the golden section algorithm. This produces a fast algorithm which is still robust.

The outline of the algorithm can be summarized as follows: on each iteration Brent's method approximates the function using an interpolating parabola through three existing points. The minimum of the parabola is taken as a guess for the minimum. If it lies within the bounds of the current interval then the interpolating point is accepted, and used to generate a smaller interval. If the interpolating point is not accepted then the algorithm falls back to an ordinary golden section step. The full details of Brent's method include some additional checks to improve convergence.

gsl_min_fminimizer_type ***gsl_min_fminimizer_quad_golden***

This is a variant of Brent's algorithm which uses the safeguarded step-length algorithm of Gill and Murray.

37.8 Examples

The following program uses the Brent algorithm to find the minimum of the function $f(x) = \cos(x) + 1$, which occurs at $x = \pi$. The starting interval is $(0, 6)$, with an initial guess for the minimum of 2.

```
#include <stdio.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_min.h>

double fn1 (double x, void * params)
{
  (void)(params); /* avoid unused parameter warning */
  return cos(x) + 1.0;
}

int
main (void)
{
  int status;
  int iter = 0, max_iter = 100;
  const gsl_min_fminimizer_type *T;
  gsl_min_fminimizer *s;
  double m = 2.0, m_expected = M_PI;
  double a = 0.0, b = 6.0;
  gsl_function F;

  F.function = &fn1;
  F.params = 0;

  T = gsl_min_fminimizer_brent;
  s = gsl_min_fminimizer_alloc (T);
  gsl_min_fminimizer_set (s, &F, m, a, b);

  printf ("using %s method\n",
          gsl_min_fminimizer_name (s));

  printf ("%5s [%9s, %9s] %9s %10s %9s\n",
          "iter", "lower", "upper", "min",
```

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```
          "err", "err(est)");

  printf ("%5d [%.7f, %.7f] %.7f %+.7f %.7f\n",
          iter, a, b,
          m, m - m_expected, b - a);

  do
    {
      iter++;
      status = gsl_min_fminimizer_iterate (s);

      m = gsl_min_fminimizer_x_minimum (s);
      a = gsl_min_fminimizer_x_lower (s);
      b = gsl_min_fminimizer_x_upper (s);

      status
        = gsl_min_test_interval (a, b, 0.001, 0.0);

      if (status == GSL_SUCCESS)
        printf ("Converged:\n");

      printf ("%5d [%.7f, %.7f] "
              "%.7f %+.7f %.7f\n",
              iter, a, b,
              m, m - m_expected, b - a);
    }
  while (status == GSL_CONTINUE && iter < max_iter);

  gsl_min_fminimizer_free (s);

  return status;
}
```

Here are the results of the minimization procedure.

```
using brent method
 iter [     lower,      upper]       min        err  err(est)
    0 [0.0000000, 6.0000000] 2.0000000 -1.1415927 6.0000000
    1 [2.0000000, 6.0000000] 3.5278640 +0.3862713 4.0000000
    2 [2.0000000, 3.5278640] 3.1748217 +0.0332290 1.5278640
    3 [2.0000000, 3.1748217] 3.1264576 -0.0151351 1.1748217
    4 [3.1264576, 3.1748217] 3.1414743 -0.0001183 0.0483641
    5 [3.1414743, 3.1748217] 3.1415930 +0.0000004 0.0333474
Converged:
    6 [3.1414743, 3.1415930] 3.1415927 +0.0000000 0.0001187
```

37.9 References and Further Reading

Further information on Brent's algorithm is available in the following book,

- Richard Brent, *Algorithms for minimization without derivatives*, Prentice-Hall (1973), republished by Dover in paperback (2002), ISBN 0-486-41998-3.

CHAPTER

THIRTYEIGHT

MULTIDIMENSIONAL ROOT-FINDING

This chapter describes functions for multidimensional root-finding (solving nonlinear systems with n equations in n unknowns). The library provides low level components for a variety of iterative solvers and convergence tests. These can be combined by the user to achieve the desired solution, with full access to the intermediate steps of the iteration. Each class of methods uses the same framework, so that you can switch between solvers at runtime without needing to recompile your program. Each instance of a solver keeps track of its own state, allowing the solvers to be used in multi-threaded programs. The solvers are based on the original Fortran library MINPACK.

The header file `gsl_multiroots.h` contains prototypes for the multidimensional root finding functions and related declarations.

38.1 Overview

The problem of multidimensional root finding requires the simultaneous solution of n equations, f_i, in n variables, x_i,

$$f_i(x_1, \dots, x_n) = 0 \qquad \text{for } i = 1 \dots n.$$

In general there are no bracketing methods available for n dimensional systems, and no way of knowing whether any solutions exist. All algorithms proceed from an initial guess using a variant of the Newton iteration,

$$x \to x' = x - J^{-1} f(x)$$

where x, f are vector quantities and J is the Jacobian matrix $J_{ij} = \partial f_i / \partial x_j$. Additional strategies can be used to enlarge the region of convergence. These include requiring a decrease in the norm $|f|$ on each step proposed by Newton's method, or taking steepest-descent steps in the direction of the negative gradient of $|f|$.

Several root-finding algorithms are available within a single framework. The user provides a high-level driver for the algorithms, and the library provides the individual functions necessary for each of the steps. There are three main phases of the iteration. The steps are,

- initialize solver state, `s`, for algorithm `T`
- update `s` using the iteration `T`
- test `s` for convergence, and repeat iteration if necessary

The evaluation of the Jacobian matrix can be problematic, either because programming the derivatives is intractable or because computation of the n^2 terms of the matrix becomes too expensive. For these reasons the algorithms provided by the library are divided into two classes according to whether the derivatives are available or not.

The state for solvers with an analytic Jacobian matrix is held in a *`gsl_multiroot_fdfsolver`* struct. The updating procedure requires both the function and its derivatives to be supplied by the user.

The state for solvers which do not use an analytic Jacobian matrix is held in a *`gsl_multiroot_fsolver`* struct. The updating procedure uses only function evaluations (not derivatives). The algorithms estimate the matrix J or J^{-1} by approximate methods.

38.2 Initializing the Solver

The following functions initialize a multidimensional solver, either with or without derivatives. The solver itself depends only on the dimension of the problem and the algorithm and can be reused for different problems.

type **gsl_multiroot_fsolver**

This is a workspace for multidimensional root-finding without derivatives.

type **gsl_multiroot_fdfsolver**

This is a workspace for multidimensional root-finding with derivatives.

gsl_multiroot_fsolver ***gsl_multiroot_fsolver_alloc**(const *gsl_multiroot_fsolver_type* *T, size_t n)

This function returns a pointer to a newly allocated instance of a solver of type *T* for a system of *n* dimensions. For example, the following code creates an instance of a hybrid solver, to solve a 3-dimensional system of equations:

```
const gsl_multiroot_fsolver_type * T = gsl_multiroot_fsolver_hybrid;
gsl_multiroot_fsolver * s = gsl_multiroot_fsolver_alloc (T, 3);
```

If there is insufficient memory to create the solver then the function returns a null pointer and the error handler is invoked with an error code of *GSL_ENOMEM*.

gsl_multiroot_fdfsolver ***gsl_multiroot_fdfsolver_alloc**(const *gsl_multiroot_fdfsolver_type* *T, size_t n)

This function returns a pointer to a newly allocated instance of a derivative solver of type *T* for a system of *n* dimensions. For example, the following code creates an instance of a Newton-Raphson solver, for a 2-dimensional system of equations:

```
const gsl_multiroot_fdfsolver_type * T = gsl_multiroot_fdfsolver_newton;
gsl_multiroot_fdfsolver * s = gsl_multiroot_fdfsolver_alloc (T, 2);
```

If there is insufficient memory to create the solver then the function returns a null pointer and the error handler is invoked with an error code of *GSL_ENOMEM*.

int **gsl_multiroot_fsolver_set**(*gsl_multiroot_fsolver* *s, *gsl_multiroot_function* *f, const *gsl_vector* *x)

int **gsl_multiroot_fdfsolver_set**(*gsl_multiroot_fdfsolver* *s, *gsl_multiroot_function_fdf* *fdf, const *gsl_vector* *x)

These functions set, or reset, an existing solver *s* to use the function f or function and derivative *fdf*, and the initial guess *x*. Note that the initial position is copied from *x*, this argument is not modified by subsequent iterations.

void **gsl_multiroot_fsolver_free**(*gsl_multiroot_fsolver* *s)

void **gsl_multiroot_fdfsolver_free**(*gsl_multiroot_fdfsolver* *s)

These functions free all the memory associated with the solver *s*.

const char ***gsl_multiroot_fsolver_name**(const *gsl_multiroot_fsolver* *s)

const char ***gsl_multiroot_fdfsolver_name**(const *gsl_multiroot_fdfsolver* *s)

These functions return a pointer to the name of the solver. For example:

```
printf ("s is a '%s' solver\n", gsl_multiroot_fdfsolver_name (s));
```

would print something like `s is a 'newton' solver`.

38.3 Providing the function to solve

You must provide n functions of n variables for the root finders to operate on. In order to allow for general parameters the functions are defined by the following data types:

type **gsl_multiroot_function**

This data type defines a general system of functions with parameters.

`int (* f) (const gsl_vector * x, void * params, gsl_vector * f)`

this function should store the vector result $f(x, params)$ in `f` for argument `x` and parameters `params`, returning an appropriate error code if the function cannot be computed.

`size_t n`

the dimension of the system, i.e. the number of components of the vectors `x` and `f`.

`void * params`

a pointer to the parameters of the function.

Here is an example using Powell's test function,

$$f_1(x) = Ax_0x_1 - 1$$
$$f_2(x) = \exp(-x_0) + \exp(-x_1) - (1 + 1/A)$$

with $A = 10^4$. The following code defines a *gsl_multiroot_function* system `F` which you could pass to a solver:

```
struct powell_params { double A; };

int
powell (gsl_vector * x, void * p, gsl_vector * f) {
   struct powell_params * params
     = (struct powell_params *)p;
   const double A = (params->A);
   const double x0 = gsl_vector_get(x,0);
   const double x1 = gsl_vector_get(x,1);

   gsl_vector_set (f, 0, A * x0 * x1 - 1);
   gsl_vector_set (f, 1, (exp(-x0) + exp(-x1)
                          - (1.0 + 1.0/A)));
   return GSL_SUCCESS
}

gsl_multiroot_function F;
struct powell_params params = { 10000.0 };

F.f = &powell;
F.n = 2;
F.params = &params;
```

type **gsl_multiroot_function_fdf**

This data type defines a general system of functions with parameters and the corresponding Jacobian matrix of derivatives,

`int (* f) (const gsl_vector * x, void * params, gsl_vector * f)`

this function should store the vector result $f(x, params)$ in `f` for argument `x` and parameters `params`, returning an appropriate error code if the function cannot be computed.

`int (* df) (const gsl_vector * x, void * params, gsl_matrix * J)`

this function should store the `n`-by-`n` matrix result

$$J_{ij} = \partial f_i(x, params) / \partial x_j$$

in `J` for argument `x` and parameters `params`, returning an appropriate error code if the function cannot be computed.

`int (* fdf) (const gsl_vector * x, void * params, gsl_vector * f, gsl_matrix * J)`

This function should set the values of the `f` and `J` as above, for arguments `x` and parameters `params`. This function provides an optimization of the separate functions for $f(x)$ and $J(x)$—it is always faster to compute the function and its derivative at the same time.

`size_t n`

the dimension of the system, i.e. the number of components of the vectors `x` and `f`.

`void * params`

a pointer to the parameters of the function.

The example of Powell's test function defined above can be extended to include analytic derivatives using the following code:

```
int
powell_df (gsl_vector * x, void * p, gsl_matrix * J)
{
   struct powell_params * params
     = (struct powell_params *)p;
   const double A = (params->A);
   const double x0 = gsl_vector_get(x,0);
   const double x1 = gsl_vector_get(x,1);
   gsl_matrix_set (J, 0, 0, A * x1);
   gsl_matrix_set (J, 0, 1, A * x0);
   gsl_matrix_set (J, 1, 0, -exp(-x0));
   gsl_matrix_set (J, 1, 1, -exp(-x1));
   return GSL_SUCCESS
}

int
powell_fdf (gsl_vector * x, void * p,
            gsl_matrix * f, gsl_matrix * J) {
   struct powell_params * params
     = (struct powell_params *)p;
   const double A = (params->A);
   const double x0 = gsl_vector_get(x,0);
   const double x1 = gsl_vector_get(x,1);

   const double u0 = exp(-x0);
   const double u1 = exp(-x1);

   gsl_vector_set (f, 0, A * x0 * x1 - 1);
   gsl_vector_set (f, 1, u0 + u1 - (1 + 1/A));

   gsl_matrix_set (J, 0, 0, A * x1);
   gsl_matrix_set (J, 0, 1, A * x0);
```

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```
   gsl_matrix_set (J, 1, 0, -u0);
   gsl_matrix_set (J, 1, 1, -u1);
   return GSL_SUCCESS
}

gsl_multiroot_function_fdf FDF;

FDF.f = &powell_f;
FDF.df = &powell_df;
FDF.fdf = &powell_fdf;
FDF.n = 2;
FDF.params = 0;
```

Note that the function `powell_fdf` is able to reuse existing terms from the function when calculating the Jacobian, thus saving time.

38.4 Iteration

The following functions drive the iteration of each algorithm. Each function performs one iteration to update the state of any solver of the corresponding type. The same functions work for all solvers so that different methods can be substituted at runtime without modifications to the code.

int **gsl_multiroot_fsolver_iterate**(*gsl_multiroot_fsolver* *s)

int **gsl_multiroot_fdfsolver_iterate**(*gsl_multiroot_fdfsolver* *s)

These functions perform a single iteration of the solver `s`. If the iteration encounters an unexpected problem then an error code will be returned,

`GSL_EBADFUNC`

the iteration encountered a singular point where the function or its derivative evaluated to `Inf` or `NaN`.

`GSL_ENOPROG`

the iteration is not making any progress, preventing the algorithm from continuing.

The solver maintains a current best estimate of the root `s->x` and its function value `s->f` at all times. This information can be accessed with the following auxiliary functions,

gsl_vector ***gsl_multiroot_fsolver_root**(const *gsl_multiroot_fsolver* *s)

gsl_vector ***gsl_multiroot_fdfsolver_root**(const *gsl_multiroot_fdfsolver* *s)

These functions return the current estimate of the root for the solver `s`, given by `s->x`.

gsl_vector ***gsl_multiroot_fsolver_f**(const *gsl_multiroot_fsolver* *s)

gsl_vector ***gsl_multiroot_fdfsolver_f**(const *gsl_multiroot_fdfsolver* *s)

These functions return the function value $f(x)$ at the current estimate of the root for the solver `s`, given by `s->f`.

gsl_vector ***gsl_multiroot_fsolver_dx**(const *gsl_multiroot_fsolver* *s)

gsl_vector ***gsl_multiroot_fdfsolver_dx**(const *gsl_multiroot_fdfsolver* *s)

These functions return the last step dx taken by the solver `s`, given by `s->dx`.

38.5 Search Stopping Parameters

A root finding procedure should stop when one of the following conditions is true:

- A multidimensional root has been found to within the user-specified precision.
- A user-specified maximum number of iterations has been reached.
- An error has occurred.

The handling of these conditions is under user control. The functions below allow the user to test the precision of the current result in several standard ways.

int **gsl_multiroot_test_delta**(const *gsl_vector* *dx, const *gsl_vector* *x, double epsabs, double epsrel)

This function tests for the convergence of the sequence by comparing the last step `dx` with the absolute error `epsabs` and relative error `epsrel` to the current position `x`. The test returns `GSL_SUCCESS` if the following condition is achieved,

$$|dx_i| < epsabs + epsrel\,|x_i|$$

for each component of `x` and returns `GSL_CONTINUE` otherwise.

int **gsl_multiroot_test_residual**(const *gsl_vector* *f, double epsabs)

This function tests the residual value `f` against the absolute error bound `epsabs`. The test returns `GSL_SUCCESS` if the following condition is achieved,

$$\sum_i |f_i| < epsabs$$

and returns `GSL_CONTINUE` otherwise. This criterion is suitable for situations where the precise location of the root, x, is unimportant provided a value can be found where the residual is small enough.

38.6 Algorithms using Derivatives

The root finding algorithms described in this section make use of both the function and its derivative. They require an initial guess for the location of the root, but there is no absolute guarantee of convergence—the function must be suitable for this technique and the initial guess must be sufficiently close to the root for it to work. When the conditions are satisfied then convergence is quadratic.

type **gsl_multiroot_fdfsolver_type**

The following are available algorithms for minimizing functions using derivatives.

gsl_multiroot_fdfsolver_type ***gsl_multiroot_fdfsolver_hybridsj**

This is a modified version of Powell's Hybrid method as implemented in the HYBRJ algorithm in MINPACK. Minpack was written by Jorge J. Moré, Burton S. Garbow and Kenneth E. Hillstrom. The Hybrid algorithm retains the fast convergence of Newton's method but will also reduce the residual when Newton's method is unreliable.

The algorithm uses a generalized trust region to keep each step under control. In order to be accepted a proposed new position x' must satisfy the condition $|D(x' - x)| < \delta$, where D is a diagonal scaling matrix and δ is the size of the trust region. The components of D are computed internally, using the column norms of the Jacobian to estimate the sensitivity of the residual to each component of x. This improves the behavior of the algorithm for badly scaled functions.

On each iteration the algorithm first determines the standard Newton step by solving the system $Jdx = -f$. If this step falls inside the trust region it is used as a trial step in the next stage. If not, the algorithm uses the linear combination of the Newton and gradient directions which is predicted to minimize the norm of the function while staying inside the trust region,

$$dx = -\alpha J^{-1} f(x) - \beta \nabla |f(x)|^2$$

This combination of Newton and gradient directions is referred to as a *dogleg step*.

The proposed step is now tested by evaluating the function at the resulting point, x'. If the step reduces the norm of the function sufficiently then it is accepted and size of the trust region is increased. If the proposed step fails to improve the solution then the size of the trust region is decreased and another trial step is computed.

The speed of the algorithm is increased by computing the changes to the Jacobian approximately, using a rank-1 update. If two successive attempts fail to reduce the residual then the full Jacobian is recomputed. The algorithm also monitors the progress of the solution and returns an error if several steps fail to make any improvement,

`GSL_ENOPROG`

the iteration is not making any progress, preventing the algorithm from continuing.

`GSL_ENOPROGJ`

re-evaluations of the Jacobian indicate that the iteration is not making any progress, preventing the algorithm from continuing.

gsl_multiroot_fdfsolver_type ***gsl_multiroot_fdfsolver_hybridj**

This algorithm is an unscaled version of HYBRIDSJ. The steps are controlled by a spherical trust region $|x' - x| < \delta$, instead of a generalized region. This can be useful if the generalized region estimated by HYBRIDSJ is inappropriate.

gsl_multiroot_fdfsolver_type ***gsl_multiroot_fdfsolver_newton**

Newton's Method is the standard root-polishing algorithm. The algorithm begins with an initial guess for the location of the solution. On each iteration a linear approximation to the function F is used to estimate the step which will zero all the components of the residual. The iteration is defined by the following sequence,

$$x \to x' = x - J^{-1} f(x)$$

where the Jacobian matrix J is computed from the derivative functions provided by `f`. The step dx is obtained by solving the linear system,

$$J dx = -f(x)$$

using LU decomposition. If the Jacobian matrix is singular, an error code of `GSL_EDOM` is returned.

gsl_multiroot_fdfsolver_type ***gsl_multiroot_fdfsolver_gnewton**

This is a modified version of Newton's method which attempts to improve global convergence by requiring every step to reduce the Euclidean norm of the residual, $|f(x)|$. If the Newton step leads to an increase in the norm then a reduced step of relative size,

$$t = (\sqrt{1 + 6r} - 1)/(3r)$$

is proposed, with r being the ratio of norms $|f(x')|^2/|f(x)|^2$. This procedure is repeated until a suitable step size is found.

38.7 Algorithms without Derivatives

The algorithms described in this section do not require any derivative information to be supplied by the user. Any derivatives needed are approximated by finite differences. Note that if the finite-differencing step size chosen by these routines is inappropriate, an explicit user-supplied numerical derivative can always be used with the algorithms described in the previous section.

type **`gsl_multiroot_fsolver_type`**

The following are available algorithms for minimizing functions without derivatives.

gsl_multiroot_fsolver_type ***`gsl_multiroot_fsolver_hybrids`**

This is a version of the Hybrid algorithm which replaces calls to the Jacobian function by its finite difference approximation. The finite difference approximation is computed using `gsl_multiroots_fdjac()` with a relative step size of `GSL_SQRT_DBL_EPSILON`. Note that this step size will not be suitable for all problems.

gsl_multiroot_fsolver_type ***`gsl_multiroot_fsolver_hybrid`**

This is a finite difference version of the Hybrid algorithm without internal scaling.

gsl_multiroot_fsolver_type ***`gsl_multiroot_fsolver_dnewton`**

The *discrete Newton algorithm* is the simplest method of solving a multidimensional system. It uses the Newton iteration

$$x \to x - J^{-1} f(x)$$

where the Jacobian matrix J is approximated by taking finite differences of the function `f`. The approximation scheme used by this implementation is,

$$J_{ij} = (f_i(x + \delta_j) - f_i(x))/\delta_j$$

where δ_j is a step of size $\sqrt{\epsilon}|x_j|$ with ϵ being the machine precision ($\epsilon \approx 2.22 \times 10^{-16}$). The order of convergence of Newton's algorithm is quadratic, but the finite differences require n^2 function evaluations on each iteration. The algorithm may become unstable if the finite differences are not a good approximation to the true derivatives.

gsl_multiroot_fsolver_type ***`gsl_multiroot_fsolver_broyden`**

The *Broyden algorithm* is a version of the discrete Newton algorithm which attempts to avoids the expensive update of the Jacobian matrix on each iteration. The changes to the Jacobian are also approximated, using a rank-1 update,

$$J^{-1} \to J^{-1} - (J^{-1} df - dx) dx^T J^{-1} / dx^T J^{-1} df$$

where the vectors dx and df are the changes in x and f. On the first iteration the inverse Jacobian is estimated using finite differences, as in the discrete Newton algorithm.

This approximation gives a fast update but is unreliable if the changes are not small, and the estimate of the inverse Jacobian becomes worse as time passes. The algorithm has a tendency to become unstable unless it starts close to the root. The Jacobian is refreshed if this instability is detected (consult the source for details).

This algorithm is included only for demonstration purposes, and is not recommended for serious use.

38.8 Examples

The multidimensional solvers are used in a similar way to the one-dimensional root finding algorithms. This first example demonstrates the HYBRIDS scaled-hybrid algorithm, which does not require derivatives. The program solves the Rosenbrock system of equations,

$$f_1(x,y) = a(1-x)$$
$$f_2(x,y) = b(y-x^2)$$

with $a = 1, b = 10$. The solution of this system lies at $(x, y) = (1, 1)$ in a narrow valley.

The first stage of the program is to define the system of equations:

```
#include <stdlib.h>
#include <stdio.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_multiroots.h>

struct rparams
  {
    double a;
    double b;
  };

int
rosenbrock_f (const gsl_vector * x, void *params,
              gsl_vector * f)
{
  double a = ((struct rparams *) params)->a;
  double b = ((struct rparams *) params)->b;

  const double x0 = gsl_vector_get (x, 0);
  const double x1 = gsl_vector_get (x, 1);

  const double y0 = a * (1 - x0);
  const double y1 = b * (x1 - x0 * x0);

  gsl_vector_set (f, 0, y0);
  gsl_vector_set (f, 1, y1);

  return GSL_SUCCESS;
}
```

The main program begins by creating the function object `f`, with the arguments `(x,y)` and parameters `(a,b)`. The solver `s` is initialized to use this function, with the `gsl_multiroot_fsolver_hybrids` method:

```
int
main (void)
{
  const gsl_multiroot_fsolver_type *T;
  gsl_multiroot_fsolver *s;

  int status;
  size_t i, iter = 0;
```

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```
  const size_t n = 2;
  struct rparams p = {1.0, 10.0};
  gsl_multiroot_function f = {&rosenbrock_f, n, &p};

  double x_init[2] = {-10.0, -5.0};
  gsl_vector *x = gsl_vector_alloc (n);

  gsl_vector_set (x, 0, x_init[0]);
  gsl_vector_set (x, 1, x_init[1]);

  T = gsl_multiroot_fsolver_hybrids;
  s = gsl_multiroot_fsolver_alloc (T, 2);
  gsl_multiroot_fsolver_set (s, &f, x);

  print_state (iter, s);

  do
    {
      iter++;
      status = gsl_multiroot_fsolver_iterate (s);

      print_state (iter, s);

      if (status)   /* check if solver is stuck */
        break;

      status =
        gsl_multiroot_test_residual (s->f, 1e-7);
    }
  while (status == GSL_CONTINUE && iter < 1000);

  printf ("status = %s\n", gsl_strerror (status));

  gsl_multiroot_fsolver_free (s);
  gsl_vector_free (x);
  return 0;
}
```

Note that it is important to check the return status of each solver step, in case the algorithm becomes stuck. If an error condition is detected, indicating that the algorithm cannot proceed, then the error can be reported to the user, a new starting point chosen or a different algorithm used.

The intermediate state of the solution is displayed by the following function. The solver state contains the vector `s->x` which is the current position, and the vector `s->f` with corresponding function values:

```
int
print_state (size_t iter, gsl_multiroot_fsolver * s)
{
  printf ("iter = %3u x = % .3f % .3f "
          "f(x) = % .3e % .3e\n",
          iter,
          gsl_vector_get (s->x, 0),
```

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```
          gsl_vector_get (s->x, 1),
          gsl_vector_get (s->f, 0),
          gsl_vector_get (s->f, 1));
}
```

Here are the results of running the program. The algorithm is started at $(-10, -5)$ far from the solution. Since the solution is hidden in a narrow valley the earliest steps follow the gradient of the function downhill, in an attempt to reduce the large value of the residual. Once the root has been approximately located, on iteration 8, the Newton behavior takes over and convergence is very rapid:

```
iter =  0 x = -10.000  -5.000  f(x) = 1.100e+01 -1.050e+03
iter =  1 x = -10.000  -5.000  f(x) = 1.100e+01 -1.050e+03
iter =  2 x =  -3.976  24.827  f(x) = 4.976e+00  9.020e+01
iter =  3 x =  -3.976  24.827  f(x) = 4.976e+00  9.020e+01
iter =  4 x =  -3.976  24.827  f(x) = 4.976e+00  9.020e+01
iter =  5 x =  -1.274  -5.680  f(x) = 2.274e+00 -7.302e+01
iter =  6 x =  -1.274  -5.680  f(x) = 2.274e+00 -7.302e+01
iter =  7 x =   0.249   0.298  f(x) = 7.511e-01  2.359e+00
iter =  8 x =   0.249   0.298  f(x) = 7.511e-01  2.359e+00
iter =  9 x =   1.000   0.878  f(x) = 1.268e-10 -1.218e+00
iter = 10 x =   1.000   0.989  f(x) = 1.124e-11 -1.080e-01
iter = 11 x =   1.000   1.000  f(x) = 0.000e+00  0.000e+00
status = success
```

Note that the algorithm does not update the location on every iteration. Some iterations are used to adjust the trust-region parameter, after trying a step which was found to be divergent, or to recompute the Jacobian, when poor convergence behavior is detected.

The next example program adds derivative information, in order to accelerate the solution. There are two derivative functions `rosenbrock_df` and `rosenbrock_fdf`. The latter computes both the function and its derivative simultaneously. This allows the optimization of any common terms. For simplicity we substitute calls to the separate `f` and `df` functions at this point in the code below:

```
int
rosenbrock_df (const gsl_vector * x, void *params,
               gsl_matrix * J)
{
  const double a = ((struct rparams *) params)->a;
  const double b = ((struct rparams *) params)->b;

  const double x0 = gsl_vector_get (x, 0);

  const double df00 = -a;
  const double df01 = 0;
  const double df10 = -2 * b  * x0;
  const double df11 = b;

  gsl_matrix_set (J, 0, 0, df00);
  gsl_matrix_set (J, 0, 1, df01);
  gsl_matrix_set (J, 1, 0, df10);
  gsl_matrix_set (J, 1, 1, df11);

  return GSL_SUCCESS;
```

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```
}

int
rosenbrock_fdf (const gsl_vector * x, void *params,
                gsl_vector * f, gsl_matrix * J)
{
  rosenbrock_f (x, params, f);
  rosenbrock_df (x, params, J);

  return GSL_SUCCESS;
}
```

The main program now makes calls to the corresponding `fdfsolver` versions of the functions:

```
int
main (void)
{
  const gsl_multiroot_fdfsolver_type *T;
  gsl_multiroot_fdfsolver *s;

  int status;
  size_t i, iter = 0;

  const size_t n = 2;
  struct rparams p = {1.0, 10.0};
  gsl_multiroot_function_fdf f = {&rosenbrock_f,
                                  &rosenbrock_df,
                                  &rosenbrock_fdf,
                                  n, &p};

  double x_init[2] = {-10.0, -5.0};
  gsl_vector *x = gsl_vector_alloc (n);

  gsl_vector_set (x, 0, x_init[0]);
  gsl_vector_set (x, 1, x_init[1]);

  T = gsl_multiroot_fdfsolver_gnewton;
  s = gsl_multiroot_fdfsolver_alloc (T, n);
  gsl_multiroot_fdfsolver_set (s, &f, x);

  print_state (iter, s);

  do
    {
      iter++;

      status = gsl_multiroot_fdfsolver_iterate (s);

      print_state (iter, s);

      if (status)
        break;
```

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```
      status = gsl_multiroot_test_residual (s->f, 1e-7);
    }
  while (status == GSL_CONTINUE && iter < 1000);

  printf ("status = %s\n", gsl_strerror (status));

  gsl_multiroot_fdfsolver_free (s);
  gsl_vector_free (x);
  return 0;
}
```

The addition of derivative information to the `gsl_multiroot_fsolver_hybrids` solver does not make any significant difference to its behavior, since it able to approximate the Jacobian numerically with sufficient accuracy. To illustrate the behavior of a different derivative solver we switch to `gsl_multiroot_fdfsolver_gnewton`. This is a traditional Newton solver with the constraint that it scales back its step if the full step would lead "uphill". Here is the output for the `gsl_multiroot_fdfsolver_gnewton` algorithm:

```
iter = 0 x = -10.000  -5.000 f(x) =  1.100e+01 -1.050e+03
iter = 1 x =  -4.231 -65.317 f(x) =  5.231e+00 -8.321e+02
iter = 2 x =   1.000 -26.358 f(x) = -8.882e-16 -2.736e+02
iter = 3 x =   1.000   1.000 f(x) = -2.220e-16 -4.441e-15
status = success
```

The convergence is much more rapid, but takes a wide excursion out to the point $(-4.23, -65.3)$. This could cause the algorithm to go astray in a realistic application. The hybrid algorithm follows the downhill path to the solution more reliably.

38.9 References and Further Reading

The original version of the Hybrid method is described in the following articles by Powell,

- M.J.D. Powell, "A Hybrid Method for Nonlinear Equations" (Chap 6, p 87–114) and "A Fortran Subroutine for Solving systems of Nonlinear Algebraic Equations" (Chap 7, p 115–161), in *Numerical Methods for Nonlinear Algebraic Equations*, P. Rabinowitz, editor. Gordon and Breach, 1970.

The following papers are also relevant to the algorithms described in this section,

- J.J. Moré, M.Y. Cosnard, "Numerical Solution of Nonlinear Equations", *ACM Transactions on Mathematical Software*, Vol 5, No 1, (1979), p 64–85
- C.G. Broyden, "A Class of Methods for Solving Nonlinear Simultaneous Equations", *Mathematics of Computation*, Vol 19 (1965), p 577–593
- J.J. Moré, B.S. Garbow, K.E. Hillstrom, "Testing Unconstrained Optimization Software", ACM Transactions on Mathematical Software, Vol 7, No 1 (1981), p 17–41

CHAPTER

THIRTYNINE

MULTIDIMENSIONAL MINIMIZATION

This chapter describes routines for finding minima of arbitrary multidimensional functions. The library provides low level components for a variety of iterative minimizers and convergence tests. These can be combined by the user to achieve the desired solution, while providing full access to the intermediate steps of the algorithms. Each class of methods uses the same framework, so that you can switch between minimizers at runtime without needing to recompile your program. Each instance of a minimizer keeps track of its own state, allowing the minimizers to be used in multi-threaded programs. The minimization algorithms can be used to maximize a function by inverting its sign.

The header file `gsl_multimin.h` contains prototypes for the minimization functions and related declarations.

39.1 Overview

The problem of multidimensional minimization requires finding a point x such that the scalar function,

$$f(x_1, \dots, x_n)$$

takes a value which is lower than at any neighboring point. For smooth functions the gradient $g = \nabla f$ vanishes at the minimum. In general there are no bracketing methods available for the minimization of n-dimensional functions. The algorithms proceed from an initial guess using a search algorithm which attempts to move in a downhill direction.

Algorithms making use of the gradient of the function perform a one-dimensional line minimisation along this direction until the lowest point is found to a suitable tolerance. The search direction is then updated with local information from the function and its derivatives, and the whole process repeated until the true n-dimensional minimum is found.

Algorithms which do not require the gradient of the function use different strategies. For example, the Nelder-Mead Simplex algorithm maintains $n+1$ trial parameter vectors as the vertices of a n-dimensional simplex. On each iteration it tries to improve the worst vertex of the simplex by geometrical transformations. The iterations are continued until the overall size of the simplex has decreased sufficiently.

Both types of algorithms use a standard framework. The user provides a high-level driver for the algorithms, and the library provides the individual functions necessary for each of the steps. There are three main phases of the iteration. The steps are,

- initialize minimizer state, `s`, for algorithm `T`
- update `s` using the iteration `T`
- test `s` for convergence, and repeat iteration if necessary

Each iteration step consists either of an improvement to the line-minimisation in the current direction or an update to the search direction itself. The state for the minimizers is held in a *`gsl_multimin_fdfminimizer`* struct or a *`gsl_multimin_fminimizer`* struct.

39.2 Caveats

Note that the minimization algorithms can only search for one local minimum at a time. When there are several local minima in the search area, the first minimum to be found will be returned; however it is difficult to predict which of the minima this will be. In most cases, no error will be reported if you try to find a local minimum in an area where there is more than one.

It is also important to note that the minimization algorithms find local minima; there is no way to determine whether a minimum is a global minimum of the function in question.

39.3 Initializing the Multidimensional Minimizer

The following function initializes a multidimensional minimizer. The minimizer itself depends only on the dimension of the problem and the algorithm and can be reused for different problems.

type **gsl_multimin_fdfminimizer**

This is a workspace for minimizing functions using derivatives.

type **gsl_multimin_fminimizer**

This is a workspace for minimizing functions without derivatives.

gsl_multimin_fdfminimizer ***gsl_multimin_fdfminimizer_alloc**(const *gsl_multimin_fdfminimizer_type* *T, size_t n)

gsl_multimin_fminimizer ***gsl_multimin_fminimizer_alloc**(const *gsl_multimin_fminimizer_type* *T, size_t n)

This function returns a pointer to a newly allocated instance of a minimizer of type `T` for an `n`-dimension function. If there is insufficient memory to create the minimizer then the function returns a null pointer and the error handler is invoked with an error code of `GSL_ENOMEM`.

int **gsl_multimin_fdfminimizer_set**(*gsl_multimin_fdfminimizer* *s, *gsl_multimin_function_fdf* *fdf, const *gsl_vector* *x, double step_size, double tol)

int **gsl_multimin_fminimizer_set**(*gsl_multimin_fminimizer* *s, *gsl_multimin_function* *f, const *gsl_vector* *x, const *gsl_vector* *step_size)

The function `gsl_multimin_fdfminimizer_set()` initializes the minimizer `s` to minimize the function `fdf` starting from the initial point `x`. The size of the first trial step is given by `step_size`. The accuracy of the line minimization is specified by `tol`. The precise meaning of this parameter depends on the method used. Typically the line minimization is considered successful if the gradient of the function g is orthogonal to the current search direction p to a relative accuracy of `tol`, where $p \cdot g < tol|p||g|$. A `tol` value of 0.1 is suitable for most purposes, since line minimization only needs to be carried out approximately. Note that setting `tol` to zero will force the use of "exact" line-searches, which are extremely expensive.

The function `gsl_multimin_fminimizer_set()` initializes the minimizer `s` to minimize the function `f`, starting from the initial point `x`. The size of the initial trial steps is given in vector `step_size`. The precise meaning of this parameter depends on the method used.

void **gsl_multimin_fdfminimizer_free**(*gsl_multimin_fdfminimizer* *s)

void **gsl_multimin_fminimizer_free**(*gsl_multimin_fminimizer* *s)

This function frees all the memory associated with the minimizer `s`.

const char ***gsl_multimin_fdfminimizer_name**(const *gsl_multimin_fdfminimizer* *s)

const char ***gsl_multimin_fminimizer_name**(const *gsl_multimin_fminimizer* *s)

This function returns a pointer to the name of the minimizer. For example:

```
printf ("s is a '%s' minimizer\n", gsl_multimin_fdfminimizer_name (s));
```

would print something like `s is a 'conjugate_pr' minimizer`.

39.4 Providing a function to minimize

You must provide a parametric function of n variables for the minimizers to operate on. You may also need to provide a routine which calculates the gradient of the function and a third routine which calculates both the function value and the gradient together. In order to allow for general parameters the functions are defined by the following data types:

type **`gsl_multimin_function_fdf`**

This data type defines a general function of n variables with parameters and the corresponding gradient vector of derivatives,

`double (* f) (const gsl_vector * x, void * params)`

this function should return the result $f(x, params)$ for argument `x` and parameters `params`. If the function cannot be computed, an error value of *`GSL_NAN`* should be returned.

`void (* df) (const gsl_vector * x, void * params, gsl_vector * g)`

this function should store the `n`-dimensional gradient

$$g_i = \partial f(x, params)/\partial x_i$$

in the vector `g` for argument `x` and parameters `params`, returning an appropriate error code if the function cannot be computed.

`void (* fdf) (const gsl_vector * x, void * params, double * f, gsl_vector * g)`

This function should set the values of the `f` and `g` as above, for arguments `x` and parameters `params`. This function provides an optimization of the separate functions for $f(x)$ and $g(x)$—it is always faster to compute the function and its derivative at the same time.

`size_t n`

the dimension of the system, i.e. the number of components of the vectors `x`.

`void * params`

a pointer to the parameters of the function.

type **`gsl_multimin_function`**

This data type defines a general function of n variables with parameters,

`double (* f) (const gsl_vector * x, void * params)`

this function should return the result $f(x, params)$ for argument `x` and parameters `params`. If the function cannot be computed, an error value of *`GSL_NAN`* should be returned.

`size_t n`

the dimension of the system, i.e. the number of components of the vectors `x`.

`void * params`

a pointer to the parameters of the function.

The following example function defines a simple two-dimensional paraboloid with five parameters,

```
/* Paraboloid centered on (p[0],p[1]), with
   scale factors (p[2],p[3]) and minimum p[4] */

double
my_f (const gsl_vector *v, void *params)
{
  double x, y;
  double *p = (double *)params;

  x = gsl_vector_get(v, 0);
  y = gsl_vector_get(v, 1);

  return p[2] * (x - p[0]) * (x - p[0]) +
           p[3] * (y - p[1]) * (y - p[1]) + p[4];
}

/* The gradient of f, df = (df/dx, df/dy). */
void
my_df (const gsl_vector *v, void *params,
       gsl_vector *df)
{
  double x, y;
  double *p = (double *)params;

  x = gsl_vector_get(v, 0);
  y = gsl_vector_get(v, 1);

  gsl_vector_set(df, 0, 2.0 * p[2] * (x - p[0]));
  gsl_vector_set(df, 1, 2.0 * p[3] * (y - p[1]));
}

/* Compute both f and df together. */
void
my_fdf (const gsl_vector *x, void *params,
        double *f, gsl_vector *df)
{
  *f = my_f(x, params);
  my_df(x, params, df);
}
```

The function can be initialized using the following code:

```
gsl_multimin_function_fdf my_func;

/* Paraboloid center at (1,2), scale factors (10, 20),
   minimum value 30 */
double p[5] = { 1.0, 2.0, 10.0, 20.0, 30.0 };

my_func.n = 2;  /* number of function components */
my_func.f = &my_f;
my_func.df = &my_df;
my_func.fdf = &my_fdf;
my_func.params = (void *)p;
```

39.5 Iteration

The following function drives the iteration of each algorithm. The function performs one iteration to update the state of the minimizer. The same function works for all minimizers so that different methods can be substituted at runtime without modifications to the code.

int **gsl_multimin_fdfminimizer_iterate**(*gsl_multimin_fdfminimizer* *s)

int **gsl_multimin_fminimizer_iterate**(*gsl_multimin_fminimizer* *s)

These functions perform a single iteration of the minimizer `s`. If the iteration encounters an unexpected problem then an error code will be returned. The error code `GSL_ENOPROG` signifies that the minimizer is unable to improve on its current estimate, either due to numerical difficulty or because a genuine local minimum has been reached.

The minimizer maintains a current best estimate of the minimum at all times. This information can be accessed with the following auxiliary functions,

gsl_vector ***gsl_multimin_fdfminimizer_x**(const *gsl_multimin_fdfminimizer* *s)

gsl_vector ***gsl_multimin_fminimizer_x**(const *gsl_multimin_fminimizer* *s)

double **gsl_multimin_fdfminimizer_minimum**(const *gsl_multimin_fdfminimizer* *s)

double **gsl_multimin_fminimizer_minimum**(const *gsl_multimin_fminimizer* *s)

gsl_vector ***gsl_multimin_fdfminimizer_gradient**(const *gsl_multimin_fdfminimizer* *s)

gsl_vector ***gsl_multimin_fdfminimizer_dx**(const *gsl_multimin_fdfminimizer* *s)

double **gsl_multimin_fminimizer_size**(const *gsl_multimin_fminimizer* *s)

These functions return the current best estimate of the location of the minimum, the value of the function at that point, its gradient, the last step increment of the estimate, and minimizer specific characteristic size for the minimizer `s`.

int **gsl_multimin_fdfminimizer_restart**(*gsl_multimin_fdfminimizer* *s)

This function resets the minimizer `s` to use the current point as a new starting point.

39.6 Stopping Criteria

A minimization procedure should stop when one of the following conditions is true:

- A minimum has been found to within the user-specified precision.
- A user-specified maximum number of iterations has been reached.
- An error has occurred.

The handling of these conditions is under user control. The functions below allow the user to test the precision of the current result.

int **gsl_multimin_test_gradient**(const *gsl_vector* *g, double epsabs)

This function tests the norm of the gradient `g` against the absolute tolerance `epsabs`. The gradient of a multi-dimensional function goes to zero at a minimum. The test returns `GSL_SUCCESS` if the following condition is achieved,

$$|g| < epsabs$$

and returns `GSL_CONTINUE` otherwise. A suitable choice of *epsabs* can be made from the desired accuracy in the function for small variations in x. The relationship between these quantities is given by $\delta f = g\,\delta x$.

int **`gsl_multimin_test_size`**(const double size, double epsabs)

This function tests the minimizer specific characteristic size (if applicable to the used minimizer) against absolute tolerance *epsabs*. The test returns `GSL_SUCCESS` if the size is smaller than tolerance, otherwise `GSL_CONTINUE` is returned.

39.7 Algorithms with Derivatives

There are several minimization methods available. The best choice of algorithm depends on the problem. The algorithms described in this section use the value of the function and its gradient at each evaluation point.

type **`gsl_multimin_fdfminimizer_type`**

This type specifies a minimization algorithm using gradients.

gsl_multimin_fdfminimizer_type ***`gsl_multimin_fdfminimizer_conjugate_fr`**

This is the Fletcher-Reeves conjugate gradient algorithm. The conjugate gradient algorithm proceeds as a succession of line minimizations. The sequence of search directions is used to build up an approximation to the curvature of the function in the neighborhood of the minimum.

An initial search direction `p` is chosen using the gradient, and line minimization is carried out in that direction. The accuracy of the line minimization is specified by the parameter `tol`. The minimum along this line occurs when the function gradient `g` and the search direction `p` are orthogonal. The line minimization terminates when $p \cdot g < tol|p||g|$. The search direction is updated using the Fletcher-Reeves formula $p' = g' - \beta p$ where $\beta = -|g'|^2/|g|^2$, and the line minimization is then repeated for the new search direction.

gsl_multimin_fdfminimizer_type ***`gsl_multimin_fdfminimizer_conjugate_pr`**

This is the Polak-Ribiere conjugate gradient algorithm. It is similar to the Fletcher-Reeves method, differing only in the choice of the coefficient β. Both methods work well when the evaluation point is close enough to the minimum of the objective function that it is well approximated by a quadratic hypersurface.

gsl_multimin_fdfminimizer_type ***`gsl_multimin_fdfminimizer_vector_bfgs2`**

gsl_multimin_fdfminimizer_type ***`gsl_multimin_fdfminimizer_vector_bfgs`**

These methods use the vector Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. This is a quasi-Newton method which builds up an approximation to the second derivatives of the function f using the difference between successive gradient vectors. By combining the first and second derivatives the algorithm is able to take Newton-type steps towards the function minimum, assuming quadratic behavior in that region.

The `bfgs2` version of this minimizer is the most efficient version available, and is a faithful implementation of the line minimization scheme described in Fletcher's *Practical Methods of Optimization*, Algorithms 2.6.2 and 2.6.4. It supersedes the original `bfgs` routine and requires substantially fewer function and gradient evaluations. The user-supplied tolerance `tol` corresponds to the parameter σ used by Fletcher. A value of 0.1 is recommended for typical use (larger values correspond to less accurate line searches).

gsl_multimin_fdfminimizer_type ***`gsl_multimin_fdfminimizer_steepest_descent`**

The steepest descent algorithm follows the downhill gradient of the function at each step. When a downhill step is successful the step-size is increased by a factor of two. If the downhill step leads to a higher function value then the algorithm backtracks and the step size is decreased using the parameter `tol`. A suitable value of `tol` for most applications is 0.1. The steepest descent method is inefficient and is included only for demonstration purposes.

39.8 Algorithms without Derivatives

The algorithms described in this section use only the value of the function at each evaluation point.

type **gsl_multimin_fminimizer_type**

This type specifies minimization algorithms which do not use gradients.

gsl_multimin_fminimizer_type ***gsl_multimin_fminimizer_nmsimplex2**

gsl_multimin_fminimizer_type ***gsl_multimin_fminimizer_nmsimplex**

These methods use the Simplex algorithm of Nelder and Mead. Starting from the initial vector $x = p_0$, the algorithm constructs an additional n vectors p_i using the step size vector $s = step\_size$ as follows:

$$
\begin{aligned}
p_0 &= (x_0, x_1, \cdots, x_n) \\
p_1 &= (x_0 + s_0, x_1, \cdots, x_n) \\
p_2 &= (x_0, x_1 + s_1, \cdots, x_n) \\
\ldots &= \ldots \\
p_n &= (x_0, x_1, \cdots, x_n + s_n)
\end{aligned}
$$

These vectors form the $n + 1$ vertices of a simplex in n dimensions. On each iteration the algorithm uses simple geometrical transformations to update the vector corresponding to the highest function value. The geometric transformations are reflection, reflection followed by expansion, contraction and multiple contraction. Using these transformations the simplex moves through the space towards the minimum, where it contracts itself.

After each iteration, the best vertex is returned. Note, that due to the nature of the algorithm not every step improves the current best parameter vector. Usually several iterations are required.

The minimizer-specific characteristic size is calculated as the average distance from the geometrical center of the simplex to all its vertices. This size can be used as a stopping criteria, as the simplex contracts itself near the minimum. The size is returned by the function `gsl_multimin_fminimizer_size()`.

The `gsl_multimin_fminimizer_nmsimplex2` version of this minimiser is a new $O(N)$ operations implementation of the earlier $O(N^2)$ operations `gsl_multimin_fminimizer_nmsimplex` minimiser. It uses the same underlying algorithm, but the simplex updates are computed more efficiently for high-dimensional problems. In addition, the size of simplex is calculated as the RMS distance of each vertex from the center rather than the mean distance, allowing a linear update of this quantity on each step. The memory usage is $O(N^2)$ for both algorithms.

gsl_multimin_fminimizer_type ***gsl_multimin_fminimizer_nmsimplex2rand**

This method is a variant of `gsl_multimin_fminimizer_nmsimplex2` which initialises the simplex around the starting point `x` using a randomly-oriented set of basis vectors instead of the fixed coordinate axes. The final dimensions of the simplex are scaled along the coordinate axes by the vector `step_size`. The randomisation uses a simple deterministic generator so that repeated calls to `gsl_multimin_fminimizer_set()` for a given solver object will vary the orientation in a well-defined way.

39.9 Examples

This example program finds the minimum of the *paraboloid function* defined earlier. The location of the minimum is offset from the origin in x and y, and the function value at the minimum is non-zero. The main program is given below, it requires the example function given earlier in this chapter.

```
int
main (void)
{
  size_t iter = 0;
  int status;

  const gsl_multimin_fdfminimizer_type *T;
  gsl_multimin_fdfminimizer *s;

  /* Position of the minimum (1,2), scale factors
     10,20, height 30. */
  double par[5] = { 1.0, 2.0, 10.0, 20.0, 30.0 };

  gsl_vector *x;
  gsl_multimin_function_fdf my_func;

  my_func.n = 2;
  my_func.f = my_f;
  my_func.df = my_df;
  my_func.fdf = my_fdf;
  my_func.params = par;

  /* Starting point, x = (5,7) */
  x = gsl_vector_alloc (2);
  gsl_vector_set (x, 0, 5.0);
  gsl_vector_set (x, 1, 7.0);

  T = gsl_multimin_fdfminimizer_conjugate_fr;
  s = gsl_multimin_fdfminimizer_alloc (T, 2);

  gsl_multimin_fdfminimizer_set (s, &my_func, x, 0.01, 1e-4);

  do
    {
      iter++;
      status = gsl_multimin_fdfminimizer_iterate (s);

      if (status)
        break;

      status = gsl_multimin_test_gradient (s->gradient, 1e-3);

      if (status == GSL_SUCCESS)
        printf ("Minimum found at:\n");

      printf ("%5d %.5f %.5f %10.5f\n", iter,
              gsl_vector_get (s->x, 0),
```

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```
              gsl_vector_get (s->x, 1),
              s->f);

    }
  while (status == GSL_CONTINUE && iter < 100);

  gsl_multimin_fdfminimizer_free (s);
  gsl_vector_free (x);

  return 0;
}
```

The initial step-size is chosen as 0.01, a conservative estimate in this case, and the line minimization parameter is set at 0.0001. The program terminates when the norm of the gradient has been reduced below 0.001. The output of the program is shown below,

```
         x       y         f
    1 4.99629 6.99072  687.84780
    2 4.98886 6.97215  683.55456
    3 4.97400 6.93501  675.01278
    4 4.94429 6.86073  658.10798
    5 4.88487 6.71217  625.01340
    6 4.76602 6.41506  561.68440
    7 4.52833 5.82083  446.46694
    8 4.05295 4.63238  261.79422
    9 3.10219 2.25548   75.49762
   10 2.85185 1.62963   67.03704
   11 2.19088 1.76182   45.31640
   12 0.86892 2.02622   30.18555
Minimum found at:
   13 1.00000 2.00000   30.00000
```

Note that the algorithm gradually increases the step size as it successfully moves downhill, as can be seen by plotting the successive points in Fig. 39.1.

The conjugate gradient algorithm finds the minimum on its second direction because the function is purely quadratic. Additional iterations would be needed for a more complicated function.

Here is another example using the Nelder-Mead Simplex algorithm to minimize the same example object function, as above.

```
int
main(void)
{
  double par[5] = {1.0, 2.0, 10.0, 20.0, 30.0};

  const gsl_multimin_fminimizer_type *T =
    gsl_multimin_fminimizer_nmsimplex2;
  gsl_multimin_fminimizer *s = NULL;
  gsl_vector *ss, *x;
  gsl_multimin_function minex_func;

  size_t iter = 0;
```

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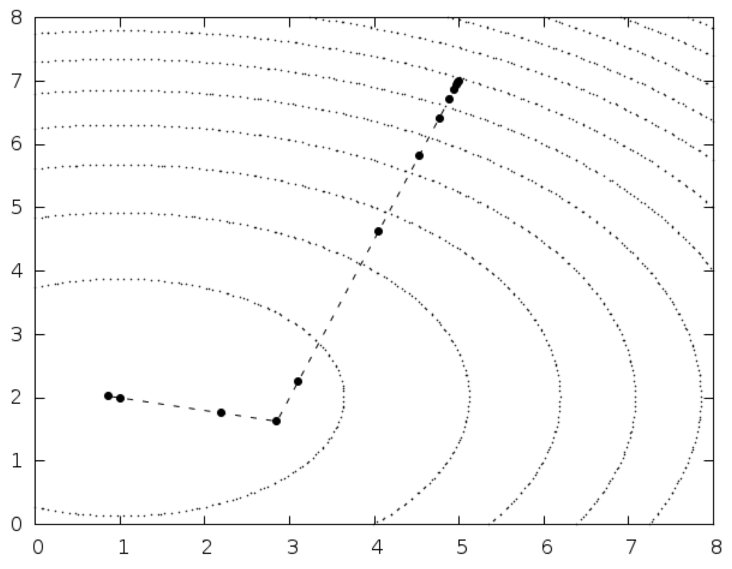

Fig. 39.1: Function contours with path taken by minimization algorithm

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```
  int status;
  double size;

  /* Starting point */
  x = gsl_vector_alloc (2);
  gsl_vector_set (x, 0, 5.0);
  gsl_vector_set (x, 1, 7.0);

  /* Set initial step sizes to 1 */
  ss = gsl_vector_alloc (2);
  gsl_vector_set_all (ss, 1.0);

  /* Initialize method and iterate */
  minex_func.n = 2;
  minex_func.f = my_f;
  minex_func.params = par;

  s = gsl_multimin_fminimizer_alloc (T, 2);
  gsl_multimin_fminimizer_set (s, &minex_func, x, ss);

  do
    {
      iter++;
      status = gsl_multimin_fminimizer_iterate(s);

      if (status)
        break;

      size = gsl_multimin_fminimizer_size (s);
      status = gsl_multimin_test_size (size, 1e-2);
```

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```
      if (status == GSL_SUCCESS)
        {
          printf ("converged to minimum at\n");
        }

      printf ("%5d %10.3e %10.3e f() = %7.3f size = %.3f\n",
              iter,
              gsl_vector_get (s->x, 0),
              gsl_vector_get (s->x, 1),
              s->fval, size);
    }
  while (status == GSL_CONTINUE && iter < 100);

  gsl_vector_free(x);
  gsl_vector_free(ss);
  gsl_multimin_fminimizer_free (s);

  return status;
}
```

The minimum search stops when the Simplex size drops to 0.01. The output is shown below.

```
    1  6.500e+00  5.000e+00 f() = 512.500 size = 1.130
    2  5.250e+00  4.000e+00 f() = 290.625 size = 1.409
    3  5.250e+00  4.000e+00 f() = 290.625 size = 1.409
    4  5.500e+00  1.000e+00 f() = 252.500 size = 1.409
    5  2.625e+00  3.500e+00 f() = 101.406 size = 1.847
    6  2.625e+00  3.500e+00 f() = 101.406 size = 1.847
    7  0.000e+00  3.000e+00 f() =  60.000 size = 1.847
    8  2.094e+00  1.875e+00 f() =  42.275 size = 1.321
    9  2.578e-01  1.906e+00 f() =  35.684 size = 1.069
   10  5.879e-01  2.445e+00 f() =  35.664 size = 0.841
   11  1.258e+00  2.025e+00 f() =  30.680 size = 0.476
   12  1.258e+00  2.025e+00 f() =  30.680 size = 0.367
   13  1.093e+00  1.849e+00 f() =  30.539 size = 0.300
   14  8.830e-01  2.004e+00 f() =  30.137 size = 0.172
   15  8.830e-01  2.004e+00 f() =  30.137 size = 0.126
   16  9.582e-01  2.060e+00 f() =  30.090 size = 0.106
   17  1.022e+00  2.004e+00 f() =  30.005 size = 0.063
   18  1.022e+00  2.004e+00 f() =  30.005 size = 0.043
   19  1.022e+00  2.004e+00 f() =  30.005 size = 0.043
   20  1.022e+00  2.004e+00 f() =  30.005 size = 0.027
   21  1.022e+00  2.004e+00 f() =  30.005 size = 0.022
   22  9.920e-01  1.997e+00 f() =  30.001 size = 0.016
   23  9.920e-01  1.997e+00 f() =  30.001 size = 0.013
converged to minimum at
   24  9.920e-01  1.997e+00 f() =  30.001 size = 0.008
```

The simplex size first increases, while the simplex moves towards the minimum. After a while the size begins to decrease as the simplex contracts around the minimum.

39.10 References and Further Reading

The conjugate gradient and BFGS methods are described in detail in the following book,

- R. Fletcher, *Practical Methods of Optimization (Second Edition)* Wiley (1987), ISBN 0471915475.

A brief description of multidimensional minimization algorithms and more recent references can be found in,

- C.W. Ueberhuber, *Numerical Computation (Volume 2)*, Chapter 14, Section 4.4 "Minimization Methods", p.: 325–335, Springer (1997), ISBN 3-540-62057-5.

The simplex algorithm is described in the following paper,

- J.A. Nelder and R. Mead, *A simplex method for function minimization*, Computer Journal vol.: 7 (1965), 308–313.

CHAPTER

FORTY

LINEAR LEAST-SQUARES FITTING

This chapter describes routines for performing least squares fits to experimental data using linear combinations of functions. The data may be weighted or unweighted, i.e. with known or unknown errors. For weighted data the functions compute the best fit parameters and their associated covariance matrix. For unweighted data the covariance matrix is estimated from the scatter of the points, giving a variance-covariance matrix.

The functions are divided into separate versions for simple one- or two-parameter regression and multiple-parameter fits.

40.1 Overview

Least-squares fits are found by minimizing χ^2 (chi-squared), the weighted sum of squared residuals over n experimental datapoints (x_i, y_i) for the model $Y(c, x)$,

$$\chi^2 = \sum_i w_i (y_i - Y(c, x_i))^2$$

The p parameters of the model are $c = \{c_0, c_1, \dots\}$. The weight factors w_i are given by $w_i = 1/\sigma_i^2$ where σ_i is the experimental error on the data-point y_i. The errors are assumed to be Gaussian and uncorrelated. For unweighted data the chi-squared sum is computed without any weight factors.

The fitting routines return the best-fit parameters c and their $p \times p$ covariance matrix. The covariance matrix measures the statistical errors on the best-fit parameters resulting from the errors on the data, σ_i, and is defined as

$$C_{ab} = \langle \delta c_a \delta c_b \rangle$$

where $\langle \, \rangle$ denotes an average over the Gaussian error distributions of the underlying datapoints.

The covariance matrix is calculated by error propagation from the data errors σ_i. The change in a fitted parameter δc_a caused by a small change in the data δy_i is given by

$$\delta c_a = \sum_i \frac{\partial c_a}{\partial y_i} \delta y_i$$

allowing the covariance matrix to be written in terms of the errors on the data,

$$C_{ab} = \sum_{i,j} \frac{\partial c_a}{\partial y_i} \frac{\partial c_b}{\partial y_j} \langle \delta y_i \delta y_j \rangle$$

For uncorrelated data the fluctuations of the underlying datapoints satisfy

$$\langle \delta y_i \delta y_j \rangle = \sigma_i^2 \delta_{ij}$$

giving a corresponding parameter covariance matrix of

$$C_{ab} = \sum_i \frac{1}{w_i} \frac{\partial c_a}{\partial y_i} \frac{\partial c_b}{\partial y_i}$$

When computing the covariance matrix for unweighted data, i.e. data with unknown errors, the weight factors w_i in this sum are replaced by the single estimate $w = 1/\sigma^2$, where σ^2 is the computed variance of the residuals about the best-fit model, $\sigma^2 = \sum (y_i - Y(c, x_i))^2/(n-p)$. This is referred to as the *variance-covariance matrix*.

The standard deviations of the best-fit parameters are given by the square root of the corresponding diagonal elements of the covariance matrix, $\sigma_{c_a} = \sqrt{C_{aa}}$. The correlation coefficient of the fit parameters c_a and c_b is given by $\rho_{ab} = C_{ab}/\sqrt{C_{aa}C_{bb}}$.

40.2 Linear regression

The functions in this section are used to fit simple one or two parameter linear regression models. The functions are declared in the header file `gsl_fit.h`.

40.2.1 Linear regression with a constant term

The functions described in this section can be used to perform least-squares fits to a straight line model, $Y(c, x) = c_0 + c_1 x$.

int **gsl_fit_linear**(const double *x, const size_t xstride, const double *y, const size_t ystride, size_t n, double *c0, double *c1, double *cov00, double *cov01, double *cov11, double *sumsq)

This function computes the best-fit linear regression coefficients (`c0`, `c1`) of the model $Y = c_0 + c_1 X$ for the dataset (`x`, `y`), two vectors of length `n` with strides `xstride` and `ystride`. The errors on `y` are assumed unknown so the variance-covariance matrix for the parameters (`c0`, `c1`) is estimated from the scatter of the points around the best-fit line and returned via the parameters (`cov00`, `cov01`, `cov11`). The sum of squares of the residuals from the best-fit line is returned in `sumsq`. Note: the correlation coefficient of the data can be computed using `gsl_stats_correlation()`, it does not depend on the fit.

int **gsl_fit_wlinear**(const double *x, const size_t xstride, const double *w, const size_t wstride, const double *y, const size_t ystride, size_t n, double *c0, double *c1, double *cov00, double *cov01, double *cov11, double *chisq)

This function computes the best-fit linear regression coefficients (`c0`, `c1`) of the model $Y = c_0 + c_1 X$ for the weighted dataset (`x`, `y`), two vectors of length `n` with strides `xstride` and `ystride`. The vector `w`, of length `n` and stride `wstride`, specifies the weight of each datapoint. The weight is the reciprocal of the variance for each datapoint in `y`.

The covariance matrix for the parameters (`c0`, `c1`) is computed using the weights and returned via the parameters (`cov00`, `cov01`, `cov11`). The weighted sum of squares of the residuals from the best-fit line, χ^2, is returned in `chisq`.

int **gsl_fit_linear_est**(double x, double c0, double c1, double cov00, double cov01, double cov11, double *y, double *y_err)

This function uses the best-fit linear regression coefficients `c0`, `c1` and their covariance `cov00`, `cov01`, `cov11` to compute the fitted function `y` and its standard deviation `y_err` for the model $Y = c_0 + c_1 X$ at the point `x`.

40.2.2 Linear regression without a constant term

The functions described in this section can be used to perform least-squares fits to a straight line model without a constant term, $Y = c_1 X$.

int **gsl_fit_mul**(const double *x, const size_t xstride, const double *y, const size_t ystride, size_t n, double *c1, double *cov11, double *sumsq)

This function computes the best-fit linear regression coefficient *c1* of the model $Y = c_1 X$ for the datasets (*x*, *y*), two vectors of length *n* with strides *xstride* and *ystride*. The errors on *y* are assumed unknown so the variance of the parameter *c1* is estimated from the scatter of the points around the best-fit line and returned via the parameter *cov11*. The sum of squares of the residuals from the best-fit line is returned in *sumsq*.

int **gsl_fit_wmul**(const double *x, const size_t xstride, const double *w, const size_t wstride, const double *y, const size_t ystride, size_t n, double *c1, double *cov11, double *sumsq)

This function computes the best-fit linear regression coefficient *c1* of the model $Y = c_1 X$ for the weighted datasets (*x*, *y*), two vectors of length *n* with strides *xstride* and *ystride*. The vector *w*, of length *n* and stride *wstride*, specifies the weight of each datapoint. The weight is the reciprocal of the variance for each datapoint in *y*.

The variance of the parameter *c1* is computed using the weights and returned via the parameter *cov11*. The weighted sum of squares of the residuals from the best-fit line, χ^2, is returned in `chisq`.

int **gsl_fit_mul_est**(double x, double c1, double cov11, double *y, double *y_err)

This function uses the best-fit linear regression coefficient *c1* and its covariance *cov11* to compute the fitted function *y* and its standard deviation *y_err* for the model $Y = c_1 X$ at the point *x*.

40.3 Multi-parameter regression

This section describes routines which perform least squares fits to a linear model by minimizing the cost function

$$\chi^2 = \sum_i w_i (y_i - \sum_j X_{ij} c_j)^2 = ||y - Xc||_W^2$$

where y is a vector of n observations, X is an n-by-p matrix of predictor variables, c is a vector of the p unknown best-fit parameters to be estimated, and $||r||_W^2 = r^T W r$. The matrix $W = \mathrm{diag}(w_1, w_2, ..., w_n)$ defines the weights or uncertainties of the observation vector.

This formulation can be used for fits to any number of functions and/or variables by preparing the n-by-p matrix X appropriately. For example, to fit to a p-th order polynomial in `x`, use the following matrix,

$$X_{ij} = x_i^j$$

where the index i runs over the observations and the index j runs from 0 to $p - 1$.

To fit to a set of p sinusoidal functions with fixed frequencies $\omega_1, \omega_2, \ldots, \omega_p$, use,

$$X_{ij} = \sin(\omega_j x_i)$$

To fit to p independent variables $x_1, x_2, \ldots, x_p$, use,

$$X_{ij} = x_j(i)$$

where $x_j(i)$ is the i-th value of the predictor variable x_j.

The solution of the general linear least-squares system requires an additional working space for intermediate results, such as the singular value decomposition of the matrix X.

These functions are declared in the header file `gsl_multifit.h`.

type **gsl_multifit_linear_workspace**

This workspace contains internal variables for fitting multi-parameter models.

gsl_multifit_linear_workspace ***gsl_multifit_linear_alloc**(const size_t n, const size_t p)

This function allocates a workspace for fitting a model to a maximum of `n` observations using a maximum of `p` parameters. The user may later supply a smaller least squares system if desired. The size of the workspace is $O(np + p^2)$.

void **gsl_multifit_linear_free**(*gsl_multifit_linear_workspace* *work)

This function frees the memory associated with the workspace `w`.

int **gsl_multifit_linear_svd**(const *gsl_matrix* *X, *gsl_multifit_linear_workspace* *work)

This function performs a singular value decomposition of the matrix `X` and stores the SVD factors internally in `work`.

int **gsl_multifit_linear_bsvd**(const *gsl_matrix* *X, *gsl_multifit_linear_workspace* *work)

This function performs a singular value decomposition of the matrix `X` and stores the SVD factors internally in `work`. The matrix `X` is first balanced by applying column scaling factors to improve the accuracy of the singular values.

int **gsl_multifit_linear**(const *gsl_matrix* *X, const *gsl_vector* *y, *gsl_vector* *c, *gsl_matrix* *cov, double *chisq, *gsl_multifit_linear_workspace* *work)

This function computes the best-fit parameters `c` of the model $y = Xc$ for the observations `y` and the matrix of predictor variables `X`, using the preallocated workspace provided in `work`. The p-by-p variance-covariance matrix of the model parameters `cov` is set to $\sigma^2(X^T X)^{-1}$, where σ is the standard deviation of the fit residuals. The sum of squares of the residuals from the best-fit, χ^2, is returned in `chisq`. If the coefficient of determination is desired, it can be computed from the expression $R^2 = 1 - \chi^2/TSS$, where the total sum of squares (TSS) of the observations `y` may be computed from `gsl_stats_tss()`.

The best-fit is found by singular value decomposition of the matrix `X` using the modified Golub-Reinsch SVD algorithm, with column scaling to improve the accuracy of the singular values. Any components which have zero singular value (to machine precision) are discarded from the fit.

int **gsl_multifit_linear_tsvd**(const *gsl_matrix* *X, const *gsl_vector* *y, const double tol, *gsl_vector* *c, *gsl_matrix* *cov, double *chisq, size_t *rank, *gsl_multifit_linear_workspace* *work)

This function computes the best-fit parameters `c` of the model $y = Xc$ for the observations `y` and the matrix of predictor variables `X`, using a truncated SVD expansion. Singular values which satisfy $s_i \leq tol \times s_0$ are discarded from the fit, where s_0 is the largest singular value. The p-by-p variance-covariance matrix of the model parameters `cov` is set to $\sigma^2(X^T X)^{-1}$, where σ is the standard deviation of the fit residuals. The sum of squares of the residuals from the best-fit, χ^2, is returned in `chisq`. The effective rank (number of singular values used in solution) is returned in `rank`. If the coefficient of determination is desired, it can be computed from the expression $R^2 = 1 - \chi^2/TSS$, where the total sum of squares (TSS) of the observations `y` may be computed from `gsl_stats_tss()`.

int **gsl_multifit_wlinear**(const *gsl_matrix* *X, const *gsl_vector* *w, const *gsl_vector* *y, *gsl_vector* *c, *gsl_matrix* *cov, double *chisq, *gsl_multifit_linear_workspace* *work)

This function computes the best-fit parameters `c` of the weighted model $y = Xc$ for the observations `y` with weights `w` and the matrix of predictor variables `X`, using the preallocated workspace provided in `work`. The p-by-p covariance matrix of the model parameters `cov` is computed as $(X^T W X)^{-1}$. The weighted sum of squares of the residuals from the best-fit, χ^2, is returned in `chisq`. If the coefficient of determination is desired, it can be computed from the expression $R^2 = 1 - \chi^2/WTSS$, where the weighted total sum of squares (WTSS) of the observations `y` may be computed from `gsl_stats_wtss()`.

int **gsl_multifit_wlinear_tsvd**(const *gsl_matrix* *X, const *gsl_vector* *w, const *gsl_vector* *y, const double tol, *gsl_vector* *c, *gsl_matrix* *cov, double *chisq, size_t *rank, *gsl_multifit_linear_workspace* *work)

This function computes the best-fit parameters `c` of the weighted model $y = Xc$ for the observations `y` with weights `w` and the matrix of predictor variables `X`, using a truncated SVD expansion. Singular values which satisfy $s_i \leq tol \times s_0$ are discarded from the fit, where s_0 is the largest singular value. The p-by-p covariance matrix of the model parameters `cov` is computed as $(X^T W X)^{-1}$. The weighted sum of squares of the residuals from the best-fit, χ^2, is returned in `chisq`. The effective rank of the system (number of singular values used in the solution) is returned in `rank`. If the coefficient of determination is desired, it can be computed from the expression $R^2 = 1 - \chi^2/WTSS$, where the weighted total sum of squares (WTSS) of the observations `y` may be computed from `gsl_stats_wtss()`.

int **gsl_multifit_linear_est**(const *gsl_vector* *x, const *gsl_vector* *c, const *gsl_matrix* *cov, double *y, double *y_err)

This function uses the best-fit multilinear regression coefficients `c` and their covariance matrix `cov` to compute the fitted function value `y` and its standard deviation `y_err` for the model $y = x.c$ at the point `x`.

int **gsl_multifit_linear_residuals**(const *gsl_matrix* *X, const *gsl_vector* *y, const *gsl_vector* *c, *gsl_vector* *r)

This function computes the vector of residuals $r = y - Xc$ for the observations `y`, coefficients `c` and matrix of predictor variables `X`.

size_t **gsl_multifit_linear_rank**(const double tol, const *gsl_multifit_linear_workspace* *work)

This function returns the rank of the matrix X which must first have its singular value decomposition computed. The rank is computed by counting the number of singular values σ_j which satisfy $\sigma_j > tol \times \sigma_0$, where σ_0 is the largest singular value.

40.4 Regularized regression

Ordinary weighted least squares models seek a solution vector c which minimizes the residual

$$\chi^2 = ||y - Xc||_W^2$$

where y is the n-by-1 observation vector, X is the n-by-p design matrix, c is the p-by-1 solution vector, $W = \mathrm{diag}(w_1, ..., w_n)$ is the data weighting matrix, and $||r||_W^2 = r^T W r$. In cases where the least squares matrix X is ill-conditioned, small perturbations (ie: noise) in the observation vector could lead to widely different solution vectors c. One way of dealing with ill-conditioned matrices is to use a "truncated SVD" in which small singular values, below some given tolerance, are discarded from the solution. The truncated SVD method is available using the functions `gsl_multifit_linear_tsvd()` and `gsl_multifit_wlinear_tsvd()`. Another way to help solve ill-posed problems is to include a regularization term in the least squares minimization

$$\chi^2 = ||y - Xc||_W^2 + \lambda^2 ||Lc||^2$$

for a suitably chosen regularization parameter λ and matrix L. This type of regularization is known as Tikhonov, or ridge, regression. In some applications, L is chosen as the identity matrix, giving preference to solution vectors c with smaller norms. Including this regularization term leads to the explicit "normal equations" solution

$$c = \left(X^T W X + \lambda^2 L^T L\right)^{-1} X^T W y$$

which reduces to the ordinary least squares solution when $L = 0$. In practice, it is often advantageous to transform a regularized least squares system into the form

$$\chi^2 = ||\tilde{y} - \tilde{X}\tilde{c}||^2 + \lambda^2 ||\tilde{c}||^2$$

This is known as the Tikhonov "standard form" and has the normal equations solution

$$\tilde{c} = \left(\tilde{X}^T \tilde{X} + \lambda^2 I\right)^{-1} \tilde{X}^T \tilde{y}$$

For an m-by-p matrix L which is full rank and has $m >= p$ (ie: L is square or has more rows than columns), we can calculate the "thin" QR decomposition of L, and note that $||Lc|| = ||Rc||$ since the Q factor will not change the norm. Since R is p-by-p, we can then use the transformation

$$\tilde{X} = W^{\frac{1}{2}} X R^{-1}$$
$$\tilde{y} = W^{\frac{1}{2}} y$$
$$\tilde{c} = Rc$$

to achieve the standard form. For a rectangular matrix L with $m < p$, a more sophisticated approach is needed (see Hansen 1998, chapter 2.3). In practice, the normal equations solution above is not desirable due to numerical instabilities, and so the system is solved using the singular value decomposition of the matrix $\tilde{X}$. The matrix L is often chosen as the identity matrix, or as a first or second finite difference operator, to ensure a smoothly varying coefficient vector c, or as a diagonal matrix to selectively damp each model parameter differently. If $L \neq I$, the user must first convert the least squares problem to standard form using `gsl_multifit_linear_stdform1()` or `gsl_multifit_linear_stdform2()`, solve the system, and then backtransform the solution vector to recover the solution of the original problem (see `gsl_multifit_linear_genform1()` and `gsl_multifit_linear_genform2()`).

In many regularization problems, care must be taken when choosing the regularization parameter λ. Since both the residual norm $||y - Xc||$ and solution norm $||Lc||$ are being minimized, the parameter λ represents a tradeoff between minimizing either the residuals or the solution vector. A common tool for visualizing the comprimise between the minimization of these two quantities is known as the L-curve. The L-curve is a log-log plot of the residual norm $||y - Xc||$ on the horizontal axis and the solution norm $||Lc||$ on the vertical axis. This curve nearly always as an L shaped appearance, with a distinct corner separating the horizontal and vertical sections of the curve. The regularization parameter corresponding to this corner is often chosen as the optimal value. GSL provides routines to calculate the L-curve for all relevant regularization parameters as well as locating the corner.

Another method of choosing the regularization parameter is known as Generalized Cross Validation (GCV). This method is based on the idea that if an arbitrary element y_i is left out of the right hand side, the resulting regularized solution should predict this element accurately. This leads to choosing the parameter λ which minimizes the GCV function

$$G(\lambda) = \frac{||y - Xc_\lambda||^2}{\text{Tr}(I_n - XX^I_\lambda)^2}$$

where X^I_λ is the matrix which relates the solution c_λ to the right hand side y, ie: $c_\lambda = X^I_\lambda y$. GSL provides routines to compute the GCV curve and its minimum.

For most applications, the steps required to solve a regularized least squares problem are as follows:

1. Construct the least squares system (X, y, W, L)
2. Transform the system to standard form ($\tilde{X}$, $\tilde{y}$). This step can be skipped if $L = I_p$ and $W = I_n$.
3. Calculate the SVD of $\tilde{X}$.
4. Determine an appropriate regularization parameter λ (using for example L-curve or GCV analysis).
5. Solve the standard form system using the chosen λ and the SVD of $\tilde{X}$.
6. Backtransform the standard form solution $\tilde{c}$ to recover the original solution vector c.

int **gsl_multifit_linear_stdform1**(const *gsl_vector* *L, const *gsl_matrix* *X, const *gsl_vector* *y, *gsl_matrix* *Xs, *gsl_vector* *ys, *gsl_multifit_linear_workspace* *work)

int **gsl_multifit_linear_wstdform1**(const *gsl_vector* *L, const *gsl_matrix* *X, const *gsl_vector* *w, const *gsl_vector* *y, *gsl_matrix* *Xs, *gsl_vector* *ys, *gsl_multifit_linear_workspace* *work)

These functions define a regularization matrix $L = \text{diag}(l_0, l_1, ..., l_{p-1})$. The diagonal matrix element l_i is provided by the i-th element of the input vector `L`. The n-by-p least squares matrix `X` and vector `y` of length n are then converted to standard form as described above and the parameters $(\tilde{X}, \tilde{y})$ are stored in `Xs` and `ys` on output. `Xs` and `ys` have the same dimensions as `X` and `y`. Optional data weights may be supplied in the vector `w` of length n. In order to apply this transformation, L^{-1} must exist and so none of the l_i may be zero. After the standard form system has been solved, use `gsl_multifit_linear_genform1()` to recover the original solution vector. It is allowed to have `X` = `Xs` and `y` = `ys` for an in-place transform. In order to perform a weighted regularized fit with $L = I$, the user may call `gsl_multifit_linear_applyW()` to convert to standard form.

int **gsl_multifit_linear_L_decomp**(*gsl_matrix* *L, *gsl_vector* *tau)

This function factors the m-by-p regularization matrix `L` into a form needed for the later transformation to standard form. `L` may have any number of rows m. If $m \geq p$ the QR decomposition of `L` is computed and stored in `L` on output. If $m < p$, the QR decomposition of L^T is computed and stored in `L` on output. On output, the Householder scalars are stored in the vector `tau` of size $MIN(m, p)$. These outputs will be used by `gsl_multifit_linear_wstdform2()` to complete the transformation to standard form.

int **gsl_multifit_linear_stdform2**(const *gsl_matrix* *LQR, const *gsl_vector* *Ltau, const *gsl_matrix* *X, const *gsl_vector* *y, *gsl_matrix* *Xs, *gsl_vector* *ys, *gsl_matrix* *M, *gsl_multifit_linear_workspace* *work)

int **gsl_multifit_linear_wstdform2**(const *gsl_matrix* *LQR, const *gsl_vector* *Ltau, const *gsl_matrix* *X, const *gsl_vector* *w, const *gsl_vector* *y, *gsl_matrix* *Xs, *gsl_vector* *ys, *gsl_matrix* *M, *gsl_multifit_linear_workspace* *work)

These functions convert the least squares system (`X`, `y`, `W`, L) to standard form $(\tilde{X}, \tilde{y})$ which are stored in `Xs` and `ys` respectively. The m-by-p regularization matrix `L` is specified by the inputs `LQR` and `Ltau`, which are outputs from `gsl_multifit_linear_L_decomp()`. The dimensions of the standard form parameters $(\tilde{X}, \tilde{y})$ depend on whether m is larger or less than p. For $m \geq p$, `Xs` is n-by-p, `ys` is n-by-1, and `M` is not used. For $m < p$, `Xs` is $(n-p+m)$-by-m, `ys` is $(n-p+m)$-by-1, and `M` is additional n-by-p workspace, which is required to recover the original solution vector after the system has been solved (see `gsl_multifit_linear_genform2()`). Optional data weights may be supplied in the vector `w` of length n, where $W = \text{diag}(w)$.

int **gsl_multifit_linear_solve**(const double lambda, const *gsl_matrix* *Xs, const *gsl_vector* *ys, *gsl_vector* *cs, double *rnorm, double *snorm, *gsl_multifit_linear_workspace* *work)

This function computes the regularized best-fit parameters $\tilde{c}$ which minimize the cost function $\chi^2 = ||\tilde{y} - \tilde{X}\tilde{c}||^2 + \lambda^2||\tilde{c}||^2$ which is in standard form. The least squares system must therefore be converted to standard form prior to calling this function. The observation vector $\tilde{y}$ is provided in `ys` and the matrix of predictor variables $\tilde{X}$ in `Xs`. The solution vector $\tilde{c}$ is returned in `cs`, which has length min(m, p). The SVD of `Xs` must be computed prior to calling this function, using `gsl_multifit_linear_svd()`. The regularization parameter λ is provided in `lambda`. The residual norm $||\tilde{y} - \tilde{X}\tilde{c}|| = ||y - Xc||_W$ is returned in `rnorm`. The solution norm $||\tilde{c}|| = ||Lc||$ is returned in `snorm`.

int **gsl_multifit_linear_genform1**(const *gsl_vector* *L, const *gsl_vector* *cs, *gsl_vector* *c, *gsl_multifit_linear_workspace* *work)

After a regularized system has been solved with $L = \text{diag}(_0, _1, ..., _{p-1})$, this function backtransforms the standard form solution vector `cs` to recover the solution vector of the original problem `c`. The diagonal matrix elements l_i are provided in the vector `L`. It is allowed to have `c` = `cs` for an in-place transform.

int **gsl_multifit_linear_genform2**(const *gsl_matrix* *LQR, const *gsl_vector* *Ltau, const *gsl_matrix* *X, const *gsl_vector* *y, const *gsl_vector* *cs, const *gsl_matrix* *M, *gsl_vector* *c, *gsl_multifit_linear_workspace* *work)

int **gsl_multifit_linear_wgenform2**(const *gsl_matrix* *LQR, const *gsl_vector* *Ltau, const *gsl_matrix* *X, const *gsl_vector* *w, const *gsl_vector* *y, const *gsl_vector* *cs, const *gsl_matrix* *M, *gsl_vector* *c, *gsl_multifit_linear_workspace* *work)

After a regularized system has been solved with a general rectangular matrix L, specified by (`LQR`, `Ltau`), this function backtransforms the standard form solution `cs` to recover the solution vector of the original problem, which is stored in `c`, of length p. The original least squares matrix and observation vector are provided in `X` and `y` respectively. `M` is the matrix computed by `gsl_multifit_linear_stdform2()`. For weighted fits, the weight vector `w` must also be supplied.

int **gsl_multifit_linear_applyW**(const *gsl_matrix* *X, const *gsl_vector* *w, const *gsl_vector* *y, *gsl_matrix* *WX, *gsl_vector* *Wy)

For weighted least squares systems with $L = I$, this function may be used to convert the system to standard form by applying the weight matrix $W = \text{diag}(w)$ to the least squares matrix `X` and observation vector `y`. On output, `WX` is equal to $W^{1/2}X$ and `Wy` is equal to $W^{1/2}y$. It is allowed for `WX` = `X` and `Wy` = `y` for an in-place transform.

int **gsl_multifit_linear_lcurve**(const *gsl_vector* *y, *gsl_vector* *reg_param, *gsl_vector* *rho, *gsl_vector* *eta, *gsl_multifit_linear_workspace* *work)

This function computes the L-curve for a least squares system using the right hand side vector `y` and the SVD decomposition of the least squares matrix `X`, which must be provided to `gsl_multifit_linear_svd()` prior to calling this function. The output vectors `reg_param`, `rho`, and `eta` must all be the same size, and will contain the regularization parameters λ_i, residual norms $||y - Xc_i||$, and solution norms $||Lc_i||$ which compose the L-curve, where c_i is the regularized solution vector corresponding to λ_i. The user may determine the number of points on the L-curve by adjusting the size of these input arrays. The regularization parameters λ_i are estimated from the singular values of `X`, and chosen to represent the most relevant portion of the L-curve.

int **gsl_multifit_linear_lcurvature**(const *gsl_vector* *y, const *gsl_vector* *reg_param, const *gsl_vector* *rho, const *gsl_vector* *eta, *gsl_vector* *kappa, *gsl_multifit_linear_workspace* *work)

This function computes the curvature of the L-curve as a function of the regularization parameter λ, using the right hand side vector `y`, the vector of regularization parameters, `reg_param`, vector of residual norms, `rho`, and vector of solution norms, `eta`. The arrays `reg_param`, `rho`, and `eta` can be computed by `gsl_multifit_linear_lcurve()`. The curvature is defined as

$$\kappa(\lambda) = \frac{\hat{\rho}'\hat{\eta}'' - \hat{\rho}''\hat{\eta}'}{\left((\hat{\rho}')^2 + (\hat{\eta}')^2\right)^{\frac{3}{2}}}$$

where $\hat{\rho}(\lambda) = \log ||y - Xc_\lambda||$ and $\hat{\eta}(\lambda) = \log ||Lc_\lambda||$. The curvature values are stored in `kappa` on output.

int **gsl_multifit_linear_lcorner**(const *gsl_vector* *rho, const *gsl_vector* *eta, size_t *idx)

This function attempts to locate the corner of the L-curve $(||y - Xc||, ||Lc||)$ defined by the `rho` and `eta` input arrays respectively. The corner is defined as the point of maximum curvature of the L-curve in log-log scale. The `rho` and `eta` arrays can be outputs of `gsl_multifit_linear_lcurve()`. The algorithm used simply fits a circle to 3 consecutive points on the L-curve and uses the circle's radius to determine the curvature at the middle point. Therefore, the input array sizes must be ≥ 3. With more points provided for the L-curve, a better estimate of the curvature can be obtained. The array index corresponding to maximum curvature (ie: the corner) is returned in `idx`. If the input arrays contain colinear points, this function could fail and return `GSL_EINVAL`.

int **gsl_multifit_linear_lcorner2**(const *gsl_vector* *reg_param, const *gsl_vector* *eta, size_t *idx)

This function attempts to locate the corner of an alternate L-curve $(\lambda^2, ||Lc||^2)$ studied by Rezghi and Hosseini, 2009. This alternate L-curve can provide better estimates of the regularization parameter for smooth solution vectors. The regularization parameters λ and solution norms $||Lc||$ are provided in the `reg_param` and `eta` input arrays respectively. The corner is defined as the point of maximum curvature of this alternate L-curve in linear scale. The `reg_param` and `eta` arrays can be outputs of `gsl_multifit_linear_lcurve()`. The algorithm used simply fits a circle to 3 consecutive points on the L-curve and uses the circle's radius to determine the curvature at the middle point. Therefore, the input array sizes must be ≥ 3. With more points provided for the L-curve, a better estimate of the curvature can be obtained. The array index corresponding to maximum curvature (ie: the corner) is returned in `idx`. If the input arrays contain colinear points, this function could fail and return `GSL_EINVAL`.

int **gsl_multifit_linear_gcv_init**(const *gsl_vector* *y, *gsl_vector* *reg_param, *gsl_vector* *UTy, double *delta0, *gsl_multifit_linear_workspace* *work)

This function performs some initialization in preparation for computing the GCV curve and its minimum. The right hand side vector is provided in `y`. On output, `reg_param` is set to a vector of regularization parameters in decreasing order and may be of any size. The vector *UTy* of size p is set to $U^T y$. The parameter *delta0* is needed for subsequent steps of the GCV calculation.

int **gsl_multifit_linear_gcv_curve**(const *gsl_vector* *reg_param, const *gsl_vector* *UTy, const double delta0, *gsl_vector* *G, *gsl_multifit_linear_workspace* *work)

This funtion calculates the GCV curve $G(\lambda)$ and stores it in *G* on output, which must be the same size as *reg_param*. The inputs *reg_param*, *UTy* and *delta0* are computed in `gsl_multifit_linear_gcv_init()`.

int **gsl_multifit_linear_gcv_min**(const *gsl_vector* *reg_param, const *gsl_vector* *UTy, const *gsl_vector* *G, const double delta0, double *lambda, *gsl_multifit_linear_workspace* *work)

This function computes the value of the regularization parameter which minimizes the GCV curve $G(\lambda)$ and stores it in *lambda*. The input *G* is calculated by `gsl_multifit_linear_gcv_curve()` and the inputs *reg_param*, *UTy* and *delta0* are computed by `gsl_multifit_linear_gcv_init()`.

double **gsl_multifit_linear_gcv_calc**(const double lambda, const *gsl_vector* *UTy, const double delta0, *gsl_multifit_linear_workspace* *work)

This function returns the value of the GCV curve $G(\lambda)$ corresponding to the input *lambda*.

int **gsl_multifit_linear_gcv**(const *gsl_vector* *y, *gsl_vector* *reg_param, *gsl_vector* *G, double *lambda, double *G_lambda, *gsl_multifit_linear_workspace* *work)

This function combines the steps `gcv_init`, `gcv_curve`, and `gcv_min` defined above into a single function. The input *y* is the right hand side vector. On output, *reg_param* and *G*, which must be the same size, are set to vectors of λ and $G(\lambda)$ values respectively. The output *lambda* is set to the optimal value of λ which minimizes the GCV curve. The minimum value of the GCV curve is returned in *G_lambda*.

int **gsl_multifit_linear_Lk**(const size_t p, const size_t k, *gsl_matrix* *L)

This function computes the discrete approximation to the derivative operator L_k of order *k* on a regular grid of *p* points and stores it in *L*. The dimensions of *L* are $(p - k)$-by-p.

int **gsl_multifit_linear_Lsobolev**(const size_t p, const size_t kmax, const *gsl_vector* *alpha, *gsl_matrix* *L, *gsl_multifit_linear_workspace* *work)

This function computes the regularization matrix *L* corresponding to the weighted Sobolov norm $||Lc||^2 = \sum_k \alpha_k^2 ||L_k c||^2$ where L_k approximates the derivative operator of order k. This regularization norm can be useful in applications where it is necessary to smooth several derivatives of the solution. *p* is the number of model parameters, *kmax* is the highest derivative to include in the summation above, and *alpha* is the vector of weights of size *kmax* + 1, where `alpha[k]` = α_k is the weight assigned to the derivative of order k. The output matrix *L* is size *p*-by-*p* and upper triangular.

double **gsl_multifit_linear_rcond**(const *gsl_multifit_linear_workspace* *work)

This function returns the reciprocal condition number of the least squares matrix X, defined as the ratio of the smallest and largest singular values, rcond = $\sigma_{min}/\sigma_{max}$. The routine `gsl_multifit_linear_svd()` must first be called to compute the SVD of X.

40.5 Robust linear regression

Ordinary least squares (OLS) models are often heavily influenced by the presence of outliers. Outliers are data points which do not follow the general trend of the other observations, although there is strictly no precise definition of an outlier. Robust linear regression refers to regression algorithms which are robust to outliers. The most common type of robust regression is M-estimation. The general M-estimator minimizes the objective function

$$\sum_i \rho(e_i) = \sum_i \rho(y_i - Y(c, x_i))$$

where $e_i = y_i - Y(c, x_i)$ is the residual of the ith data point, and $\rho(e_i)$ is a function which should have the following properties:

- $\rho(e) \geq 0$

- $\rho(0) = 0$
- $\rho(-e) = \rho(e)$
- $\rho(e_1) > \rho(e_2)$ for $|e_1| > |e_2|$

The special case of ordinary least squares is given by $\rho(e_i) = e_i^2$. Letting $\psi = \rho'$ be the derivative of ρ, differentiating the objective function with respect to the coefficients c and setting the partial derivatives to zero produces the system of equations

$$\sum_i \psi(e_i) X_i = 0$$

where X_i is a vector containing row i of the design matrix X. Next, we define a weight function $w(e) = \psi(e)/e$, and let $w_i = w(e_i)$:

$$\sum_i w_i e_i X_i = 0$$

This system of equations is equivalent to solving a weighted ordinary least squares problem, minimizing $\chi^2 = \sum_i w_i e_i^2$. The weights however, depend on the residuals e_i, which depend on the coefficients c, which depend on the weights. Therefore, an iterative solution is used, called Iteratively Reweighted Least Squares (IRLS).

1. Compute initial estimates of the coefficients $c^{(0)}$ using ordinary least squares
2. For iteration k, form the residuals $e_i^{(k)} = (y_i - X_i c^{(k-1)})/(t\sigma^{(k)}\sqrt{1 - h_i})$, where t is a tuning constant depending on the choice of ψ, and h_i are the statistical leverages (diagonal elements of the matrix $X(X^T X)^{-1} X^T$). Including t and h_i in the residual calculation has been shown to improve the convergence of the method. The residual standard deviation is approximated as $\sigma^{(k)} = MAD/0.6745$, where MAD is the Median-Absolute-Deviation of the $n - p$ largest residuals from the previous iteration.
3. Compute new weights $w_i^{(k)} = \psi(e_i^{(k)})/e_i^{(k)}$.
4. Compute new coefficients $c^{(k)}$ by solving the weighted least squares problem with weights $w_i^{(k)}$.
5. Steps 2 through 4 are iterated until the coefficients converge or until some maximum iteration limit is reached. Coefficients are tested for convergence using the critera:

   $$|c_i^{(k)} - c_i^{(k-1)}| \le \epsilon \times \max(|c_i^{(k)}|, |c_i^{(k-1)}|)$$

   for all $0 \le i < p$ where ϵ is a small tolerance factor.

The key to this method lies in selecting the function $\psi(e_i)$ to assign smaller weights to large residuals, and larger weights to smaller residuals. As the iteration proceeds, outliers are assigned smaller and smaller weights, eventually having very little or no effect on the fitted model.

type **gsl_multifit_robust_workspace**

This workspace is used for robust least squares fitting.

gsl_multifit_robust_workspace ***gsl_multifit_robust_alloc**(const *gsl_multifit_robust_type* *T, const size_t n, const size_t p)

This function allocates a workspace for fitting a model to `n` observations using `p` parameters. The size of the workspace is $O(np + p^2)$. The type `T` specifies the function ψ and can be selected from the following choices.

type **gsl_multifit_robust_type**

gsl_multifit_robust_type ***gsl_multifit_robust_default**

This specifies the `gsl_multifit_robust_bisquare` type (see below) and is a good general purpose choice for robust regression.

gsl_multifit_robust_type ***gsl_multifit_robust_bisquare***

This is Tukey's biweight (bisquare) function and is a good general purpose choice for robust regression. The weight function is given by

$$w(e) = \begin{cases} (1-e^2)^2, & |e| \le 1 \\ 0, & |e| > 1 \end{cases}$$

and the default tuning constant is $t = 4.685$.

gsl_multifit_robust_type ***gsl_multifit_robust_cauchy***

This is Cauchy's function, also known as the Lorentzian function. This function does not guarantee a unique solution, meaning different choices of the coefficient vector `c` could minimize the objective function. Therefore this option should be used with care. The weight function is given by

$$w(e) = \frac{1}{1+e^2}$$

and the default tuning constant is $t = 2.385$.

gsl_multifit_robust_type ***gsl_multifit_robust_fair***

This is the fair ρ function, which guarantees a unique solution and has continuous derivatives to three orders. The weight function is given by

$$w(e) = \frac{1}{1+|e|}$$

and the default tuning constant is $t = 1.400$.

gsl_multifit_robust_type ***gsl_multifit_robust_huber***

This specifies Huber's ρ function, which is a parabola in the vicinity of zero and increases linearly for a given threshold $|e| > t$. This function is also considered an excellent general purpose robust estimator, however, occasional difficulties can be encountered due to the discontinuous first derivative of the ψ function. The weight function is given by

$$w(e) = \begin{cases} 1, & |e| \le 1 \\ \frac{1}{|e|}, & |e| > 1 \end{cases}$$

and the default tuning constant is $t = 1.345$.

gsl_multifit_robust_type ***gsl_multifit_robust_ols***

This specifies the ordinary least squares solution, which can be useful for quickly checking the difference between the various robust and OLS solutions. The weight function is given by

$$w(e) = 1$$

and the default tuning constant is $t = 1$.

gsl_multifit_robust_type ***gsl_multifit_robust_welsch***

This specifies the Welsch function which can perform well in cases where the residuals have an exponential distribution. The weight function is given by

$$w(e) = \exp\left(-e^2\right)$$

and the default tuning constant is $t = 2.985$.

void **gsl_multifit_robust_free**(*gsl_multifit_robust_workspace* *w)

This function frees the memory associated with the workspace `w`.

const char ***gsl_multifit_robust_name**(const *gsl_multifit_robust_workspace* *w)

This function returns the name of the robust type `T` specified to `gsl_multifit_robust_alloc()`.

int **gsl_multifit_robust_tune**(const double tune, *gsl_multifit_robust_workspace* *w)

This function sets the tuning constant t used to adjust the residuals at each iteration to `tune`. Decreasing the tuning constant increases the downweight assigned to large residuals, while increasing the tuning constant decreases the downweight assigned to large residuals.

int **gsl_multifit_robust_maxiter**(const size_t maxiter, *gsl_multifit_robust_workspace* *w)

This function sets the maximum number of iterations in the iteratively reweighted least squares algorithm to `maxiter`. By default, this value is set to 100 by `gsl_multifit_robust_alloc()`.

int **gsl_multifit_robust_weights**(const *gsl_vector* *r, *gsl_vector* *wts, *gsl_multifit_robust_workspace* *w)

This function assigns weights to the vector `wts` using the residual vector `r` and previously specified weighting function. The output weights are given by $wts_i = w(r_i/(t\sigma))$, where the weighting functions w are detailed in `gsl_multifit_robust_alloc()`. σ is an estimate of the residual standard deviation based on the Median-Absolute-Deviation and t is the tuning constant. This function is useful if the user wishes to implement their own robust regression rather than using the supplied `gsl_multifit_robust()` routine below.

int **gsl_multifit_robust**(const *gsl_matrix* *X, const *gsl_vector* *y, *gsl_vector* *c, *gsl_matrix* *cov, *gsl_multifit_robust_workspace* *w)

This function computes the best-fit parameters `c` of the model $y = Xc$ for the observations `y` and the matrix of predictor variables `X`, attemping to reduce the influence of outliers using the algorithm outlined above. The p-by-p variance-covariance matrix of the model parameters `cov` is estimated as $\sigma^2(X^T X)^{-1}$, where σ is an approximation of the residual standard deviation using the theory of robust regression. Special care must be taken when estimating σ and other statistics such as R^2, and so these are computed internally and are available by calling the function `gsl_multifit_robust_statistics()`.

If the coefficients do not converge within the maximum iteration limit, the function returns `GSL_EMAXITER`. In this case, the current estimates of the coefficients and covariance matrix are returned in `c` and `cov` and the internal fit statistics are computed with these estimates.

int **gsl_multifit_robust_est**(const *gsl_vector* *x, const *gsl_vector* *c, const *gsl_matrix* *cov, double *y, double *y_err)

This function uses the best-fit robust regression coefficients `c` and their covariance matrix `cov` to compute the fitted function value `y` and its standard deviation `y_err` for the model $y = x \cdot c$ at the point `x`.

int **gsl_multifit_robust_residuals**(const *gsl_matrix* *X, const *gsl_vector* *y, const *gsl_vector* *c, *gsl_vector* *r, *gsl_multifit_robust_workspace* *w)

This function computes the vector of studentized residuals $r_i = \frac{y_i - (Xc)_i}{\sigma\sqrt{1-h_i}}$ for the observations `y`, coefficients `c` and matrix of predictor variables `X`. The routine `gsl_multifit_robust()` must first be called to compute the statisical leverages h_i of the matrix `X` and residual standard deviation estimate σ.

gsl_multifit_robust_stats **gsl_multifit_robust_statistics**(const *gsl_multifit_robust_workspace* *w)

This function returns a structure containing relevant statistics from a robust regression. The function `gsl_multifit_robust()` must be called first to perform the regression and calculate these statistics. The returned `gsl_multifit_robust_stats` structure contains the following fields.

type **gsl_multifit_robust_stats**

`double sigma_ols`

This contains the standard deviation of the residuals as computed from ordinary least squares (OLS).

`double sigma_mad`

This contains an estimate of the standard deviation of the final residuals using the Median-Absolute-Deviation statistic

`double sigma_rob`

This contains an estimate of the standard deviation of the final residuals from the theory of robust regression (see Street et al, 1988).

`double sigma`

This contains an estimate of the standard deviation of the final residuals by attemping to reconcile `sigma_rob` and `sigma_ols` in a reasonable way.

`double Rsq`

This contains the R^2 coefficient of determination statistic using the estimate `sigma`.

`double adj_Rsq`

This contains the adjusted R^2 coefficient of determination statistic using the estimate `sigma`.

`double rmse`

This contains the root mean squared error of the final residuals

`double sse`

This contains the residual sum of squares taking into account the robust covariance matrix.

`size_t dof`

This contains the number of degrees of freedom $n - p$

`size_t numit`

Upon successful convergence, this contains the number of iterations performed

`gsl_vector * weights`

This contains the final weight vector of length `n`

`gsl_vector * r`

This contains the final residual vector of length `n`, $r = y - Xc$

40.6 Large dense linear systems

This module is concerned with solving large dense least squares systems $Xc = y$ where the n-by-p matrix X has $n >> p$ (ie: many more rows than columns). This type of matrix is called a "tall skinny" matrix, and for some applications, it may not be possible to fit the entire matrix in memory at once to use the standard SVD approach. Therefore, the algorithms in this module are designed to allow the user to construct smaller blocks of the matrix X and accumulate those blocks into the larger system one at a time. The algorithms in this module never need to store the entire matrix X in memory. The large linear least squares routines support data weights and Tikhonov regularization, and are designed to minimize the residual

$$\chi^2 = ||y - Xc||_W^2 + \lambda^2 ||Lc||^2$$

where y is the n-by-1 observation vector, X is the n-by-p design matrix, c is the p-by-1 solution vector, $W = \mathrm{diag}(w_1, ..., w_n)$ is the data weighting matrix, L is an m-by-p regularization matrix, λ is a regularization parameter, and $||r||_W^2 = r^T W r$. In the discussion which follows, we will assume that the system has been converted into Tikhonov standard form,

$$\chi^2 = ||\tilde{y} - \tilde{X}\tilde{c}||^2 + \lambda^2 ||\tilde{c}||^2$$

and we will drop the tilde characters from the various parameters. For a discussion of the transformation to standard form, see *Regularized regression*.

The basic idea is to partition the matrix X and observation vector y as

$$\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ \vdots \\ X_k \end{pmatrix} c = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_k \end{pmatrix}$$

into k blocks, where each block (X_i, y_i) may have any number of rows, but each X_i has p columns. The sections below describe the methods available for solving this partitioned system. The functions are declared in the header file `gsl_multilarge.h`.

40.6.1 Normal Equations Approach

The normal equations approach to the large linear least squares problem described above is popular due to its speed and simplicity. Since the normal equations solution to the problem is given by

$$c = \left(X^T X + \lambda^2 I\right)^{-1} X^T y$$

only the p-by-p matrix $X^T X$ and p-by-1 vector $X^T y$ need to be stored. Using the partition scheme described above, these are given by

$$X^T X = \sum_i X_i^T X_i$$
$$X^T y = \sum_i X_i^T y_i$$

Since the matrix $X^T X$ is symmetric, only half of it needs to be calculated. Once all of the blocks (X_i, y_i) have been accumulated into the final $X^T X$ and $X^T y$, the system can be solved with a Cholesky factorization of the $X^T X$ matrix. The $X^T X$ matrix is first transformed via a diagonal scaling transformation to attempt to reduce its condition number as much as possible to recover a more accurate solution vector. The normal equations approach is the fastest method for solving the large least squares problem, and is accurate for well-conditioned matrices X. However, for ill-conditioned matrices, as is often the case for large systems, this method can suffer from numerical instabilities (see Trefethen and Bau, 1997). The number of operations for this method is $O(np^2 + \frac{1}{3}p^3)$.

40.6.2 Tall Skinny QR (TSQR) Approach

An algorithm which has better numerical stability for ill-conditioned problems is known as the Tall Skinny QR (TSQR) method. This method is based on computing the thin QR decomposition of the least squares matrix $X = QR$, where Q is an n-by-p matrix with orthogonal columns, and R is a p-by-p upper triangular matrix. Once these factors are calculated, the residual becomes

$$\chi^2 = ||Q^T y - Rc||^2 + \lambda^2 ||c||^2$$

which can be written as the matrix equation

$$\begin{pmatrix} R \\ \lambda I \end{pmatrix} c = \begin{pmatrix} Q^T y \\ 0 \end{pmatrix}$$

The matrix on the left hand side is now a much smaller $2p$-by-p matrix which can be solved with a standard SVD approach. The Q matrix is just as large as the original matrix X, however it does not need to be explicitly constructed. The TSQR algorithm computes only the p-by-p matrix R and the p-by-1 vector $Q^T y$, and updates these quantities as new blocks are added to the system. Each time a new block of rows (X_i, y_i) is added, the algorithm performs a QR decomposition of the matrix

$$\begin{pmatrix} R_{i-1} \\ X_i \end{pmatrix}$$

where R_{i-1} is the upper triangular R factor for the matrix

$$\begin{pmatrix} X_1 \\ \vdots \\ X_{i-1} \end{pmatrix}$$

This QR decomposition is done efficiently taking into account the sparse structure of R_{i-1}. See Demmel et al, 2008 for more details on how this is accomplished. The number of operations for this method is $O(2np^2 - \frac{2}{3}p^3)$.

40.6.3 Large Dense Linear Systems Solution Steps

The typical steps required to solve large regularized linear least squares problems are as follows:

1. Choose the regularization matrix L.
2. Construct a block of rows of the least squares matrix, right hand side vector, and weight vector (X_i, y_i, w_i).
3. Transform the block to standard form $(\tilde{X}_i, \tilde{y}_i)$. This step can be skipped if $L = I$ and $W = I$.
4. Accumulate the standard form block $(\tilde{X}_i, \tilde{y}_i)$ into the system.
5. Repeat steps 2-4 until the entire matrix and right hand side vector have been accumulated.
6. Determine an appropriate regularization parameter λ (using for example L-curve analysis).
7. Solve the standard form system using the chosen λ.
8. Backtransform the standard form solution $\tilde{c}$ to recover the original solution vector c.

40.6.4 Large Dense Linear Least Squares Routines

type **gsl_multilarge_linear_workspace**

This workspace contains parameters for solving large linear least squares problems.

gsl_multilarge_linear_workspace ***gsl_multilarge_linear_alloc**(const *gsl_multilarge_linear_type* *T, const size_t p)

This function allocates a workspace for solving large linear least squares systems. The least squares matrix X has `p` columns, but may have any number of rows.

type **gsl_multilarge_linear_type**

The parameter `T` specifies the method to be used for solving the large least squares system and may be selected from the following choices

gsl_multilarge_linear_type ***gsl_multilarge_linear_normal**

This specifies the normal equations approach for solving the least squares system. This method is suitable in cases where performance is critical and it is known that the least squares matrix X is well conditioned. The size of this workspace is $O(p^2)$.

gsl_multilarge_linear_type ***gsl_multilarge_linear_tsqr**

This specifies the sequential Tall Skinny QR (TSQR) approach for solving the least squares system. This method is a good general purpose choice for large systems, but requires about twice as many operations as the normal equations method for $n >> p$. The size of this workspace is $O(p^2)$.

void **gsl_multilarge_linear_free**(*gsl_multilarge_linear_workspace* *w)
: This function frees the memory associated with the workspace `w`.

const char ***gsl_multilarge_linear_name**(*gsl_multilarge_linear_workspace* *w)
: This function returns a string pointer to the name of the multilarge solver.

int **gsl_multilarge_linear_reset**(*gsl_multilarge_linear_workspace* *w)
: This function resets the workspace `w` so it can begin to accumulate a new least squares system.

int **gsl_multilarge_linear_stdform1**(const *gsl_vector* *L, const *gsl_matrix* *X, const *gsl_vector* *y, *gsl_matrix* *Xs, *gsl_vector* *ys, *gsl_multilarge_linear_workspace* *work)

int **gsl_multilarge_linear_wstdform1**(const *gsl_vector* *L, const *gsl_matrix* *X, const *gsl_vector* *w, const *gsl_vector* *y, *gsl_matrix* *Xs, *gsl_vector* *ys, *gsl_multilarge_linear_workspace* *work)
: These functions define a regularization matrix $L = \mathrm{diag}(l_0, l_1, ..., l_{p-1})$. The diagonal matrix element l_i is provided by the i-th element of the input vector `L`. The block (`X`, `y`) is converted to standard form and the parameters $(\tilde{X}, \tilde{y})$ are stored in `Xs` and `ys` on output. `Xs` and `ys` have the same dimensions as `X` and `y`. Optional data weights may be supplied in the vector `w`. In order to apply this transformation, L^{-1} must exist and so none of the l_i may be zero. After the standard form system has been solved, use `gsl_multilarge_linear_genform1()` to recover the original solution vector. It is allowed to have `X` = `Xs` and `y` = `ys` for an in-place transform.

int **gsl_multilarge_linear_L_decomp**(*gsl_matrix* *L, *gsl_vector* *tau)
: This function calculates the QR decomposition of the m-by-p regularization matrix `L`. `L` must have $m \geq p$. On output, the Householder scalars are stored in the vector `tau` of size p. These outputs will be used by `gsl_multilarge_linear_wstdform2()` to complete the transformation to standard form.

int **gsl_multilarge_linear_stdform2**(const *gsl_matrix* *LQR, const *gsl_vector* *Ltau, const *gsl_matrix* *X, const *gsl_vector* *y, *gsl_matrix* *Xs, *gsl_vector* *ys, *gsl_multilarge_linear_workspace* *work)

int **gsl_multilarge_linear_wstdform2**(const *gsl_matrix* *LQR, const *gsl_vector* *Ltau, const *gsl_matrix* *X, const *gsl_vector* *w, const *gsl_vector* *y, *gsl_matrix* *Xs, *gsl_vector* *ys, *gsl_multilarge_linear_workspace* *work)
: These functions convert a block of rows (`X`, `y`, `w`) to standard form ($\tilde{X}$, $\tilde{y}$) which are stored in `Xs` and `ys` respectively. `X`, `y`, and `w` must all have the same number of rows. The m-by-p regularization matrix L is specified by the inputs `LQR` and `Ltau`, which are outputs from `gsl_multilarge_linear_L_decomp()`. `Xs` and `ys` have the same dimensions as `X` and `y`. After the standard form system has been solved, use `gsl_multilarge_linear_genform2()` to recover the original solution vector. Optional data weights may be supplied in the vector `w`, where $W = \mathrm{diag}(w)$.

int **gsl_multilarge_linear_accumulate**(*gsl_matrix* *X, *gsl_vector* *y, *gsl_multilarge_linear_workspace* *w)
: This function accumulates the standard form block (X, y) into the current least squares system. `X` and `y` have the same number of rows, which can be arbitrary. `X` must have p columns. For the TSQR method, `X` and `y` are destroyed on output. For the normal equations method, they are both unchanged.

int **gsl_multilarge_linear_solve**(const double lambda, *gsl_vector* *c, double *rnorm, double *snorm, *gsl_multilarge_linear_workspace* *w)
: After all blocks (X_i, y_i) have been accumulated into the large least squares system, this function will compute the solution vector which is stored in `c` on output. The regularization parameter λ is provided in `lambda`. On output, `rnorm` contains the residual norm $||y - Xc||_W$ and `snorm` contains the solution norm $||Lc||$.

int **gsl_multilarge_linear_genform1**(const *gsl_vector* *L, const *gsl_vector* *cs, *gsl_vector* *c, *gsl_multilarge_linear_workspace* *work)
: After a regularized system has been solved with $L = \mathrm{diag}(_0, _1, ..., _{p-1})$, this function backtransforms the standard form solution vector `cs` to recover the solution vector of the original problem `c`. The diagonal matrix elements l_i are provided in the vector `L`. It is allowed to have `c` = `cs` for an in-place transform.

int **gsl_multilarge_linear_genform2**(const *gsl_matrix* *LQR, const *gsl_vector* *Ltau, const *gsl_vector* *cs, *gsl_vector* *c, *gsl_multilarge_linear_workspace* *work)

After a regularized system has been solved with a regularization matrix L, specified by (`LQR`, `Ltau`), this function backtransforms the standard form solution `cs` to recover the solution vector of the original problem, which is stored in `c`, of length p.

int **gsl_multilarge_linear_lcurve**(*gsl_vector* *reg_param, *gsl_vector* *rho, *gsl_vector* *eta, *gsl_multilarge_linear_workspace* *work)

This function computes the L-curve for a large least squares system after it has been fully accumulated into the workspace `work`. The output vectors `reg_param`, `rho`, and `eta` must all be the same size, and will contain the regularization parameters λ_i, residual norms $||y - Xc_i||$, and solution norms $||Lc_i||$ which compose the L-curve, where c_i is the regularized solution vector corresponding to λ_i. The user may determine the number of points on the L-curve by adjusting the size of these input arrays. For the TSQR method, the regularization parameters λ_i are estimated from the singular values of the triangular R factor. For the normal equations method, they are estimated from the eigenvalues of the $X^T X$ matrix.

const *gsl_matrix* ***gsl_multilarge_linear_matrix_ptr**(const *gsl_multilarge_linear_workspace* *work)

For the normal equations method, this function returns a pointer to the $X^T X$ matrix. For the TSQR method, this function returns a pointer to the upper triangular R matrix.

const *gsl_vector* ***gsl_multilarge_linear_rhs_ptr**(const *gsl_multilarge_linear_workspace* *work)

For the normal equations method, this function returns a pointer to the $X^T y$ right hand side vector. For the TSQR method, this function returns a pointer to the $Q^T y$ right hand side vector.

int **gsl_multilarge_linear_rcond**(double *rcond, *gsl_multilarge_linear_workspace* *work)

This function computes the reciprocal condition number, stored in `rcond`, of the least squares matrix after it has been accumulated into the workspace `work`. For the TSQR algorithm, this is accomplished by calculating the SVD of the R factor, which has the same singular values as the matrix X. For the normal equations method, this is done by computing the eigenvalues of $X^T X$, which could be inaccurate for ill-conditioned matrices X.

40.7 Troubleshooting

When using models based on polynomials, care should be taken when constructing the design matrix X. If the x values are large, then the matrix X could be ill-conditioned since its columns are powers of x, leading to unstable least-squares solutions. In this case it can often help to center and scale the x values using the mean and standard deviation:

$$x' = \frac{x - \mu(x)}{\sigma(x)}$$

and then construct the X matrix using the transformed values x'.

40.8 Examples

The example programs in this section demonstrate the various linear regression methods.

40.8.1 Simple Linear Regression Example

The following program computes a least squares straight-line fit to a simple dataset, and outputs the best-fit line and its associated one standard-deviation error bars.

```
#include <stdio.h>
#include <gsl/gsl_fit.h>

int
main (void)
{
  int i, n = 4;
  double x[4] = { 1970, 1980, 1990, 2000 };
  double y[4] = {   12,   11,   14,   13 };
  double w[4] = {  0.1,  0.2,  0.3,  0.4 };

  double c0, c1, cov00, cov01, cov11, chisq;

  gsl_fit_wlinear (x, 1, w, 1, y, 1, n,
                   &c0, &c1, &cov00, &cov01, &cov11,
                   &chisq);

  printf ("# best fit: Y = %g + %g X\n", c0, c1);
  printf ("# covariance matrix:\n");
  printf ("# [ %g, %g\n#   %g, %g]\n",
          cov00, cov01, cov01, cov11);
  printf ("# chisq = %g\n", chisq);

  for (i = 0; i < n; i++)
    printf ("data: %g %g %g\n",
                   x[i], y[i], 1/sqrt(w[i]));

  printf ("\n");

  for (i = -30; i < 130; i++)
    {
      double xf = x[0] + (i/100.0) * (x[n-1] - x[0]);
      double yf, yf_err;

      gsl_fit_linear_est (xf,
                          c0, c1,
                          cov00, cov01, cov11,
                          &yf, &yf_err);

      printf ("fit: %g %g\n", xf, yf);
      printf ("hi : %g %g\n", xf, yf + yf_err);
      printf ("lo : %g %g\n", xf, yf - yf_err);
    }
  return 0;
}
```

The following commands extract the data from the output of the program and display it using the GNU plotutils "graph" utility:

```
$ ./demo > tmp
$ more tmp
# best fit: Y = -106.6 + 0.06 X
# covariance matrix:
# [ 39602, -19.9
#   -19.9, 0.01]
# chisq = 0.8

$ for n in data fit hi lo ;
   do
     grep "^$n" tmp | cut -d: -f2 > $n ;
   done
$ graph -T X -X x -Y y -y 0 20 -m 0 -S 2 -Ie data
     -S 0 -I a -m 1 fit -m 2 hi -m 2 lo
```

The result is shown in Fig. 40.1.

40.8.2 Multi-parameter Linear Regression Example

The following program performs a quadratic fit $y = c_0 + c_1 x + c_2 x^2$ to a weighted dataset using the generalised linear fitting function `gsl_multifit_wlinear()`. The model matrix X for a quadratic fit is given by,

$$X = \begin{pmatrix} 1 & x_0 & x_0^2 \\ 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \dots & \dots & \dots \end{pmatrix}$$

where the column of ones corresponds to the constant term c_0. The two remaining columns corresponds to the terms $c_1 x$ and $c_2 x^2$.

The program reads `n` lines of data in the format (`x`, `y`, `err`) where `err` is the error (standard deviation) in the value `y`.

```c
#include <stdio.h>
#include <gsl/gsl_multifit.h>

int
main (int argc, char **argv)
{
  int i, n;
  double xi, yi, ei, chisq;
  gsl_matrix *X, *cov;
  gsl_vector *y, *w, *c;

  if (argc != 2)
    {
      fprintf (stderr,"usage: fit n < data\n");
      exit (-1);
    }

  n = atoi (argv[1]);

  X = gsl_matrix_alloc (n, 3);
  y = gsl_vector_alloc (n);
```

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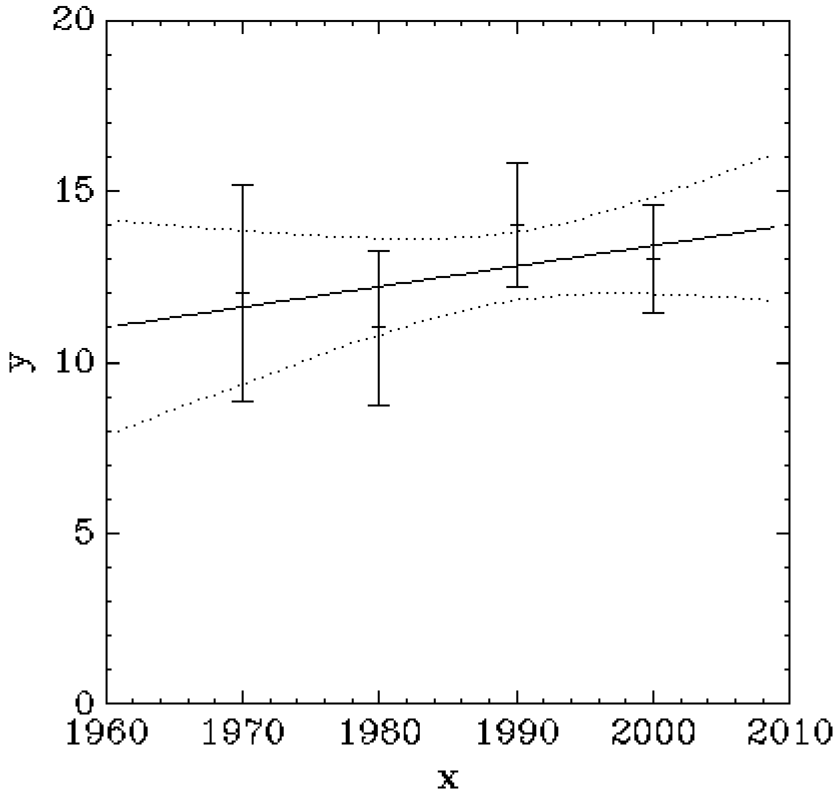

Fig. 40.1: Straight line fit with 1-σ error bars

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```
  w = gsl_vector_alloc (n);

  c = gsl_vector_alloc (3);
  cov = gsl_matrix_alloc (3, 3);

  for (i = 0; i < n; i++)
    {
      int count = fscanf (stdin, "%lg %lg %lg",
                          &xi, &yi, &ei);

      if (count != 3)
        {
          fprintf (stderr, "error reading file\n");
          exit (-1);
        }

      printf ("%g %g +/- %g\n", xi, yi, ei);

      gsl_matrix_set (X, i, 0, 1.0);
      gsl_matrix_set (X, i, 1, xi);
      gsl_matrix_set (X, i, 2, xi*xi);

      gsl_vector_set (y, i, yi);
      gsl_vector_set (w, i, 1.0/(ei*ei));
    }

  {
    gsl_multifit_linear_workspace * work
      = gsl_multifit_linear_alloc (n, 3);
    gsl_multifit_wlinear (X, w, y, c, cov,
                          &chisq, work);
    gsl_multifit_linear_free (work);
  }

#define C(i) (gsl_vector_get(c,(i)))
#define COV(i,j) (gsl_matrix_get(cov,(i),(j)))

  {
    printf ("# best fit: Y = %g + %g X + %g X^2\n",
            C(0), C(1), C(2));

    printf ("# covariance matrix:\n");
    printf ("[ %+.5e, %+.5e, %+.5e  \n",
               COV(0,0), COV(0,1), COV(0,2));
    printf ("  %+.5e, %+.5e, %+.5e  \n",
               COV(1,0), COV(1,1), COV(1,2));
    printf ("  %+.5e, %+.5e, %+.5e ]\n",
               COV(2,0), COV(2,1), COV(2,2));
    printf ("# chisq = %g\n", chisq);
  }

  gsl_matrix_free (X);
```

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```
  gsl_vector_free (y);
  gsl_vector_free (w);
  gsl_vector_free (c);
  gsl_matrix_free (cov);

  return 0;
}
```

A suitable set of data for fitting can be generated using the following program. It outputs a set of points with gaussian errors from the curve $y = e^x$ in the region $0 < x < 2$.

```
#include <stdio.h>
#include <math.h>
#include <gsl/gsl_randist.h>

int
main (void)
{
  double x;
  const gsl_rng_type * T;
  gsl_rng * r;

  gsl_rng_env_setup ();

  T = gsl_rng_default;
  r = gsl_rng_alloc (T);

  for (x = 0.1; x < 2; x+= 0.1)
    {
      double y0 = exp (x);
      double sigma = 0.1 * y0;
      double dy = gsl_ran_gaussian (r, sigma);

      printf ("%g %g %g\n", x, y0 + dy, sigma);
    }

  gsl_rng_free(r);

  return 0;
}
```

The data can be prepared by running the resulting executable program:

```
$ GSL_RNG_TYPE=mt19937_1999 ./generate > exp.dat
$ more exp.dat
0.1 0.97935 0.110517
0.2 1.3359 0.12214
0.3 1.52573 0.134986
0.4 1.60318 0.149182
0.5 1.81731 0.164872
0.6 1.92475 0.182212
....
```

To fit the data use the previous program, with the number of data points given as the first argument. In this case there are 19 data points:

```
$ ./fit 19 < exp.dat
0.1 0.97935 +/- 0.110517
0.2 1.3359 +/- 0.12214
...
# best fit: Y = 1.02318 + 0.956201 X + 0.876796 X^2
# covariance matrix:
[ +1.25612e-02, -3.64387e-02, +1.94389e-02
  -3.64387e-02, +1.42339e-01, -8.48761e-02
  +1.94389e-02, -8.48761e-02, +5.60243e-02 ]
# chisq = 23.0987
```

The parameters of the quadratic fit match the coefficients of the expansion of e^x, taking into account the errors on the parameters and the $O(x^3)$ difference between the exponential and quadratic functions for the larger values of x. The errors on the parameters are given by the square-root of the corresponding diagonal elements of the covariance matrix. The chi-squared per degree of freedom is 1.4, indicating a reasonable fit to the data.

Fig. 40.2 shows the resulting fit.

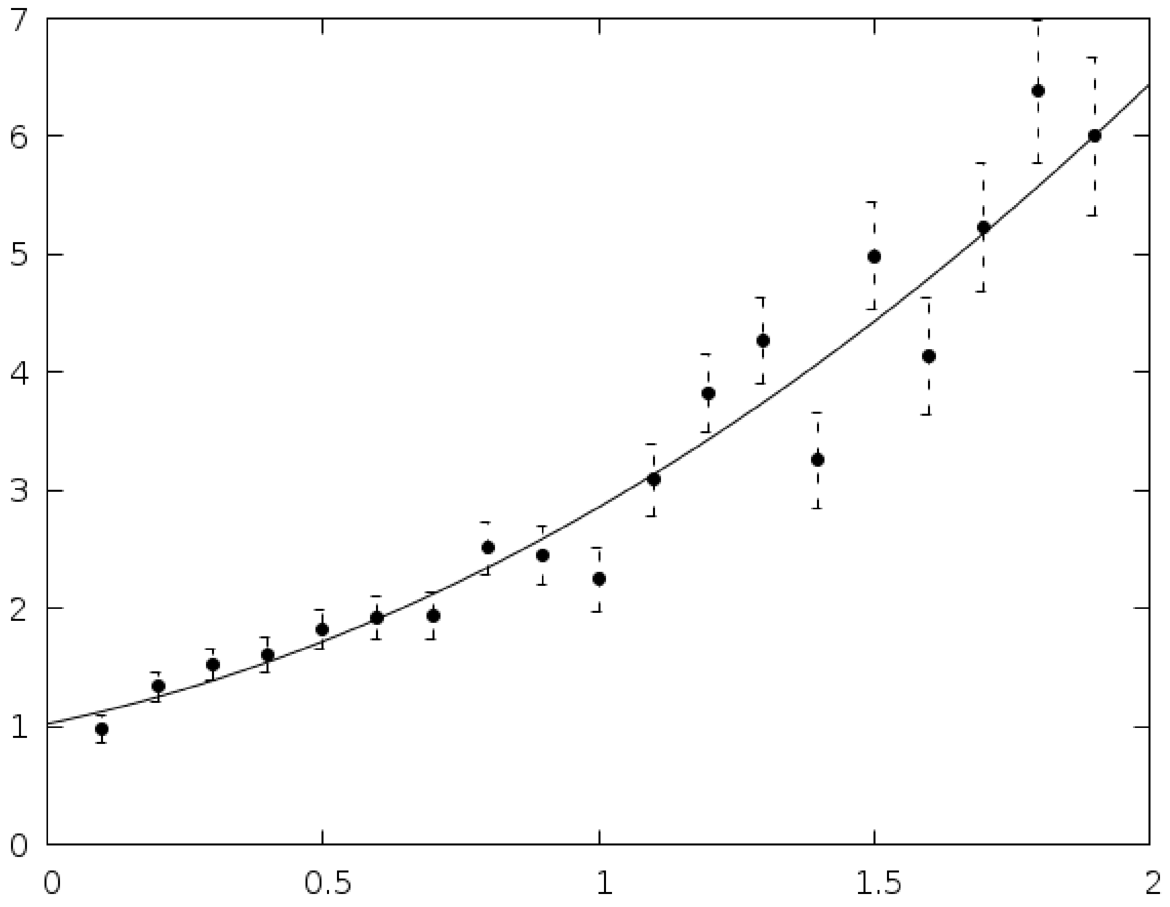

Fig. 40.2: Weighted fit example with error bars

40.8.3 Regularized Linear Regression Example 1

The next program demonstrates the difference between ordinary and regularized least squares when the design matrix is near-singular. In this program, we generate two random normally distributed variables u and v, with $v = u + noise$ so that u and v are nearly colinear. We then set a third dependent variable $y = u + v + noise$ and solve for the coefficients c_1, c_2 of the model $Y(c_1, c_2) = c_1 u + c_2 v$. Since $u \approx v$, the design matrix X is nearly singular, leading to unstable ordinary least squares solutions.

Here is the program output:

```
matrix condition number = 1.025113e+04

=== Unregularized fit ===
best fit: y = -43.6588 u + 45.6636 v
residual norm = 31.6248
solution norm = 63.1764
chisq/dof = 1.00213

=== Regularized fit (L-curve) ===
optimal lambda: 4.51103
best fit: y = 1.00113 u + 1.0032 v
residual norm = 31.6547
solution norm = 1.41728
chisq/dof = 1.04499

=== Regularized fit (GCV) ===
optimal lambda: 0.0232029
best fit: y = -19.8367 u + 21.8417 v
residual norm = 31.6332
solution norm = 29.5051
chisq/dof = 1.00314
```

We see that the ordinary least squares solution is completely wrong, while the L-curve regularized method with the optimal $\lambda = 4.51103$ finds the correct solution $c_1 \approx c_2 \approx 1$. The GCV regularized method finds a regularization parameter $\lambda = 0.0232029$ which is too small to give an accurate solution, although it performs better than OLS. The L-curve and its computed corner, as well as the GCV curve and its minimum are plotted in Fig. 40.3.

The program is given below.

```
#include <gsl/gsl_math.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_multifit.h>

int
main()
{
  const size_t n = 1000; /* number of observations */
  const size_t p = 2;    /* number of model parameters */
  size_t i;
  gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
  gsl_matrix *X = gsl_matrix_alloc(n, p);
  gsl_vector *y = gsl_vector_alloc(n);
```

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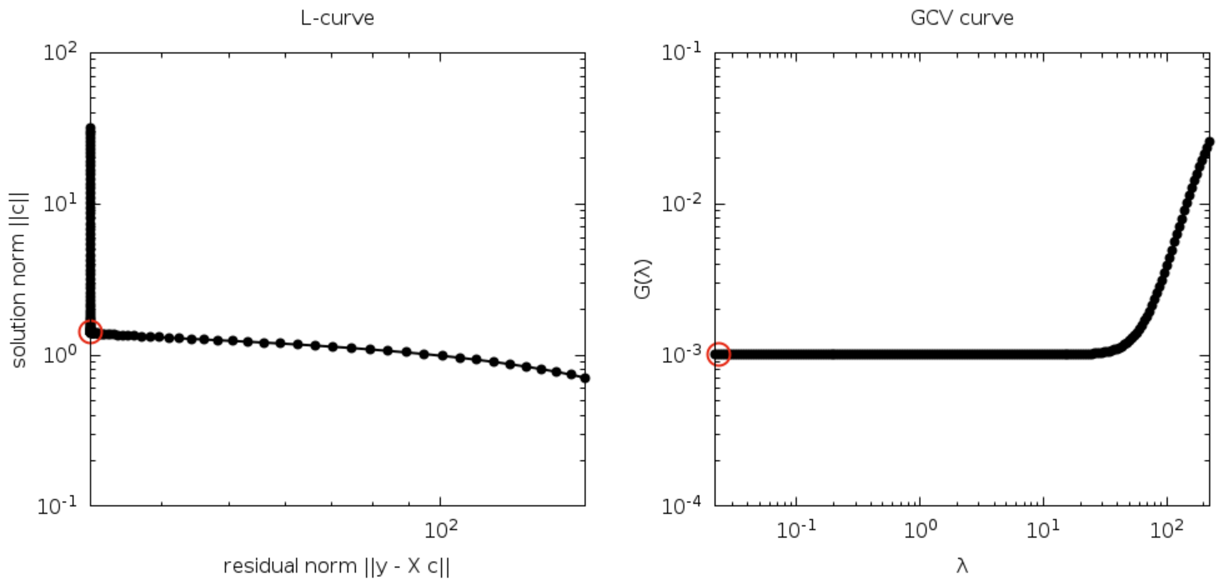

Fig. 40.3: L-curve and GCV curve for example program.

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```
  for (i = 0; i < n; ++i)
    {
      /* generate first random variable u */
      double ui = 5.0 * gsl_ran_gaussian(r, 1.0);

      /* set v = u + noise */
      double vi = ui + gsl_ran_gaussian(r, 0.001);

      /* set y = u + v + noise */
      double yi = ui + vi + gsl_ran_gaussian(r, 1.0);

      /* since u =~ v, the matrix X is ill-conditioned */
      gsl_matrix_set(X, i, 0, ui);
      gsl_matrix_set(X, i, 1, vi);

      /* rhs vector */
      gsl_vector_set(y, i, yi);
    }

  {
    const size_t npoints = 200;                   /* number of points on L-curve and GCV␣
↪curve */
    gsl_multifit_linear_workspace *w =
      gsl_multifit_linear_alloc(n, p);
    gsl_vector *c = gsl_vector_alloc(p);          /* OLS solution */
    gsl_vector *c_lcurve = gsl_vector_alloc(p);   /* regularized solution (L-curve) */
    gsl_vector *c_gcv = gsl_vector_alloc(p);      /* regularized solution (GCV) */
    gsl_vector *reg_param = gsl_vector_alloc(npoints);
```

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```
  gsl_vector *rho = gsl_vector_alloc(npoints);  /* residual norms */
  gsl_vector *eta = gsl_vector_alloc(npoints);  /* solution norms */
  gsl_vector *G = gsl_vector_alloc(npoints);    /* GCV function values */
  double lambda_l;                              /* optimal regularization parameter (L-
↪curve) */
  double lambda_gcv;                            /* optimal regularization parameter␣
↪(GCV) */
  double G_gcv;                                 /* G(lambda_gcv) */
  size_t reg_idx;                               /* index of optimal lambda */
  double rcond;                                 /* reciprocal condition number of X */
  double chisq, rnorm, snorm;

  /* compute SVD of X */
  gsl_multifit_linear_svd(X, w);

  rcond = gsl_multifit_linear_rcond(w);
  fprintf(stderr, "matrix condition number = %e\n\n", 1.0 / rcond);

  /* unregularized (standard) least squares fit, lambda = 0 */
  gsl_multifit_linear_solve(0.0, X, y, c, &rnorm, &snorm, w);
  chisq = pow(rnorm, 2.0);

  fprintf(stderr, "=== Unregularized fit ===\n");
  fprintf(stderr, "best fit: y = %g u + %g v\n",
    gsl_vector_get(c, 0), gsl_vector_get(c, 1));
  fprintf(stderr, "residual norm = %g\n", rnorm);
  fprintf(stderr, "solution norm = %g\n", snorm);
  fprintf(stderr, "chisq/dof = %g\n", chisq / (n - p));

  /* calculate L-curve and find its corner */
  gsl_multifit_linear_lcurve(y, reg_param, rho, eta, w);
  gsl_multifit_linear_lcorner(rho, eta, &reg_idx);

  /* store optimal regularization parameter */
  lambda_l = gsl_vector_get(reg_param, reg_idx);

  /* regularize with lambda_l */
  gsl_multifit_linear_solve(lambda_l, X, y, c_lcurve, &rnorm, &snorm, w);
  chisq = pow(rnorm, 2.0) + pow(lambda_l * snorm, 2.0);

  fprintf(stderr, "\n=== Regularized fit (L-curve) ===\n");
  fprintf(stderr, "optimal lambda: %g\n", lambda_l);
  fprintf(stderr, "best fit: y = %g u + %g v\n",
          gsl_vector_get(c_lcurve, 0), gsl_vector_get(c_lcurve, 1));
  fprintf(stderr, "residual norm = %g\n", rnorm);
  fprintf(stderr, "solution norm = %g\n", snorm);
  fprintf(stderr, "chisq/dof = %g\n", chisq / (n - p));

  /* calculate GCV curve and find its minimum */
  gsl_multifit_linear_gcv(y, reg_param, G, &lambda_gcv, &G_gcv, w);

  /* regularize with lambda_gcv */
```

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```
    gsl_multifit_linear_solve(lambda_gcv, X, y, c_gcv, &rnorm, &snorm, w);
    chisq = pow(rnorm, 2.0) + pow(lambda_gcv * snorm, 2.0);

    fprintf(stderr, "\n=== Regularized fit (GCV) ===\n");
    fprintf(stderr, "optimal lambda: %g\n", lambda_gcv);
    fprintf(stderr, "best fit: y = %g u + %g v\n",
            gsl_vector_get(c_gcv, 0), gsl_vector_get(c_gcv, 1));
    fprintf(stderr, "residual norm = %g\n", rnorm);
    fprintf(stderr, "solution norm = %g\n", snorm);
    fprintf(stderr, "chisq/dof = %g\n", chisq / (n - p));

    /* output L-curve and GCV curve */
    for (i = 0; i < npoints; ++i)
      {
        printf("%e %e %e %e\n",
               gsl_vector_get(reg_param, i),
               gsl_vector_get(rho, i),
               gsl_vector_get(eta, i),
               gsl_vector_get(G, i));
      }

    /* output L-curve corner point */
    printf("\n\n%f %f\n",
           gsl_vector_get(rho, reg_idx),
           gsl_vector_get(eta, reg_idx));

    /* output GCV curve corner minimum */
    printf("\n\n%e %e\n",
           lambda_gcv,
           G_gcv);

    gsl_multifit_linear_free(w);
    gsl_vector_free(c);
    gsl_vector_free(c_lcurve);
    gsl_vector_free(reg_param);
    gsl_vector_free(rho);
    gsl_vector_free(eta);
    gsl_vector_free(G);
  }

  gsl_rng_free(r);
  gsl_matrix_free(X);
  gsl_vector_free(y);

  return 0;
}
```

40.8.4 Regularized Linear Regression Example 2

The following example program minimizes the cost function

$$||y - Xc||^2 + \lambda^2 ||x||^2$$

where X is the 10-by-8 Hilbert matrix whose entries are given by

$$X_{ij} = \frac{1}{i + j - 1}$$

and the right hand side vector is given by $y = [1, -1, 1, -1, 1, -1, 1, -1, 1, -1]^T$. Solutions are computed for $\lambda = 0$ (unregularized) as well as for optimal parameters λ chosen by analyzing the L-curve and GCV curve.

Here is the program output:

```
matrix condition number = 3.565872e+09

=== Unregularized fit ===
residual norm = 2.15376
solution norm = 2.92217e+09
chisq/dof = 2.31934

=== Regularized fit (L-curve) ===
optimal lambda: 7.11407e-07
residual norm = 2.60386
solution norm = 424507
chisq/dof = 3.43565

=== Regularized fit (GCV) ===
optimal lambda: 1.72278
residual norm = 3.1375
solution norm = 0.139357
chisq/dof = 4.95076
```

Here we see the unregularized solution results in a large solution norm due to the ill-conditioned matrix. The L-curve solution finds a small value of $\lambda = 7.11e - 7$ which still results in a badly conditioned system and a large solution norm. The GCV method finds a parameter $\lambda = 1.72$ which results in a well-conditioned system and small solution norm.

The L-curve and its computed corner, as well as the GCV curve and its minimum are plotted in Fig. 40.4.

The program is given below.

```
#include <gsl/gsl_math.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_multifit.h>
#include <gsl/gsl_blas.h>

static int
hilbert_matrix(gsl_matrix * m)
{
  const size_t N = m->size1;
  const size_t M = m->size2;
  size_t i, j;
```

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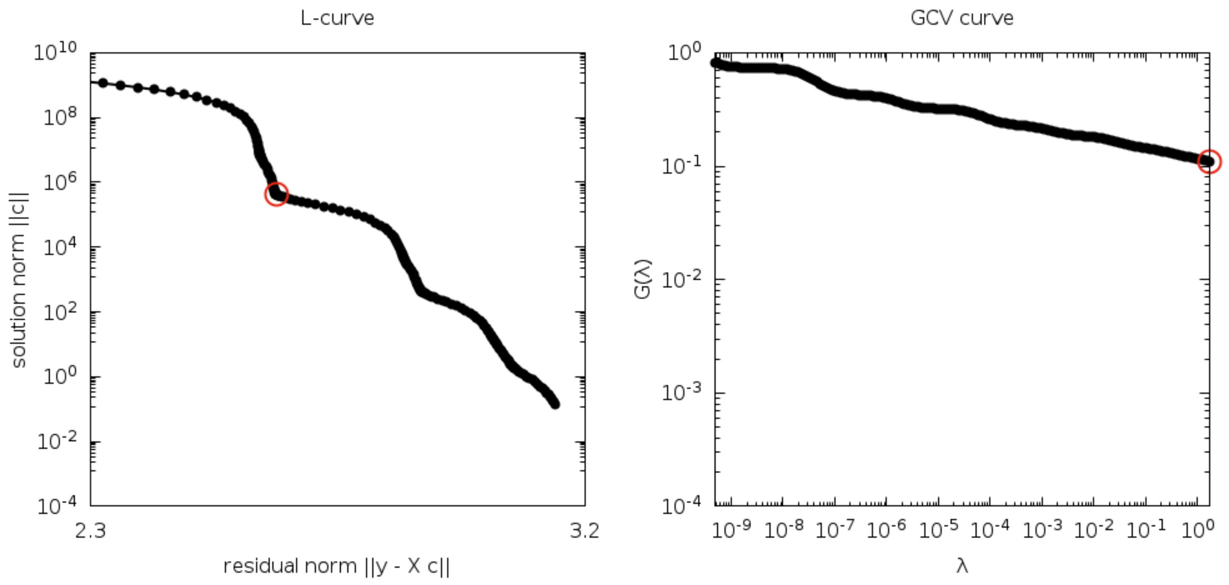

Fig. 40.4: L-curve and GCV curve for example program.

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```
  for (i = 0; i < N; i++)
    {
      for (j = 0; j < M; j++)
        {
          gsl_matrix_set(m, i, j, 1.0/(i+j+1.0));
        }
    }

  return GSL_SUCCESS;
}

int
main()
{
  const size_t n = 10; /* number of observations */
  const size_t p = 8;  /* number of model parameters */
  size_t i;
  gsl_matrix *X = gsl_matrix_alloc(n, p);
  gsl_vector *y = gsl_vector_alloc(n);

  /* construct Hilbert matrix and rhs vector */
  hilbert_matrix(X);

  {
    double val = 1.0;
    for (i = 0; i < n; ++i)
      {
        gsl_vector_set(y, i, val);
```

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```
        val *= -1.0;
      }
  }

  {
    const size_t npoints = 200;                   /* number of points on L-curve and GCV␣
↪curve */
    gsl_multifit_linear_workspace *w =
      gsl_multifit_linear_alloc(n, p);
    gsl_vector *c = gsl_vector_alloc(p);          /* OLS solution */
    gsl_vector *c_lcurve = gsl_vector_alloc(p);   /* regularized solution (L-curve) */
    gsl_vector *c_gcv = gsl_vector_alloc(p);      /* regularized solution (GCV) */
    gsl_vector *reg_param = gsl_vector_alloc(npoints);
    gsl_vector *rho = gsl_vector_alloc(npoints);  /* residual norms */
    gsl_vector *eta = gsl_vector_alloc(npoints);  /* solution norms */
    gsl_vector *G = gsl_vector_alloc(npoints);    /* GCV function values */
    double lambda_l;                              /* optimal regularization parameter (L-
↪curve) */
    double lambda_gcv;                            /* optimal regularization parameter␣
↪(GCV) */
    double G_gcv;                                 /* G(lambda_gcv) */
    size_t reg_idx;                               /* index of optimal lambda */
    double rcond;                                 /* reciprocal condition number of X */
    double chisq, rnorm, snorm;

    /* compute SVD of X */
    gsl_multifit_linear_svd(X, w);

    rcond = gsl_multifit_linear_rcond(w);
    fprintf(stderr, "matrix condition number = %e\n", 1.0 / rcond);

    /* unregularized (standard) least squares fit, lambda = 0 */
    gsl_multifit_linear_solve(0.0, X, y, c, &rnorm, &snorm, w);
    chisq = pow(rnorm, 2.0);

    fprintf(stderr, "\n=== Unregularized fit ===\n");
    fprintf(stderr, "residual norm = %g\n", rnorm);
    fprintf(stderr, "solution norm = %g\n", snorm);
    fprintf(stderr, "chisq/dof = %g\n", chisq / (n - p));

    /* calculate L-curve and find its corner */
    gsl_multifit_linear_lcurve(y, reg_param, rho, eta, w);
    gsl_multifit_linear_lcorner(rho, eta, &reg_idx);

    /* store optimal regularization parameter */
    lambda_l = gsl_vector_get(reg_param, reg_idx);

    /* regularize with lambda_l */
    gsl_multifit_linear_solve(lambda_l, X, y, c_lcurve, &rnorm, &snorm, w);
    chisq = pow(rnorm, 2.0) + pow(lambda_l * snorm, 2.0);

    fprintf(stderr, "\n=== Regularized fit (L-curve) ===\n");
```

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```
    fprintf(stderr, "optimal lambda: %g\n", lambda_l);
    fprintf(stderr, "residual norm = %g\n", rnorm);
    fprintf(stderr, "solution norm = %g\n", snorm);
    fprintf(stderr, "chisq/dof = %g\n", chisq / (n - p));

    /* calculate GCV curve and find its minimum */
    gsl_multifit_linear_gcv(y, reg_param, G, &lambda_gcv, &G_gcv, w);

    /* regularize with lambda_gcv */
    gsl_multifit_linear_solve(lambda_gcv, X, y, c_gcv, &rnorm, &snorm, w);
    chisq = pow(rnorm, 2.0) + pow(lambda_gcv * snorm, 2.0);

    fprintf(stderr, "\n=== Regularized fit (GCV) ===\n");
    fprintf(stderr, "optimal lambda: %g\n", lambda_gcv);
    fprintf(stderr, "residual norm = %g\n", rnorm);
    fprintf(stderr, "solution norm = %g\n", snorm);
    fprintf(stderr, "chisq/dof = %g\n", chisq / (n - p));

    /* output L-curve and GCV curve */
    for (i = 0; i < npoints; ++i)
      {
        printf("%e %e %e %e\n",
               gsl_vector_get(reg_param, i),
               gsl_vector_get(rho, i),
               gsl_vector_get(eta, i),
               gsl_vector_get(G, i));
      }

    /* output L-curve corner point */
    printf("\n\n%f %f\n",
           gsl_vector_get(rho, reg_idx),
           gsl_vector_get(eta, reg_idx));

    /* output GCV curve corner minimum */
    printf("\n\n%e %e\n",
           lambda_gcv,
           G_gcv);

    gsl_multifit_linear_free(w);
    gsl_vector_free(c);
    gsl_vector_free(c_lcurve);
    gsl_vector_free(reg_param);
    gsl_vector_free(rho);
    gsl_vector_free(eta);
    gsl_vector_free(G);
  }

  gsl_matrix_free(X);
  gsl_vector_free(y);

  return 0;
}
```

40.8.5 Robust Linear Regression Example

The next program demonstrates the advantage of robust least squares on a dataset with outliers. The program generates linear (x, y) data pairs on the line $y = 1.45x + 3.88$, adds some random noise, and inserts 3 outliers into the dataset. Both the robust and ordinary least squares (OLS) coefficients are computed for comparison.

```
#include <stdio.h>
#include <gsl/gsl_multifit.h>
#include <gsl/gsl_randist.h>

int
dofit(const gsl_multifit_robust_type *T,
      const gsl_matrix *X, const gsl_vector *y,
      gsl_vector *c, gsl_matrix *cov)
{
  int s;
  gsl_multifit_robust_workspace * work
    = gsl_multifit_robust_alloc (T, X->size1, X->size2);

  s = gsl_multifit_robust (X, y, c, cov, work);
  gsl_multifit_robust_free (work);

  return s;
}

int
main (int argc, char **argv)
{
  size_t i;
  size_t n;
  const size_t p = 2; /* linear fit */
  gsl_matrix *X, *cov;
  gsl_vector *x, *y, *c, *c_ols;
  const double a = 1.45; /* slope */
  const double b = 3.88; /* intercept */
  gsl_rng *r;

  if (argc != 2)
    {
      fprintf (stderr,"usage: robfit n\n");
      exit (-1);
    }

  n = atoi (argv[1]);

  X = gsl_matrix_alloc (n, p);
  x = gsl_vector_alloc (n);
  y = gsl_vector_alloc (n);

  c = gsl_vector_alloc (p);
  c_ols = gsl_vector_alloc (p);
  cov = gsl_matrix_alloc (p, p);
```

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```
  r = gsl_rng_alloc(gsl_rng_default);

  /* generate linear dataset */
  for (i = 0; i < n - 3; i++)
    {
      double dx = 10.0 / (n - 1.0);
      double ei = gsl_rng_uniform(r);
      double xi = -5.0 + i * dx;
      double yi = a * xi + b;

      gsl_vector_set (x, i, xi);
      gsl_vector_set (y, i, yi + ei);
    }

  /* add a few outliers */
  gsl_vector_set(x, n - 3, 4.7);
  gsl_vector_set(y, n - 3, -8.3);

  gsl_vector_set(x, n - 2, 3.5);
  gsl_vector_set(y, n - 2, -6.7);

  gsl_vector_set(x, n - 1, 4.1);
  gsl_vector_set(y, n - 1, -6.0);

  /* construct design matrix X for linear fit */
  for (i = 0; i < n; ++i)
    {
      double xi = gsl_vector_get(x, i);

      gsl_matrix_set (X, i, 0, 1.0);
      gsl_matrix_set (X, i, 1, xi);
    }

  /* perform robust and OLS fit */
  dofit(gsl_multifit_robust_ols, X, y, c_ols, cov);
  dofit(gsl_multifit_robust_bisquare, X, y, c, cov);

  /* output data and model */
  for (i = 0; i < n; ++i)
    {
      double xi = gsl_vector_get(x, i);
      double yi = gsl_vector_get(y, i);
      gsl_vector_view v = gsl_matrix_row(X, i);
      double y_ols, y_rob, y_err;

      gsl_multifit_robust_est(&v.vector, c, cov, &y_rob, &y_err);
      gsl_multifit_robust_est(&v.vector, c_ols, cov, &y_ols, &y_err);

      printf("%g %g %g %g\n", xi, yi, y_rob, y_ols);
    }

#define C(i) (gsl_vector_get(c,(i)))
```

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```
#define COV(i,j) (gsl_matrix_get(cov,(i),(j)))

  {
    printf ("# best fit: Y = %g + %g X\n",
            C(0), C(1));

    printf ("# covariance matrix:\n");
    printf ("# [ %+.5e, %+.5e\n",
               COV(0,0), COV(0,1));
    printf ("#   %+.5e, %+.5e\n",
               COV(1,0), COV(1,1));
  }

  gsl_matrix_free (X);
  gsl_vector_free (x);
  gsl_vector_free (y);
  gsl_vector_free (c);
  gsl_vector_free (c_ols);
  gsl_matrix_free (cov);
  gsl_rng_free(r);

  return 0;
}
```

The output from the program is shown in Fig. 40.5.

40.8.6 Large Dense Linear Regression Example

The following program demostrates the large dense linear least squares solvers. This example is adapted from Trefethen and Bau, and fits the function $f(t) = \exp(\sin^3(10t))$ on the interval $[0, 1]$ with a degree 15 polynomial. The program generates $n = 50000$ equally spaced points t_i on this interval, calculates the function value and adds random noise to determine the observation value y_i. The entries of the least squares matrix are $X_{ij} = t_i^j$, representing a polynomial fit. The matrix is highly ill-conditioned, with a condition number of about $2.4 \cdot 10^{11}$. The program accumulates the matrix into the least squares system in 5 blocks, each with 10000 rows. This way the full matrix X is never stored in memory. We solve the system with both the normal equations and TSQR methods. The results are shown in Fig. 40.6. In the top left plot, the TSQR solution provides a reasonable agreement to the exact solution, while the normal equations method fails completely since the Cholesky factorization fails due to the ill-conditioning of the matrix. In the bottom left plot, we show the L-curve calculated from TSQR, which exhibits multiple corners. In the top right panel, we plot a regularized solution using $\lambda = 10^{-5}$. The TSQR and normal solutions now agree, however they are unable to provide a good fit due to the damping. This indicates that for some ill-conditioned problems, regularizing the normal equations does not improve the solution. This is further illustrated in the bottom right panel, where we plot the L-curve calculated from the normal equations. The curve agrees with the TSQR curve for larger damping parameters, but for small λ, the normal equations approach cannot provide accurate solution vectors leading to numerical inaccuracies in the left portion of the curve.

```
#include <gsl/gsl_math.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_multifit.h>
```

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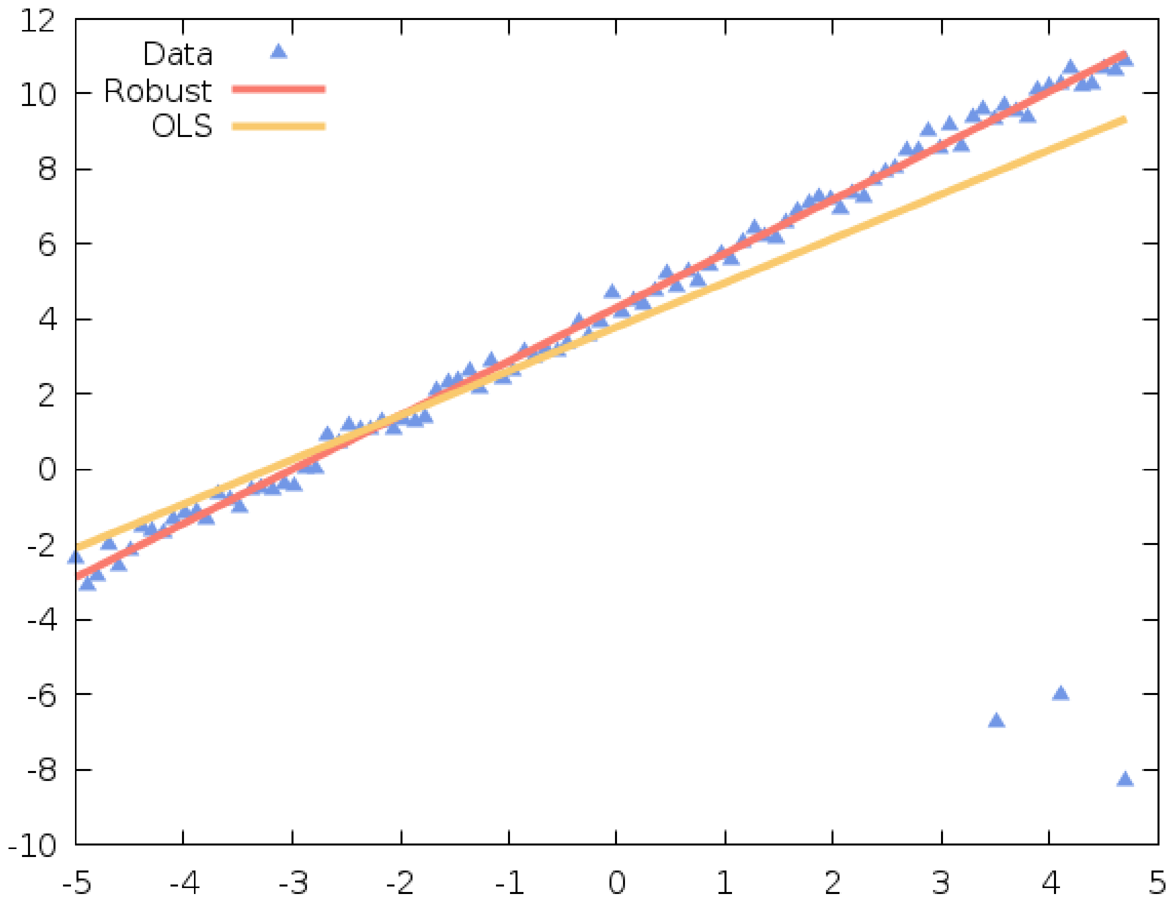

Fig. 40.5: Linear fit to dataset with outliers.

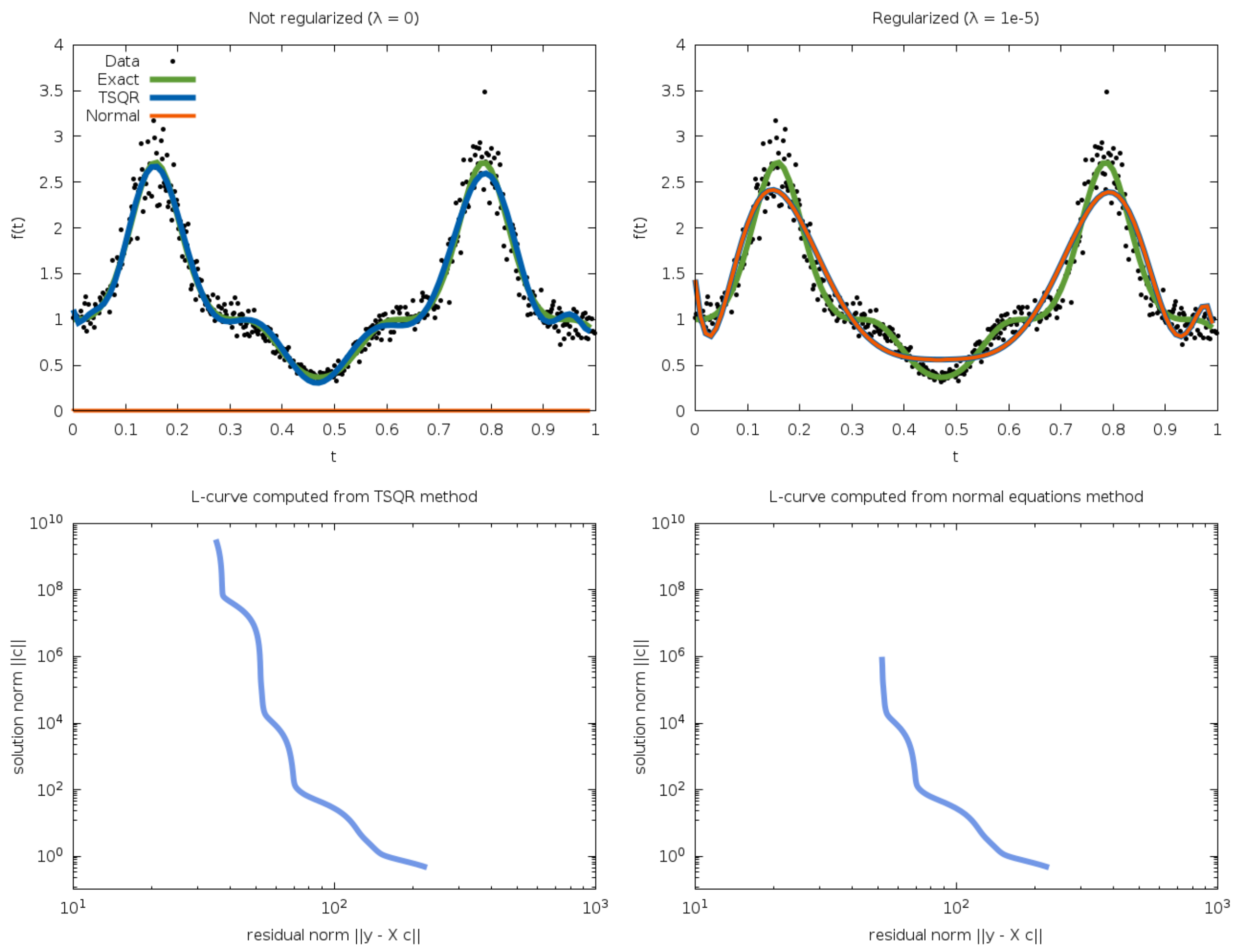

Fig. 40.6: Top left: unregularized solutions; top right: regularized solutions; bottom left: L-curve for TSQR method; bottom right: L-curve from normal equations method.

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```
#include <gsl/gsl_multilarge.h>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_errno.h>

/* function to be fitted */
double
func(const double t)
{
  double x = sin(10.0 * t);
  return exp(x*x*x);
}

/* construct a row of the least squares matrix */
int
build_row(const double t, gsl_vector *row)
{
  const size_t p = row->size;
  double Xj = 1.0;
  size_t j;

  for (j = 0; j < p; ++j)
    {
      gsl_vector_set(row, j, Xj);
      Xj *= t;
    }

  return 0;
}

int
solve_system(const int print_data, const gsl_multilarge_linear_type * T,
             const double lambda, const size_t n, const size_t p,
             gsl_vector * c)
{
  const size_t nblock = 5;         /* number of blocks to accumulate */
  const size_t nrows = n / nblock; /* number of rows per block */
  gsl_multilarge_linear_workspace * w =
    gsl_multilarge_linear_alloc(T, p);
  gsl_matrix *X = gsl_matrix_alloc(nrows, p);
  gsl_vector *y = gsl_vector_alloc(nrows);
  gsl_rng *r = gsl_rng_alloc(gsl_rng_default);
  const size_t nlcurve = 200;
  gsl_vector *reg_param = gsl_vector_alloc(nlcurve);
  gsl_vector *rho = gsl_vector_calloc(nlcurve);
  gsl_vector *eta = gsl_vector_calloc(nlcurve);
  size_t rowidx = 0;
  double rnorm, snorm, rcond;
  double t = 0.0;
  double dt = 1.0 / (n - 1.0);

  while (rowidx < n)
    {
```

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```
      size_t nleft = n - rowidx;          /* number of rows left to accumulate */
      size_t nr = GSL_MIN(nrows, nleft); /* number of rows in this block */
      gsl_matrix_view Xv = gsl_matrix_submatrix(X, 0, 0, nr, p);
      gsl_vector_view yv = gsl_vector_subvector(y, 0, nr);
      size_t i;

      /* build (X,y) block with 'nr' rows */
      for (i = 0; i < nr; ++i)
        {
          gsl_vector_view row = gsl_matrix_row(&Xv.matrix, i);
          double fi = func(t);
          double ei = gsl_ran_gaussian (r, 0.1 * fi); /* noise */
          double yi = fi + ei;

          /* construct this row of LS matrix */
          build_row(t, &row.vector);

          /* set right hand side value with added noise */
          gsl_vector_set(&yv.vector, i, yi);

          if (print_data && (i % 100 == 0))
            printf("%f %f\n", t, yi);

          t += dt;
        }

      /* accumulate (X,y) block into LS system */
      gsl_multilarge_linear_accumulate(&Xv.matrix, &yv.vector, w);

      rowidx += nr;
    }

  if (print_data)
    printf("\n\n");

  /* compute L-curve */
  gsl_multilarge_linear_lcurve(reg_param, rho, eta, w);

  /* solve large LS system and store solution in c */
  gsl_multilarge_linear_solve(lambda, c, &rnorm, &snorm, w);

  /* compute reciprocal condition number */
  gsl_multilarge_linear_rcond(&rcond, w);

  fprintf(stderr, "=== Method %s ===\n", gsl_multilarge_linear_name(w));
  fprintf(stderr, "condition number = %e\n", 1.0 / rcond);
  fprintf(stderr, "residual norm    = %e\n", rnorm);
  fprintf(stderr, "solution norm    = %e\n", snorm);

  /* output L-curve */
  {
    size_t i;
```

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```
    for (i = 0; i < nlcurve; ++i)
      {
        printf("%.12e %.12e %.12e\n",
               gsl_vector_get(reg_param, i),
               gsl_vector_get(rho, i),
               gsl_vector_get(eta, i));
      }
    printf("\n\n");
  }

  gsl_matrix_free(X);
  gsl_vector_free(y);
  gsl_multilarge_linear_free(w);
  gsl_rng_free(r);
  gsl_vector_free(reg_param);
  gsl_vector_free(rho);
  gsl_vector_free(eta);

  return 0;
}

int
main(int argc, char *argv[])
{
  const size_t n = 50000;   /* number of observations */
  const size_t p = 16;      /* polynomial order + 1 */
  double lambda = 0.0;      /* regularization parameter */
  gsl_vector *c_tsqr = gsl_vector_calloc(p);
  gsl_vector *c_normal = gsl_vector_calloc(p);

  if (argc > 1)
    lambda = atof(argv[1]);

  /* turn off error handler so normal equations method won't abort */
  gsl_set_error_handler_off();

  /* solve system with TSQR method */
  solve_system(1, gsl_multilarge_linear_tsqr, lambda, n, p, c_tsqr);

  /* solve system with Normal equations method */
  solve_system(0, gsl_multilarge_linear_normal, lambda, n, p, c_normal);

  /* output solutions */
  {
    gsl_vector *v = gsl_vector_alloc(p);
    double t;

    for (t = 0.0; t <= 1.0; t += 0.01)
      {
        double f_exact = func(t);
        double f_tsqr, f_normal;
```

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```
        build_row(t, v);
        gsl_blas_ddot(v, c_tsqr, &f_tsqr);
        gsl_blas_ddot(v, c_normal, &f_normal);

        printf("%f %e %e %e\n", t, f_exact, f_tsqr, f_normal);
      }

    gsl_vector_free(v);
  }

  gsl_vector_free(c_tsqr);
  gsl_vector_free(c_normal);

  return 0;
}
```

40.9 References and Further Reading

A summary of formulas and techniques for least squares fitting can be found in the "Statistics" chapter of the Annual Review of Particle Physics prepared by the Particle Data Group,

- *Review of Particle Properties*, R.M. Barnett et al., Physical Review D54, 1 (1996) http://pdg.lbl.gov

The Review of Particle Physics is available online at the website given above.

The tests used to prepare these routines are based on the NIST Statistical Reference Datasets. The datasets and their documentation are available from NIST at the following website,

http://www.nist.gov/itl/div898/strd/index.html

More information on Tikhonov regularization can be found in

- Hansen, P. C. (1998), Rank-Deficient and Discrete Ill-Posed Problems: Numerical Aspects of Linear Inversion. SIAM Monogr. on Mathematical Modeling and Computation, Society for Industrial and Applied Mathematics
- M. Rezghi and S. M. Hosseini (2009), A new variant of L-curve for Tikhonov regularization, Journal of Computational and Applied Mathematics, Volume 231, Issue 2, pages 914-924.

The GSL implementation of robust linear regression closely follows the publications

- DuMouchel, W. and F. O'Brien (1989), "Integrating a robust option into a multiple regression computing environment," Computer Science and Statistics: Proceedings of the 21st Symposium on the Interface, American Statistical Association
- Street, J.O., R.J. Carroll, and D. Ruppert (1988), "A note on computing robust regression estimates via iteratively reweighted least squares," The American Statistician, v. 42, pp. 152-154.

More information about the normal equations and TSQR approach for solving large linear least squares systems can be found in the publications

- Trefethen, L. N. and Bau, D. (1997), "Numerical Linear Algebra", SIAM.
- Demmel, J., Grigori, L., Hoemmen, M. F., and Langou, J. "Communication-optimal parallel and sequential QR and LU factorizations", UCB Technical Report No. UCB/EECS-2008-89, 2008.

CHAPTER

FORTYONE

NONLINEAR LEAST-SQUARES FITTING

This chapter describes functions for multidimensional nonlinear least-squares fitting. There are generally two classes of algorithms for solving nonlinear least squares problems, which fall under line search methods and trust region methods. GSL currently implements only trust region methods and provides the user with full access to intermediate steps of the iteration. The user also has the ability to tune a number of parameters which affect low-level aspects of the algorithm which can help to accelerate convergence for the specific problem at hand. GSL provides two separate interfaces for nonlinear least squares fitting. The first is designed for small to moderate sized problems, and the second is designed for very large problems, which may or may not have significant sparse structure.

The header file `gsl_multifit_nlinear.h` contains prototypes for the multidimensional nonlinear fitting functions and related declarations relating to the small to moderate sized systems.

The header file `gsl_multilarge_nlinear.h` contains prototypes for the multidimensional nonlinear fitting functions and related declarations relating to large systems.

41.1 Overview

The problem of multidimensional nonlinear least-squares fitting requires the minimization of the squared residuals of n functions, f_i, in p parameters, x_i,

$$\begin{aligned}\Phi(x) &= \frac{1}{2}||f(x)||^2\\ &= \frac{1}{2}\sum_{i=1}^{n} f_i(x_1,\ldots,x_p)^2\end{aligned}$$

In trust region methods, the objective (or cost) function $\Phi(x)$ is approximated by a model function $m_k(\delta)$ in the vicinity of some point x_k. The model function is often simply a second order Taylor series expansion around the point x_k, ie:

$$\Phi(x_k+\delta) \approx m_k(\delta) = \Phi(x_k) + g_k^T\delta + \frac{1}{2}\delta^T B_k \delta$$

where $g_k = \nabla\Phi(x_k) = J^T f$ is the gradient vector at the point x_k, $B_k = \nabla^2\Phi(x_k)$ is the Hessian matrix at x_k, or some approximation to it, and J is the n-by-p Jacobian matrix

$$J_{ij} = \partial f_i/\partial x_j$$

In order to find the next step δ, we minimize the model function $m_k(\delta)$, but search for solutions only within a region where we trust that $m_k(\delta)$ is a good approximation to the objective function $\Phi(x_k+\delta)$. In other words, we seek a solution of the trust region subproblem (TRS)

$$\min_{\delta\in R^p} m_k(\delta) = \Phi(x_k) + g_k^T\delta + \frac{1}{2}\delta^T B_k\delta, \qquad \text{s.t.} \quad ||D_k\delta|| \le \Delta_k$$

where $\Delta_k > 0$ is the trust region radius and D_k is a scaling matrix. If $D_k = I$, then the trust region is a ball of radius Δ_k centered at x_k. In some applications, the parameter vector x may have widely different scales. For example, one parameter might be a temperature on the order of 10^3 K, while another might be a length on the order of 10^{-6} m. In such cases, a spherical trust region may not be the best choice, since if Φ changes rapidly along directions with one scale, and more slowly along directions with a different scale, the model function m_k may be a poor approximation to Φ along the rapidly changing directions. In such problems, it may be best to use an elliptical trust region, by setting D_k to a diagonal matrix whose entries are designed so that the scaled step $D_k\delta$ has entries of approximately the same order of magnitude.

The trust region subproblem above normally amounts to solving a linear least squares system (or multiple systems) for the step δ. Once δ is computed, it is checked whether or not it reduces the objective function $\Phi(x)$. A useful statistic for this is to look at the ratio

$$\rho_k = \frac{\Phi(x_k) - \Phi(x_k + \delta_k)}{m_k(0) - m_k(\delta_k)}$$

where the numerator is the actual reduction of the objective function due to the step δ_k, and the denominator is the predicted reduction due to the model m_k. If ρ_k is negative, it means that the step δ_k increased the objective function and so it is rejected. If ρ_k is positive, then we have found a step which reduced the objective function and it is accepted. Furthermore, if ρ_k is close to 1, then this indicates that the model function is a good approximation to the objective function in the trust region, and so on the next iteration the trust region is enlarged in order to take more ambitious steps. When a step is rejected, the trust region is made smaller and the TRS is solved again. An outline for the general trust region method used by GSL can now be given.

Trust Region Algorithm

1. Initialize: given x_0, construct $m_0(\delta)$, D_0 and $\Delta_0 > 0$
2. For k = 0, 1, 2, …
   a. If converged, then stop
   b. Solve TRS for trial step δ_k
   c. Evaluate trial step by computing ρ_k
      1). if step is accepted, set $x_{k+1} = x_k + \delta_k$ **and increase radius,** $\Delta_{k+1} = \alpha\Delta_k$
      2). if step is rejected, set $x_{k+1} = x_k$ **and decrease radius,** $\Delta_{k+1} = \frac{\Delta_k}{\beta}$; goto 2(b)
   d. Construct $m_{k+1}(\delta)$ and D_{k+1}

GSL offers the user a number of different algorithms for solving the trust region subproblem in 2(b), as well as different choices of scaling matrices D_k and different methods of updating the trust region radius Δ_k. Therefore, while reasonable default methods are provided, the user has a lot of control to fine-tune the various steps of the algorithm for their specific problem.

41.2 Solving the Trust Region Subproblem (TRS)

Below we describe the methods available for solving the trust region subproblem. The methods available provide either exact or approximate solutions to the trust region subproblem. In all algorithms below, the Hessian matrix B_k is approximated as $B_k \approx J_k^T J_k$, where $J_k = J(x_k)$. In all methods, the solution of the TRS involves solving a linear least squares system involving the Jacobian matrix. For small to moderate sized problems (`gsl_multifit_nlinear` interface), this is accomplished by factoring the full Jacobian matrix, which is provided by the user, with the Cholesky, QR, or SVD decompositions. For large systems (`gsl_multilarge_nlinear` interface), the user has two choices. One is to solve the system iteratively, without needing to store the full Jacobian matrix in memory. With this method, the user must provide a routine to calculate the matrix-vector products Ju or $J^T u$ for a given vector u. This iterative method is particularly useful for systems where the Jacobian has sparse structure, since forming matrix-vector products can be done cheaply. The second option for large systems involves forming the normal equations matrix $J^T J$ and then factoring it using a Cholesky decomposition. The normal equations matrix is p-by-p, typically much smaller than the full n-by-p Jacobian, and can usually be stored in memory even if the full Jacobian matrix cannot. This option is useful for large, dense systems, or if the iterative method has difficulty converging.

41.2.1 Levenberg-Marquardt

There is a theorem which states that if δ_k is a solution to the trust region subproblem given above, then there exists $\mu_k \geq 0$ such that

$$\left(B_k + \mu_k D_k^T D_k\right) \delta_k = -g_k$$

with $\mu_k(\Delta_k - ||D_k \delta_k||) = 0$. This forms the basis of the Levenberg-Marquardt algorithm, which controls the trust region size by adjusting the parameter μ_k rather than the radius Δ_k directly. For each radius Δ_k, there is a unique parameter μ_k which solves the TRS, and they have an inverse relationship, so that large values of μ_k correspond to smaller trust regions, while small values of μ_k correspond to larger trust regions.

With the approximation $B_k \approx J_k^T J_k$, on each iteration, in order to calculate the step δ_k, the following linear least squares problem is solved:

$$\left[\begin{array}{c} J_k \\ \sqrt{\mu_k} D_k \end{array} \right] \delta_k = - \left[\begin{array}{c} f_k \\ 0 \end{array} \right]$$

If the step δ_k is accepted, then μ_k is decreased on the next iteration in order to take a larger step, otherwise it is increased to take a smaller step. The Levenberg-Marquardt algorithm provides an exact solution of the trust region subproblem, but typically has a higher computational cost per iteration than the approximate methods discussed below, since it may need to solve the least squares system above several times for different values of μ_k.

41.2.2 Levenberg-Marquardt with Geodesic Acceleration

This method applies a so-called geodesic acceleration correction to the standard Levenberg-Marquardt step δ_k (Transtrum et al, 2011). By interpreting δ_k as a first order step along a geodesic in the model parameter space (ie: a velocity $\delta_k = v_k$), the geodesic acceleration a_k is a second order correction along the geodesic which is determined by solving the linear least squares system

$$\left[\begin{array}{c} J_k \\ \sqrt{\mu_k} D_k \end{array} \right] a_k = - \left[\begin{array}{c} f_{vv}(x_k) \\ 0 \end{array} \right]$$

where f_{vv} is the second directional derivative of the residual vector in the velocity direction v, $f_{vv}(x) = D_v^2 f = \sum_{\alpha\beta} v_\alpha v_\beta \partial_\alpha \partial_\beta f(x)$, where α and β are summed over the p parameters. The new total step is then $\delta_k' = v_k + \frac{1}{2} a_k$. The second order correction a_k can be calculated with a modest additional cost, and has been shown to dramatically reduce the number of iterations (and expensive Jacobian evaluations) required to reach convergence on a variety of different problems. In order to utilize the geodesic acceleration, the user must supply a function which provides the second directional derivative vector $f_{vv}(x)$, or alternatively the library can use a finite difference method to estimate this vector with one additional function evaluation of $f(x + hv)$ where h is a tunable step size (see the `h_fvv` parameter description).

41.2.3 Dogleg

This is Powell's dogleg method, which finds an approximate solution to the trust region subproblem, by restricting its search to a piecewise linear "dogleg" path, composed of the origin, the Cauchy point which represents the model minimizer along the steepest descent direction, and the Gauss-Newton point, which is the overall minimizer of the unconstrained model. The Gauss-Newton step is calculated by solving

$$J_k \delta_{gn} = -f_k$$

which is the main computational task for each iteration, but only needs to be performed once per iteration. If the Gauss-Newton point is inside the trust region, it is selected as the step. If it is outside, the method then calculates the Cauchy point, which is located along the gradient direction. If the Cauchy point is also outside the trust region, the method assumes that it is still far from the minimum and so proceeds along the gradient direction, truncating the step at the trust region boundary. If the Cauchy point is inside the trust region, with the Gauss-Newton point outside, the method uses a dogleg step, which is a linear combination of the gradient direction and the Gauss-Newton direction, stopping at the trust region boundary.

41.2.4 Double Dogleg

This method is an improvement over the classical dogleg algorithm, which attempts to include information about the Gauss-Newton step while the iteration is still far from the minimum. When the Cauchy point is inside the trust region and the Gauss-Newton point is outside, the method computes a scaled Gauss-Newton point and then takes a dogleg step between the Cauchy point and the scaled Gauss-Newton point. The scaling is calculated to ensure that the reduction in the model m_k is about the same as the reduction provided by the Cauchy point.

41.2.5 Two Dimensional Subspace

The dogleg methods restrict the search for the TRS solution to a 1D curve defined by the Cauchy and Gauss-Newton points. An improvement to this is to search for a solution using the full two dimensional subspace spanned by the Cauchy and Gauss-Newton directions. The dogleg path is of course inside this subspace, and so this method solves the TRS at least as accurately as the dogleg methods. Since this method searches a larger subspace for a solution, it can converge more quickly than dogleg on some problems. Because the subspace is only two dimensional, this method is very efficient and the main computation per iteration is to determine the Gauss-Newton point.

41.2.6 Steihaug-Toint Conjugate Gradient

One difficulty of the dogleg methods is calculating the Gauss-Newton step when the Jacobian matrix is singular. The Steihaug-Toint method also computes a generalized dogleg step, but avoids solving for the Gauss-Newton step directly, instead using an iterative conjugate gradient algorithm. This method performs well at points where the Jacobian is singular, and is also suitable for large-scale problems where factoring the Jacobian matrix could be prohibitively expensive.

41.3 Weighted Nonlinear Least-Squares

Weighted nonlinear least-squares fitting minimizes the function

$$\begin{aligned}\Phi(x) &= \frac{1}{2}||f||_W^2 \\ &= \frac{1}{2}\sum_{i=1}^{n} w_i f_i(x_1,\dots,x_p)^2\end{aligned}$$

where $W = \mathrm{diag}(w_1, w_2, ..., w_n)$ is the weighting matrix, and $||f||_W^2 = f^T W f$. The weights w_i are commonly defined as $w_i = 1/\sigma_i^2$, where σ_i is the error in the i-th measurement. A simple change of variables $\tilde{f} = W^{\frac{1}{2}} f$ yields $\Phi(x) = \frac{1}{2}||\tilde{f}||^2$, which is in the same form as the unweighted case. The user can either perform this transform directly on their function residuals and Jacobian, or use the *gsl_multifit_nlinear_winit()* interface which automatically performs the correct scaling. To manually perform this transformation, the residuals and Jacobian should be modified according to

$$\begin{aligned}\tilde{f}_i &= \sqrt{w_i} f_i = \frac{f_i}{\sigma_i} \\ \tilde{J}_{ij} &= \sqrt{w_i}\frac{\partial f_i}{\partial x_j} = \frac{1}{\sigma_i}\frac{\partial f_i}{\partial x_j}\end{aligned}$$

For large systems, the user must perform their own weighting.

41.4 Tunable Parameters

The user can tune nearly all aspects of the iteration at allocation time. For the `gsl_multifit_nlinear` interface, the user may modify the *gsl_multifit_nlinear_parameters* structure, which is defined as follows:

type **gsl_multifit_nlinear_parameters**

```
typedef struct
{
  const gsl_multifit_nlinear_trs *trs;        /* trust region subproblem method */
  const gsl_multifit_nlinear_scale *scale;    /* scaling method */
  const gsl_multifit_nlinear_solver *solver;  /* solver method */
  gsl_multifit_nlinear_fdtype fdtype;         /* finite difference method */
  double factor_up;                           /* factor for increasing trust radius␣
↪*/
  double factor_down;                         /* factor for decreasing trust radius␣
↪*/
  double avmax;                               /* max allowed |a|/|v| */
  double h_df;                                /* step size for finite difference␣
↪Jacobian */
  double h_fvv;                               /* step size for finite difference␣
↪fvv */
} gsl_multifit_nlinear_parameters;
```

For the `gsl_multilarge_nlinear` interface, the user may modify the *gsl_multilarge_nlinear_parameters* structure, which is defined as follows:

type **gsl_multilarge_nlinear_parameters**

```
typedef struct
{
  const gsl_multilarge_nlinear_trs *trs;       /* trust region subproblem method */
  const gsl_multilarge_nlinear_scale *scale;   /* scaling method */
  const gsl_multilarge_nlinear_solver *solver; /* solver method */
  gsl_multilarge_nlinear_fdtype fdtype;        /* finite difference method */
  double factor_up;                            /* factor for increasing trust␣
↪radius */
  double factor_down;                          /* factor for decreasing trust␣
↪radius */
  double avmax;                                /* max allowed |a|/|v| */
  double h_df;                                 /* step size for finite difference␣
↪Jacobian */
  double h_fvv;                                /* step size for finite difference␣
↪fvv */
  size_t max_iter;                             /* maximum iterations for trs method␣
↪*/
  double tol;                                  /* tolerance for solving trs */
} gsl_multilarge_nlinear_parameters;
```

Each of these parameters is discussed in further detail below.

type **gsl_multifit_nlinear_trs**

type **gsl_multilarge_nlinear_trs**

The parameter `trs` determines the method used to solve the trust region subproblem, and may be selected from the following choices,

gsl_multifit_nlinear_trs ***gsl_multifit_nlinear_trs_lm**

gsl_multilarge_nlinear_trs ***gsl_multilarge_nlinear_trs_lm**

This selects the Levenberg-Marquardt algorithm.

gsl_multifit_nlinear_trs ***gsl_multifit_nlinear_trs_lmaccel**

gsl_multilarge_nlinear_trs ***gsl_multilarge_nlinear_trs_lmaccel**

This selects the Levenberg-Marquardt algorithm with geodesic acceleration.

gsl_multifit_nlinear_trs ***gsl_multifit_nlinear_trs_dogleg**

gsl_multilarge_nlinear_trs ***gsl_multilarge_nlinear_trs_dogleg**

This selects the dogleg algorithm.

gsl_multifit_nlinear_trs ***gsl_multifit_nlinear_trs_ddogleg**

gsl_multilarge_nlinear_trs ***gsl_multilarge_nlinear_trs_ddogleg**

This selects the double dogleg algorithm.

gsl_multifit_nlinear_trs ***gsl_multifit_nlinear_trs_subspace2D**

gsl_multilarge_nlinear_trs ***gsl_multilarge_nlinear_trs_subspace2D**

This selects the 2D subspace algorithm.

gsl_multilarge_nlinear_trs ***gsl_multilarge_nlinear_trs_cgst**

This selects the Steihaug-Toint conjugate gradient algorithm. This method is available only for large systems.

type **gsl_multifit_nlinear_scale**

type **gsl_multilarge_nlinear_scale**

The parameter `scale` determines the diagonal scaling matrix D and may be selected from the following choices, *gsl_multifit_nlinear_scale* ***gsl_multifit_nlinear_scale_more**

gsl_multilarge_nlinear_scale ***gsl_multilarge_nlinear_scale_more**

This damping strategy was suggested by Moré, and corresponds to $D^T D = \max(\text{diag}(J^T J))$, in other words the maximum elements of $\text{diag}(J^T J)$ encountered thus far in the iteration. This choice of D makes the problem scale-invariant, so that if the model parameters x_i are each scaled by an arbitrary constant, $\tilde{x}_i = a_i x_i$, then the sequence of iterates produced by the algorithm would be unchanged. This method can work very well in cases where the model parameters have widely different scales (ie: if some parameters are measured in nanometers, while others are measured in degrees Kelvin). This strategy has been proven effective on a large class of problems and so it is the library default, but it may not be the best choice for all problems.

gsl_multifit_nlinear_scale ***gsl_multifit_nlinear_scale_levenberg**

gsl_multilarge_nlinear_scale ***gsl_multilarge_nlinear_scale_levenberg**

This damping strategy was originally suggested by Levenberg, and corresponds to $D^T D = I$. This method has also proven effective on a large class of problems, but is not scale-invariant. However, some authors (e.g. Transtrum and Sethna 2012) argue that this choice is better for problems which are susceptible to parameter evaporation (ie: parameters go to infinity)

gsl_multifit_nlinear_scale ***gsl_multifit_nlinear_scale_marquardt**

gsl_multilarge_nlinear_scale ***gsl_multilarge_nlinear_scale_marquardt**

This damping strategy was suggested by Marquardt, and corresponds to $D^T D = \text{diag}(J^T J)$. This method is scale-invariant, but it is generally considered inferior to both the Levenberg and Moré strategies, though may work well on certain classes of problems.

type **gsl_multifit_nlinear_solver**

type **gsl_multilarge_nlinear_solver**

Solving the trust region subproblem on each iteration almost always requires the solution of the following linear least squares system

$$\begin{bmatrix} J \\ \sqrt{\mu} D \end{bmatrix} \delta = - \begin{bmatrix} f \\ 0 \end{bmatrix}$$

The `solver` parameter determines how the system is solved and can be selected from the following choices:

gsl_multifit_nlinear_solver ***gsl_multifit_nlinear_solver_qr**

This method solves the system using a rank revealing QR decomposition of the Jacobian J. This method will produce reliable solutions in cases where the Jacobian is rank deficient or near-singular but does require about twice as many operations as the Cholesky method discussed below.

gsl_multifit_nlinear_solver ***gsl_multifit_nlinear_solver_cholesky**

gsl_multilarge_nlinear_solver ***gsl_multilarge_nlinear_solver_cholesky**

This method solves the alternate normal equations problem

$$\left(J^T J + \mu D^T D \right) \delta = -J^T f$$

by using a Cholesky decomposition of the matrix $J^T J + \mu D^T D$. This method is faster than the QR approach, however it is susceptible to numerical instabilities if the Jacobian matrix is rank deficient or near-singular. In these cases, an attempt is made to reduce the condition number of the matrix using Jacobi preconditioning, but for highly ill-conditioned problems the QR approach is better. If it is known that the Jacobian matrix is well conditioned, this method is accurate and will perform faster than the QR approach.

gsl_multifit_nlinear_solver ***gsl_multifit_nlinear_solver_mcholesky**

gsl_multilarge_nlinear_solver ***gsl_multilarge_nlinear_solver_mcholesky**

This method solves the alternate normal equations problem

$$\left(J^T J + \mu D^T D \right) \delta = -J^T f$$

by using a modified Cholesky decomposition of the matrix $J^T J + \mu D^T D$. This is more suitable for the dogleg methods where the parameter $\mu = 0$, and the matrix $J^T J$ may be ill-conditioned or indefinite causing the standard Cholesky decomposition to fail. This method is based on Level 2 BLAS and is thus slower than the standard Cholesky decomposition, which is based on Level 3 BLAS.

gsl_multifit_nlinear_solver ***gsl_multifit_nlinear_solver_svd**

This method solves the system using a singular value decomposition of the Jacobian J. This method will produce the most reliable solutions for ill-conditioned Jacobians but is also the slowest solver method.

type **gsl_multifit_nlinear_fdtype**

The parameter `fdtype` specifies whether to use forward or centered differences when approximating the Jacobian. This is only used when an analytic Jacobian is not provided to the solver. This parameter may be set to one of the following choices.

GSL_MULTIFIT_NLINEAR_FWDIFF

This specifies a forward finite difference to approximate the Jacobian matrix. The Jacobian matrix will be calculated as

$$J_{ij} = \frac{1}{\Delta_j} \left(f_i(x + \Delta_j e_j) - f_i(x) \right)$$

where $\Delta_j = h|x_j|$ and e_j is the standard j-th Cartesian unit basis vector so that $x + \Delta_j e_j$ represents a small (forward) perturbation of the j-th parameter by an amount Δ_j. The perturbation Δ_j is proportional to the current value $|x_j|$ which helps to calculate an accurate Jacobian when the various parameters have different scale sizes. The value of h is specified by the `h_df` parameter. The accuracy of this method is $O(h)$, and evaluating this matrix requires an additional p function evaluations.

GSL_MULTIFIT_NLINEAR_CTRDIFF

This specifies a centered finite difference to approximate the Jacobian matrix. The Jacobian matrix will be calculated as

$$J_{ij} = \frac{1}{\Delta_j} \left(f_i(x + \frac{1}{2}\Delta_j e_j) - f_i(x - \frac{1}{2}\Delta_j e_j) \right)$$

See above for a description of Δ_j. The accuracy of this method is $O(h^2)$, but evaluating this matrix requires an additional $2p$ function evaluations.

`double factor_up`

When a step is accepted, the trust region radius will be increased by this factor. The default value is 3.

`double factor_down`

When a step is rejected, the trust region radius will be decreased by this factor. The default value is 2.

`double avmax`

When using geodesic acceleration to solve a nonlinear least squares problem, an important parameter to monitor is the ratio of the acceleration term to the velocity term,

$$\frac{||a||}{||v||}$$

If this ratio is small, it means the acceleration correction is contributing very little to the step. This could be because the problem is not "nonlinear" enough to benefit from the acceleration. If the ratio is large (> 1) it means that the acceleration is larger than the velocity, which shouldn't happen since the step represents a truncated series and so the second order term a should be smaller than the first order term v to guarantee convergence. Therefore any steps with a ratio larger than the parameter `avmax` are rejected. `avmax` is set to 0.75 by default. For problems which experience difficulty converging, this threshold could be lowered.

`double h_df`

This parameter specifies the step size for approximating the Jacobian matrix with finite differences. It is set to $\sqrt{\epsilon}$ by default, where ϵ is `GSL_DBL_EPSILON`.

`double h_fvv`

When using geodesic acceleration, the user must either supply a function to calculate $f_{vv}(x)$ or the library can estimate this second directional derivative using a finite difference method. When using finite differences, the library must calculate $f(x + hv)$ where h represents a small step in the velocity direction. The parameter **h_fvv** defines this step size and is set to 0.02 by default.

41.5 Initializing the Solver

type **gsl_multifit_nlinear_type**

This structure specifies the type of algorithm which will be used to solve a nonlinear least squares problem. It may be selected from the following choices,

gsl_multifit_nlinear_type ***gsl_multifit_nlinear_trust**

This specifies a trust region method. It is currently the only implemented nonlinear least squares method.

gsl_multifit_nlinear_workspace ***gsl_multifit_nlinear_alloc**(const *gsl_multifit_nlinear_type* *T, const *gsl_multifit_nlinear_parameters* *params, const size_t n, const size_t p)

gsl_multilarge_nlinear_workspace ***gsl_multilarge_nlinear_alloc**(const gsl_multilarge_nlinear_type *T, const *gsl_multilarge_nlinear_parameters* *params, const size_t n, const size_t p)

These functions return a pointer to a newly allocated instance of a derivative solver of type *T* for *n* observations and *p* parameters. The *params* input specifies a tunable set of parameters which will affect important details in each iteration of the trust region subproblem algorithm. It is recommended to start with the suggested default parameters (see *gsl_multifit_nlinear_default_parameters()* and *gsl_multilarge_nlinear_default_parameters()*) and then tune the parameters once the code is working correctly. See *Tunable Parameters*. for descriptions of the various parameters. For example, the following code creates an instance of a Levenberg-Marquardt solver for 100 data points and 3 parameters, using suggested defaults:

```
const gsl_multifit_nlinear_type * T = gsl_multifit_nlinear_trust;
gsl_multifit_nlinear_parameters params = gsl_multifit_nlinear_default_parameters();
gsl_multifit_nlinear_workspace * w = gsl_multifit_nlinear_alloc (T, &params, 100,␣
↪3);
```

The number of observations *n* must be greater than or equal to parameters *p*.

If there is insufficient memory to create the solver then the function returns a null pointer and the error handler is invoked with an error code of *GSL_ENOMEM*.

gsl_multifit_nlinear_parameters **gsl_multifit_nlinear_default_parameters**(void)

gsl_multilarge_nlinear_parameters **gsl_multilarge_nlinear_default_parameters**(void)

These functions return a set of recommended default parameters for use in solving nonlinear least squares problems. The user can tune each parameter to improve the performance on their particular problem, see *Tunable Parameters*.

int **gsl_multifit_nlinear_init**(const *gsl_vector* *x, *gsl_multifit_nlinear_fdf* *fdf, gsl_multifit_nlinear_workspace *w) int **gsl_multifit_nlinear_winit**(const *gsl_vector* *x, const *gsl_vector* *wts, *gsl_multifit_nlinear_fdf* *fdf, gsl_multifit_nlinear_workspace *w)

int **gsl_multilarge_nlinear_init**(const *gsl_vector* *x, *gsl_multilarge_nlinear_fdf* *fdf, gsl_multilarge_nlinear_workspace *w)

These functions initialize, or reinitialize, an existing workspace `w` to use the system `fdf` and the initial guess `x`. See *Providing the Function to be Minimized* for a description of the `fdf` structure.

Optionally, a weight vector `wts` can be given to perform a weighted nonlinear regression. Here, the weighting matrix is $W = \text{diag}(w_1, w_2, ..., w_n)$.

void **gsl_multifit_nlinear_free**(gsl_multifit_nlinear_workspace *w)

void **gsl_multilarge_nlinear_free**(gsl_multilarge_nlinear_workspace *w)

These functions free all the memory associated with the workspace `w`.

const char ***gsl_multifit_nlinear_name**(const gsl_multifit_nlinear_workspace *w)

const char ***gsl_multilarge_nlinear_name**(const gsl_multilarge_nlinear_workspace *w)

These functions return a pointer to the name of the solver. For example:

```
printf ("w is a '%s' solver\n", gsl_multifit_nlinear_name (w));
```

would print something like `w is a 'trust-region' solver`.

const char ***gsl_multifit_nlinear_trs_name**(const gsl_multifit_nlinear_workspace *w)

const char ***gsl_multilarge_nlinear_trs_name**(const gsl_multilarge_nlinear_workspace *w)

These functions return a pointer to the name of the trust region subproblem method. For example:

```
printf ("w is a '%s' solver\n", gsl_multifit_nlinear_trs_name (w));
```

would print something like `w is a 'levenberg-marquardt' solver`.

41.6 Providing the Function to be Minimized

The user must provide n functions of p variables for the minimization algorithm to operate on. In order to allow for arbitrary parameters the functions are defined by the following data types:

type **gsl_multifit_nlinear_fdf**

This data type defines a general system of functions with arbitrary parameters, the corresponding Jacobian matrix of derivatives, and optionally the second directional derivative of the functions for geodesic acceleration.

`int (* f) (const gsl_vector * x, void * params, gsl_vector * f)`

This function should store the n components of the vector $f(x)$ in `f` for argument `x` and arbitrary parameters `params`, returning an appropriate error code if the function cannot be computed.

`int (* df) (const gsl_vector * x, void * params, gsl_matrix * J)`

This function should store the `n`-by-`p` matrix result

$$J_{ij} = \partial f_i(x)/\partial x_j$$

in `J` for argument `x` and arbitrary parameters `params`, returning an appropriate error code if the matrix cannot be computed. If an analytic Jacobian is unavailable, or too expensive to compute, this function pointer may be set to NULL, in which case the Jacobian will be internally computed using finite difference approximations of the function f.

`int (* fvv) (const gsl_vector * x, const gsl_vector * v, void * params, gsl_vector * fvv)`

When geodesic acceleration is enabled, this function should store the n components of the vector $f_{vv}(x) = \sum_{\alpha\beta} v_\alpha v_\beta \frac{\partial}{\partial x_\alpha} \frac{\partial}{\partial x_\beta} f(x)$, representing second directional derivatives of the function to be minimized, into the output fvv. The parameter vector is provided in x and the velocity vector is provided in v, both of which have p components. The arbitrary parameters are given in params. If analytic expressions for $f_{vv}(x)$ are unavailable or too difficult to compute, this function pointer may be set to NULL, in which case $f_{vv}(x)$ will be computed internally using a finite difference approximation.

`size_t n`

the number of functions, i.e. the number of components of the vector f.

`size_t p`

the number of independent variables, i.e. the number of components of the vector x.

`void * params`

a pointer to the arbitrary parameters of the function.

`size_t nevalf`

This does not need to be set by the user. It counts the number of function evaluations and is initialized by the _init function.

`size_t nevaldf`

This does not need to be set by the user. It counts the number of Jacobian evaluations and is initialized by the _init function.

`size_t nevalfvv`

This does not need to be set by the user. It counts the number of $f_{vv}(x)$ evaluations and is initialized by the _init function.

type **gsl_multilarge_nlinear_fdf**

This data type defines a general system of functions with arbitrary parameters, a function to compute Ju or $J^T u$ for a given vector u, the normal equations matrix $J^T J$, and optionally the second directional derivative of the functions for geodesic acceleration.

`int (* f) (const gsl_vector * x, void * params, gsl_vector * f)`

This function should store the n components of the vector $f(x)$ in f for argument x and arbitrary parameters params, returning an appropriate error code if the function cannot be computed.

`int (* df) (CBLAS_TRANSPOSE_t TransJ, const gsl_vector * x, const gsl_vector * u, void * params, gsl_vector * v, gsl_matrix * JTJ)`

If TransJ is equal to CblasNoTrans, then this function should compute the matrix-vector product Ju and store the result in v. If TransJ is equal to CblasTrans, then this function should compute the matrix-vector product $J^T u$ and store the result in v. Additionally, the normal equations matrix $J^T J$ should be stored in the lower half of JTJ. The input matrix JTJ could be set to NULL, for example by iterative methods which do not require this matrix, so the user should check for this prior to constructing the matrix. The input params contains the arbitrary parameters.

`int (* fvv) (const gsl_vector * x, const gsl_vector * v, void * params, gsl_vector * fvv)`

When geodesic acceleration is enabled, this function should store the n components of the vector $f_{vv}(x) = \sum_{\alpha\beta} v_\alpha v_\beta \frac{\partial}{\partial x_\alpha} \frac{\partial}{\partial x_\beta} f(x)$, representing second directional derivatives of the function to be minimized, into the output `fvv`. The parameter vector is provided in `x` and the velocity vector is provided in `v`, both of which have p components. The arbitrary parameters are given in `params`. If analytic expressions for $f_{vv}(x)$ are unavailable or too difficult to compute, this function pointer may be set to `NULL`, in which case $f_{vv}(x)$ will be computed internally using a finite difference approximation.

`size_t n`

the number of functions, i.e. the number of components of the vector `f`.

`size_t p`

the number of independent variables, i.e. the number of components of the vector `x`.

`void * params`

a pointer to the arbitrary parameters of the function.

`size_t nevalf`

This does not need to be set by the user. It counts the number of function evaluations and is initialized by the `_init` function.

`size_t nevaldfu`

This does not need to be set by the user. It counts the number of Jacobian matrix-vector evaluations (Ju or $J^T u$) and is initialized by the `_init` function.

`size_t nevaldf2`

This does not need to be set by the user. It counts the number of $J^T J$ evaluations and is initialized by the `_init` function.

`size_t nevalfvv`

This does not need to be set by the user. It counts the number of $f_{vv}(x)$ evaluations and is initialized by the `_init` function.

Note that when fitting a non-linear model against experimental data, the data is passed to the functions above using the `params` argument and the trial best-fit parameters through the `x` argument.

41.7 Iteration

The following functions drive the iteration of each algorithm. Each function performs one iteration of the trust region method and updates the state of the solver.

int **gsl_multifit_nlinear_iterate**(gsl_multifit_nlinear_workspace *w)

int **gsl_multilarge_nlinear_iterate**(gsl_multilarge_nlinear_workspace *w)

These functions perform a single iteration of the solver *w*. If the iteration encounters an unexpected problem then an error code will be returned. The solver workspace maintains a current estimate of the best-fit parameters at all times.

The solver workspace `w` contains the following entries, which can be used to track the progress of the solution:

`gsl_vector * x`

The current position, length p.

`gsl_vector * f`

The function residual vector at the current position $f(x)$, length n.

`gsl_matrix * J`

The Jacobian matrix at the current position $J(x)$, size n-by-p (only for `gsl_multifit_nlinear` interface).

`gsl_vector * dx`

The difference between the current position and the previous position, i.e. the last step δ, taken as a vector, length p.

These quantities can be accessed with the following functions,

gsl_vector ***gsl_multifit_nlinear_position**(const gsl_multifit_nlinear_workspace *w)

gsl_vector ***gsl_multilarge_nlinear_position**(const gsl_multilarge_nlinear_workspace *w)

These functions return the current position x (i.e. best-fit parameters) of the solver `w`.

gsl_vector ***gsl_multifit_nlinear_residual**(const gsl_multifit_nlinear_workspace *w)

gsl_vector ***gsl_multilarge_nlinear_residual**(const gsl_multilarge_nlinear_workspace *w)

These functions return the current residual vector $f(x)$ of the solver `w`. For weighted systems, the residual vector includes the weighting factor $\sqrt{W}$.

gsl_matrix ***gsl_multifit_nlinear_jac**(const gsl_multifit_nlinear_workspace *w)

This function returns a pointer to the n-by-p Jacobian matrix for the current iteration of the solver `w`. This function is available only for the `gsl_multifit_nlinear` interface.

size_t **gsl_multifit_nlinear_niter**(const gsl_multifit_nlinear_workspace *w)

size_t **gsl_multilarge_nlinear_niter**(const gsl_multilarge_nlinear_workspace *w)

These functions return the number of iterations performed so far. The iteration counter is updated on each call to the `_iterate` functions above, and reset to 0 in the `_init` functions.

int **gsl_multifit_nlinear_rcond**(double *rcond, const gsl_multifit_nlinear_workspace *w)

int **gsl_multilarge_nlinear_rcond**(double *rcond, const gsl_multilarge_nlinear_workspace *w)

This function estimates the reciprocal condition number of the Jacobian matrix at the current position x and stores it in `rcond`. The computed value is only an estimate to give the user a guideline as to the conditioning of their particular problem. Its calculation is based on which factorization method is used (Cholesky, QR, or SVD).

- For the Cholesky solver, the matrix $J^T J$ is factored at each iteration. Therefore this function will estimate the 1-norm condition number $rcond^2 = 1/(||J^T J||_1 \cdot ||(J^T J)^{-1}||_1)$
- For the QR solver, J is factored as $J = QR$ at each iteration. For simplicity, this function calculates the 1-norm conditioning of only the R factor, $rcond = 1/(||R||_1 \cdot ||R^{-1}||_1)$. This can be computed efficiently since R is upper triangular.
- For the SVD solver, in order to efficiently solve the trust region subproblem, the matrix which is factored is JD^{-1}, instead of J itself. The resulting singular values are used to provide the 2-norm reciprocal condition number, as $rcond = \sigma_{min}/\sigma_{max}$. Note that when using Moré scaling, $D \neq I$ and the resulting `rcond` estimate may be significantly different from the true `rcond` of J itself.

double **gsl_multifit_nlinear_avratio**(const gsl_multifit_nlinear_workspace *w)

double **gsl_multilarge_nlinear_avratio**(const gsl_multilarge_nlinear_workspace *w)

This function returns the current ratio $|a|/|v|$ of the acceleration correction term to the velocity step term. The acceleration term is computed only by the `gsl_multifit_nlinear_trs_lmaccel` and `gsl_multilarge_nlinear_trs_lmaccel` methods, so this ratio will be zero for other TRS methods.

41.8 Testing for Convergence

A minimization procedure should stop when one of the following conditions is true:

- A minimum has been found to within the user-specified precision.
- A user-specified maximum number of iterations has been reached.
- An error has occurred.

The handling of these conditions is under user control. The functions below allow the user to test the current estimate of the best-fit parameters in several standard ways.

int **gsl_multifit_nlinear_test**(const double xtol, const double gtol, const double ftol, int *info, const gsl_multifit_nlinear_workspace *w)

int **gsl_multilarge_nlinear_test**(const double xtol, const double gtol, const double ftol, int *info, const gsl_multilarge_nlinear_workspace *w)

These functions test for convergence of the minimization method using the following criteria:

- Testing for a small step size relative to the current parameter vector

$$|\delta_i| \leq xtol(|x_i| + xtol)$$

  for each $0 <= i < p$. Each element of the step vector δ is tested individually in case the different parameters have widely different scales. Adding *`xtol`* to $|x_i|$ helps the test avoid breaking down in situations where the true solution value $x_i = 0$. If this test succeeds, *`info`* is set to 1 and the function returns `GSL_SUCCESS`.

  A general guideline for selecting the step tolerance is to choose $xtol = 10^{-d}$ where d is the number of accurate decimal digits desired in the solution x. See Dennis and Schnabel for more information.

- Testing for a small gradient ($g = \nabla\Phi(x) = J^T f$) indicating a local function minimum:

$$\max_i |g_i \times \max(x_i, 1)| \leq gtol \times \max(\Phi(x), 1)$$

  This expression tests whether the ratio $(\nabla\Phi)_i x_i/\Phi$ is small. Testing this scaled gradient is a better than $\nabla\Phi$ alone since it is a dimensionless quantity and so independent of the scale of the problem. The `max` arguments help ensure the test doesn't break down in regions where x_i or $\Phi(x)$ are close to 0. If this test succeeds, *`info`* is set to 2 and the function returns `GSL_SUCCESS`.

  A general guideline for choosing the gradient tolerance is to set `gtol = GSL_DBL_EPSILON^(1/3)`. See Dennis and Schnabel for more information.

If none of the tests succeed, *`info`* is set to 0 and the function returns `GSL_CONTINUE`, indicating further iterations are required.

41.9 High Level Driver

These routines provide a high level wrapper that combines the iteration and convergence testing for easy use.

int **gsl_multifit_nlinear_driver**(const size_t maxiter, const double xtol, const double gtol, const double ftol, void (*callback)(const size_t iter, void *params, const *gsl_multifit_linear_workspace* *w), void *callback_params, int *info, gsl_multifit_nlinear_workspace *w) int **gsl_multilarge_nlinear_driver**(const size_t maxiter, const double xtol, const double gtol, const double ftol, void (*callback)(const size_t iter, void *params, const *gsl_multilarge_linear_workspace* *w), void *callback_params, int *info, gsl_multilarge_nlinear_workspace *w)

These functions iterate the nonlinear least squares solver `w` for a maximum of `maxiter` iterations. After each iteration, the system is tested for convergence with the error tolerances `xtol`, `gtol` and `ftol`. Additionally, the user may supply a callback function `callback` which is called after each iteration, so that the user may save or print relevant quantities for each iteration. The parameter `callback_params` is passed to the `callback` function. The parameters `callback` and `callback_params` may be set to `NULL` to disable this feature. Upon successful convergence, the function returns `GSL_SUCCESS` and sets `info` to the reason for convergence (see `gsl_multifit_nlinear_test()`). If the function has not converged after `maxiter` iterations, `GSL_EMAXITER` is returned. In rare cases, during an iteration the algorithm may be unable to find a new acceptable step δ to take. In this case, `GSL_ENOPROG` is returned indicating no further progress can be made. If your problem is having difficulty converging, see *Troubleshooting* for further guidance.

41.10 Covariance matrix of best fit parameters

int **gsl_multifit_nlinear_covar**(const *gsl_matrix* *J, const double epsrel, *gsl_matrix* *covar)

int **gsl_multilarge_nlinear_covar**(*gsl_matrix* *covar, gsl_multilarge_nlinear_workspace *w)

This function computes the covariance matrix of best-fit parameters using the Jacobian matrix `J` and stores it in `covar`. The parameter `epsrel` is used to remove linear-dependent columns when `J` is rank deficient.

The covariance matrix is given by,

$$C = (J^T J)^{-1}$$

or in the weighted case,

$$C = (J^T W J)^{-1}$$

and is computed using the factored form of the Jacobian (Cholesky, QR, or SVD). Any columns of R which satisfy

$$|R_{kk}| \leq epsrel|R_{11}|$$

are considered linearly-dependent and are excluded from the covariance matrix (the corresponding rows and columns of the covariance matrix are set to zero).

If the minimisation uses the weighted least-squares function $f_i = (Y(x, t_i) - y_i)/\sigma_i$ then the covariance matrix above gives the statistical error on the best-fit parameters resulting from the Gaussian errors σ_i on the underlying data y_i. This can be verified from the relation $\delta f = J\delta c$ and the fact that the fluctuations in f from the data y_i are normalised by σ_i and so satisfy

$$\langle \delta f \delta f^T \rangle = I$$

For an unweighted least-squares function $f_i = (Y(x, t_i) - y_i)$ the covariance matrix above should be multiplied by the variance of the residuals about the best-fit $\sigma^2 = \sum (y_i - Y(x, t_i))^2/(n - p)$ to give the variance-covariance matrix $\sigma^2 C$. This estimates the statistical error on the best-fit parameters from the scatter of the underlying data.

For more information about covariance matrices see *Linear Least-Squares Overview*.

41.11 Troubleshooting

When developing a code to solve a nonlinear least squares problem, here are a few considerations to keep in mind.

1. The most common difficulty is the accurate implementation of the Jacobian matrix. If the analytic Jacobian is not properly provided to the solver, this can hinder and many times prevent convergence of the method. When developing a new nonlinear least squares code, it often helps to compare the program output with the internally computed finite difference Jacobian and the user supplied analytic Jacobian. If there is a large difference in coefficients, it is likely the analytic Jacobian is incorrectly implemented.
2. If your code is having difficulty converging, the next thing to check is the starting point provided to the solver. The methods of this chapter are local methods, meaning if you provide a starting point far away from the true minimum, the method may converge to a local minimum or not converge at all. Sometimes it is possible to solve a linearized approximation to the nonlinear problem, and use the linear solution as the starting point to the nonlinear problem.
3. If the various parameters of the coefficient vector x vary widely in magnitude, then the problem is said to be badly scaled. The methods of this chapter do attempt to automatically rescale the elements of x to have roughly the same order of magnitude, but in extreme cases this could still cause problems for convergence. In these cases it is recommended for the user to scale their parameter vector x so that each parameter spans roughly the same range, say $[-1, 1]$. The solution vector can be backscaled to recover the original units of the problem.

41.12 Examples

The following example programs demonstrate the nonlinear least squares fitting capabilities.

41.12.1 Exponential Fitting Example

The following example program fits a weighted exponential model with background to experimental data, $Y = A\exp(-\lambda t) + b$. The first part of the program sets up the functions `expb_f()` and `expb_df()` to calculate the model and its Jacobian. The appropriate fitting function is given by,

$$f_i = (A\exp(-\lambda t_i) + b) - y_i$$

where we have chosen $t_i = iT/(N-1)$, where N is the number of data points fitted, so that $t_i \in [0, T]$. The Jacobian matrix J is the derivative of these functions with respect to the three parameters (A, λ, b). It is given by,

$$J_{ij} = \frac{\partial f_i}{\partial x_j}$$

where $x_0 = A$, $x_1 = \lambda$ and $x_2 = b$. The i-th row of the Jacobian is therefore

$$J_{i\cdot} = \left(\begin{array}{ccc} \exp(-\lambda t_i) & -t_i A\exp(-\lambda t_i) & 1 \end{array} \right)$$

The main part of the program sets up a Levenberg-Marquardt solver and some simulated random data. The data uses the known parameters (5.0,1.5,1.0) combined with Gaussian noise (standard deviation = 0.1) with a maximum time $T = 3$ and $N = 100$ timesteps. The initial guess for the parameters is chosen as (1.0, 1.0, 0.0). The iteration terminates when the relative change in x is smaller than 10^{-8}, or when the magnitude of the gradient falls below 10^{-8}. Here are the results of running the program:

```
iter  0: A = 1.0000, lambda = 1.0000, b = 0.0000, cond(J) =      inf, |f(x)| = 88.4448
iter  1: A = 4.5109, lambda = 2.5258, b = 1.0704, cond(J) =  26.2686, |f(x)| = 24.0646
iter  2: A = 4.8565, lambda = 1.7442, b = 1.1669, cond(J) =  23.7470, |f(x)| = 11.9797
```

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```
iter  3: A = 4.9356, lambda = 1.5713, b = 1.0767, cond(J) =  17.5849, |f(x)| = 10.7355
iter  4: A = 4.8678, lambda = 1.4838, b = 1.0252, cond(J) =  16.3428, |f(x)| = 10.5000
iter  5: A = 4.8118, lambda = 1.4481, b = 1.0076, cond(J) =  15.7925, |f(x)| = 10.4786
iter  6: A = 4.7983, lambda = 1.4404, b = 1.0041, cond(J) =  15.5840, |f(x)| = 10.4778
iter  7: A = 4.7967, lambda = 1.4395, b = 1.0037, cond(J) =  15.5396, |f(x)| = 10.4778
iter  8: A = 4.7965, lambda = 1.4394, b = 1.0037, cond(J) =  15.5344, |f(x)| = 10.4778
iter  9: A = 4.7965, lambda = 1.4394, b = 1.0037, cond(J) =  15.5339, |f(x)| = 10.4778
iter 10: A = 4.7965, lambda = 1.4394, b = 1.0037, cond(J) =  15.5339, |f(x)| = 10.4778
iter 11: A = 4.7965, lambda = 1.4394, b = 1.0037, cond(J) =  15.5339, |f(x)| = 10.4778
summary from method 'trust-region/levenberg-marquardt'
number of iterations: 11
function evaluations: 16
Jacobian evaluations: 12
reason for stopping: small gradient
initial |f(x)| = 88.444756
final   |f(x)| = 10.477801
chisq/dof = 1.1318
A      = 4.79653 +/- 0.18704
lambda = 1.43937 +/- 0.07390
b      = 1.00368 +/- 0.03473
status = success
```

The approximate values of the parameters are found correctly, and the chi-squared value indicates a good fit (the chi-squared per degree of freedom is approximately 1). In this case the errors on the parameters can be estimated from the square roots of the diagonal elements of the covariance matrix. If the chi-squared value shows a poor fit (i.e. $\chi^2/(n-p) \gg 1$ then the error estimates obtained from the covariance matrix will be too small. In the example program the error estimates are multiplied by $\sqrt{\chi^2/(n-p)}$ in this case, a common way of increasing the errors for a poor fit. Note that a poor fit will result from the use of an inappropriate model, and the scaled error estimates may then be outside the range of validity for Gaussian errors.

Additionally, we see that the condition number of $J(x)$ stays reasonably small throughout the iteration. This indicates we could safely switch to the Cholesky solver for speed improvement, although this particular system is too small to really benefit.

Fig. 41.1 shows the fitted curve with the original data.

```
#include <stdlib.h>
#include <stdio.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_multifit_nlinear.h>

#define N      100    /* number of data points to fit */
#define TMAX   (3.0)  /* time variable in [0,TMAX] */

struct data {
  size_t n;
  double * t;
  double * y;
};
```

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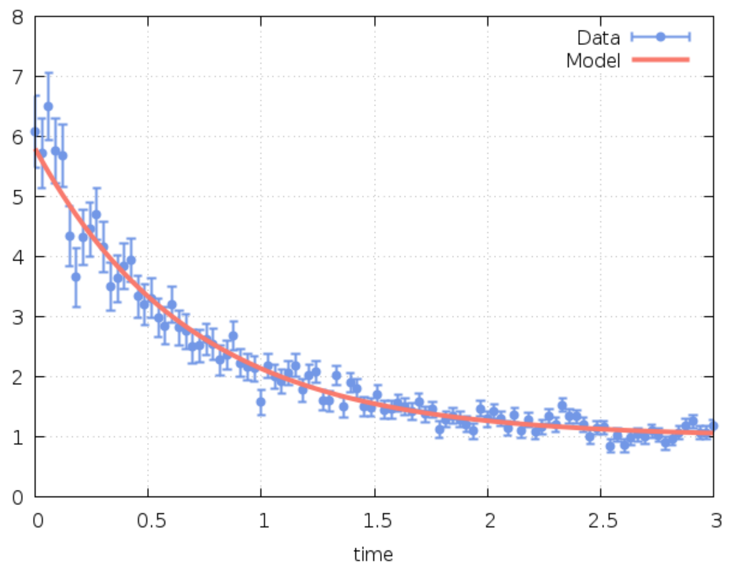

Fig. 41.1: Exponential fitted curve with data

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```

int
expb_f (const gsl_vector * x, void *data,
        gsl_vector * f)
{
  size_t n = ((struct data *)data)->n;
  double *t = ((struct data *)data)->t;
  double *y = ((struct data *)data)->y;

  double A = gsl_vector_get (x, 0);
  double lambda = gsl_vector_get (x, 1);
  double b = gsl_vector_get (x, 2);

  size_t i;

  for (i = 0; i < n; i++)
    {
      /* Model Yi = A * exp(-lambda * t_i) + b */
      double Yi = A * exp (-lambda * t[i]) + b;
      gsl_vector_set (f, i, Yi - y[i]);
    }

  return GSL_SUCCESS;
}

int
expb_df (const gsl_vector * x, void *data,
         gsl_matrix * J)
{
  size_t n = ((struct data *)data)->n;
```

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```
  double *t = ((struct data *)data)->t;

  double A = gsl_vector_get (x, 0);
  double lambda = gsl_vector_get (x, 1);

  size_t i;

  for (i = 0; i < n; i++)
    {
      /* Jacobian matrix J(i,j) = dfi / dxj, */
      /* where fi = (Yi - yi)/sigma[i],      */
      /*       Yi = A * exp(-lambda * t_i) + b  */
      /* and the xj are the parameters (A,lambda,b) */
      double e = exp(-lambda * t[i]);
      gsl_matrix_set (J, i, 0, e);
      gsl_matrix_set (J, i, 1, -t[i] * A * e);
      gsl_matrix_set (J, i, 2, 1.0);
    }

  return GSL_SUCCESS;
}

void
callback(const size_t iter, void *params,
         const gsl_multifit_nlinear_workspace *w)
{
  gsl_vector *f = gsl_multifit_nlinear_residual(w);
  gsl_vector *x = gsl_multifit_nlinear_position(w);
  double rcond;

  /* compute reciprocal condition number of J(x) */
  gsl_multifit_nlinear_rcond(&rcond, w);

  fprintf(stderr, "iter %2zu: A = %.4f, lambda = %.4f, b = %.4f, cond(J) = %8.4f, |f(x)|␣
↪= %.4f\n",
          iter,
          gsl_vector_get(x, 0),
          gsl_vector_get(x, 1),
          gsl_vector_get(x, 2),
          1.0 / rcond,
          gsl_blas_dnrm2(f));
}

int
main (void)
{
  const gsl_multifit_nlinear_type *T = gsl_multifit_nlinear_trust;
  gsl_multifit_nlinear_workspace *w;
  gsl_multifit_nlinear_fdf fdf;
  gsl_multifit_nlinear_parameters fdf_params =
    gsl_multifit_nlinear_default_parameters();
  const size_t n = N;
```

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```
  const size_t p = 3;

  gsl_vector *f;
  gsl_matrix *J;
  gsl_matrix *covar = gsl_matrix_alloc (p, p);
  double t[N], y[N], weights[N];
  struct data d = { n, t, y };
  double x_init[3] = { 1.0, 1.0, 0.0 }; /* starting values */
  gsl_vector_view x = gsl_vector_view_array (x_init, p);
  gsl_vector_view wts = gsl_vector_view_array(weights, n);
  gsl_rng * r;
  double chisq, chisq0;
  int status, info;
  size_t i;

  const double xtol = 1e-8;
  const double gtol = 1e-8;
  const double ftol = 0.0;

  gsl_rng_env_setup();
  r = gsl_rng_alloc(gsl_rng_default);

  /* define the function to be minimized */
  fdf.f = expb_f;
  fdf.df = expb_df;   /* set to NULL for finite-difference Jacobian */
  fdf.fvv = NULL;     /* not using geodesic acceleration */
  fdf.n = n;
  fdf.p = p;
  fdf.params = &d;

  /* this is the data to be fitted */
  for (i = 0; i < n; i++)
    {
      double ti = i * TMAX / (n - 1.0);
      double yi = 1.0 + 5 * exp (-1.5 * ti);
      double si = 0.1 * yi;
      double dy = gsl_ran_gaussian(r, si);

      t[i] = ti;
      y[i] = yi + dy;
      weights[i] = 1.0 / (si * si);
      printf ("data: %g %g %g\n", ti, y[i], si);
    };

  /* allocate workspace with default parameters */
  w = gsl_multifit_nlinear_alloc (T, &fdf_params, n, p);

  /* initialize solver with starting point and weights */
  gsl_multifit_nlinear_winit (&x.vector, &wts.vector, &fdf, w);

  /* compute initial cost function */
  f = gsl_multifit_nlinear_residual(w);
```

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```
  gsl_blas_ddot(f, f, &chisq0);

  /* solve the system with a maximum of 100 iterations */
  status = gsl_multifit_nlinear_driver(100, xtol, gtol, ftol,
                                       callback, NULL, &info, w);

  /* compute covariance of best fit parameters */
  J = gsl_multifit_nlinear_jac(w);
  gsl_multifit_nlinear_covar (J, 0.0, covar);

  /* compute final cost */
  gsl_blas_ddot(f, f, &chisq);

#define FIT(i) gsl_vector_get(w->x, i)
#define ERR(i) sqrt(gsl_matrix_get(covar,i,i))

  fprintf(stderr, "summary from method '%s/%s'\n",
          gsl_multifit_nlinear_name(w),
          gsl_multifit_nlinear_trs_name(w));
  fprintf(stderr, "number of iterations: %zu\n",
          gsl_multifit_nlinear_niter(w));
  fprintf(stderr, "function evaluations: %zu\n", fdf.nevalf);
  fprintf(stderr, "Jacobian evaluations: %zu\n", fdf.nevaldf);
  fprintf(stderr, "reason for stopping: %s\n",
          (info == 1) ? "small step size" : "small gradient");
  fprintf(stderr, "initial |f(x)| = %f\n", sqrt(chisq0));
  fprintf(stderr, "final   |f(x)| = %f\n", sqrt(chisq));

  {
    double dof = n - p;
    double c = GSL_MAX_DBL(1, sqrt(chisq / dof));

    fprintf(stderr, "chisq/dof = %g\n", chisq / dof);

    fprintf (stderr, "A      = %.5f +/- %.5f\n", FIT(0), c*ERR(0));
    fprintf (stderr, "lambda = %.5f +/- %.5f\n", FIT(1), c*ERR(1));
    fprintf (stderr, "b      = %.5f +/- %.5f\n", FIT(2), c*ERR(2));
  }

  fprintf (stderr, "status = %s\n", gsl_strerror (status));

  gsl_multifit_nlinear_free (w);
  gsl_matrix_free (covar);
  gsl_rng_free (r);

  return 0;
}
```

41.12.2 Geodesic Acceleration Example 1

The following example program minimizes a modified Rosenbrock function, which is characterized by a narrow canyon with steep walls. The starting point is selected high on the canyon wall, so the solver must first find the canyon bottom and then navigate to the minimum. The problem is solved both with and without using geodesic acceleration for comparison. The cost function is given by

$$\begin{aligned}\Phi(x) &= \frac{1}{2}(f_1^2 + f_2^2) \\ f_1 &= 100\left(x_2 - x_1^2\right) \\ f_2 &= 1 - x_1\end{aligned}$$

The Jacobian matrix is

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{pmatrix} = \begin{pmatrix} -200x_1 & 100 \\ -1 & 0 \end{pmatrix}$$

In order to use geodesic acceleration, the user must provide the second directional derivative of each residual in the velocity direction, $D_v^2 f_i = \sum_{\alpha\beta} v_\alpha v_\beta \partial_\alpha \partial_\beta f_i$. The velocity vector v is provided by the solver. For this example, these derivatives are

$$f_{vv} = D_v^2 \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} -200v_1^2 \\ 0 \end{pmatrix}$$

The solution of this minimization problem is

$$\begin{aligned} x^* &= \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ \Phi(x^*) &= 0 \end{aligned}$$

The program output is shown below:

```
=== Solving system without acceleration ===
NITER         = 53
NFEV          = 56
NJEV          = 54
NAEV          = 0
initial cost  = 2.250225000000e+04
final cost    = 6.674986031430e-18
final x       = (9.999999974165e-01, 9.999999948328e-01)
final cond(J) = 6.000096055094e+02
=== Solving system with acceleration ===
NITER         = 15
NFEV          = 17
NJEV          = 16
NAEV          = 16
initial cost  = 2.250225000000e+04
final cost    = 7.518932873279e-19
final x       = (9.999999991329e-01, 9.999999982657e-01)
final cond(J) = 6.000097233278e+02
```

We can see that enabling geodesic acceleration requires less than a third of the number of Jacobian evaluations in order to locate the minimum. The path taken by both methods is shown in Fig. 41.2. The contours show the cost function $\Phi(x_1, x_2)$. We see that both methods quickly find the canyon bottom, but the geodesic acceleration method navigates along the bottom to the solution with significantly fewer iterations.

The program is given below.

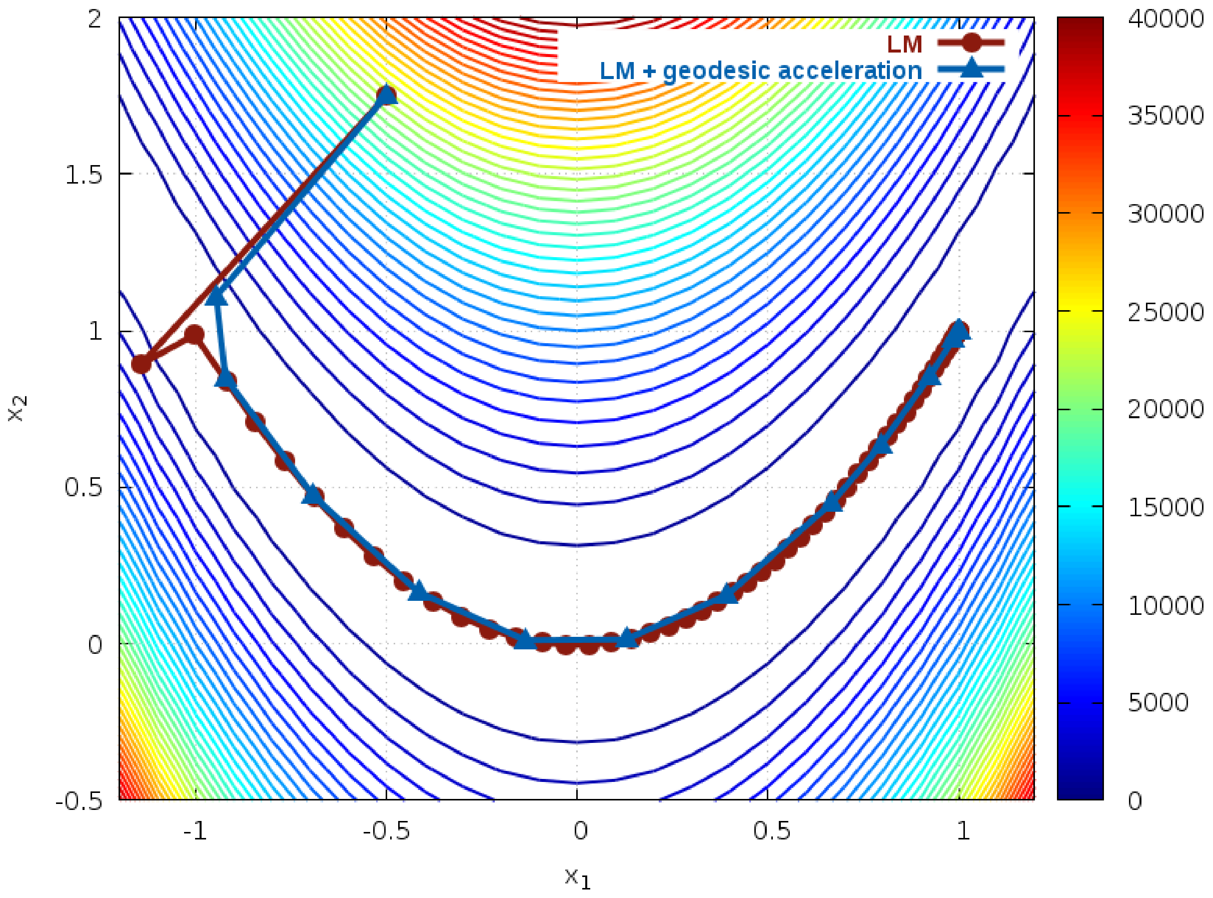

Fig. 41.2: Paths taken by solver for Rosenbrock function

```
#include <stdlib.h>
#include <stdio.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_multifit_nlinear.h>

int
func_f (const gsl_vector * x, void *params, gsl_vector * f)
{
  double x1 = gsl_vector_get(x, 0);
  double x2 = gsl_vector_get(x, 1);

  gsl_vector_set(f, 0, 100.0 * (x2 - x1*x1));
  gsl_vector_set(f, 1, 1.0 - x1);

  return GSL_SUCCESS;
}

int
func_df (const gsl_vector * x, void *params, gsl_matrix * J)
{
  double x1 = gsl_vector_get(x, 0);

  gsl_matrix_set(J, 0, 0, -200.0*x1);
  gsl_matrix_set(J, 0, 1, 100.0);
  gsl_matrix_set(J, 1, 0, -1.0);
  gsl_matrix_set(J, 1, 1, 0.0);

  return GSL_SUCCESS;
}

int
func_fvv (const gsl_vector * x, const gsl_vector * v,
          void *params, gsl_vector * fvv)
{
  double v1 = gsl_vector_get(v, 0);

  gsl_vector_set(fvv, 0, -200.0 * v1 * v1);
  gsl_vector_set(fvv, 1, 0.0);

  return GSL_SUCCESS;
}

void
callback(const size_t iter, void *params,
         const gsl_multifit_nlinear_workspace *w)
{
  gsl_vector * x = gsl_multifit_nlinear_position(w);

  /* print out current location */
  printf("%f %f\n",
         gsl_vector_get(x, 0),
```

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```
         gsl_vector_get(x, 1));
}

void
solve_system(gsl_vector *x0, gsl_multifit_nlinear_fdf *fdf,
             gsl_multifit_nlinear_parameters *params)
{
  const gsl_multifit_nlinear_type *T = gsl_multifit_nlinear_trust;
  const size_t max_iter = 200;
  const double xtol = 1.0e-8;
  const double gtol = 1.0e-8;
  const double ftol = 1.0e-8;
  const size_t n = fdf->n;
  const size_t p = fdf->p;
  gsl_multifit_nlinear_workspace *work =
    gsl_multifit_nlinear_alloc(T, params, n, p);
  gsl_vector * f = gsl_multifit_nlinear_residual(work);
  gsl_vector * x = gsl_multifit_nlinear_position(work);
  int info;
  double chisq0, chisq, rcond;

  /* initialize solver */
  gsl_multifit_nlinear_init(x0, fdf, work);

  /* store initial cost */
  gsl_blas_ddot(f, f, &chisq0);

  /* iterate until convergence */
  gsl_multifit_nlinear_driver(max_iter, xtol, gtol, ftol,
                              callback, NULL, &info, work);

  /* store final cost */
  gsl_blas_ddot(f, f, &chisq);

  /* store cond(J(x)) */
  gsl_multifit_nlinear_rcond(&rcond, work);

  /* print summary */

  fprintf(stderr, "NITER         = %zu\n", gsl_multifit_nlinear_niter(work));
  fprintf(stderr, "NFEV          = %zu\n", fdf->nevalf);
  fprintf(stderr, "NJEV          = %zu\n", fdf->nevaldf);
  fprintf(stderr, "NAEV          = %zu\n", fdf->nevalfvv);
  fprintf(stderr, "initial cost  = %.12e\n", chisq0);
  fprintf(stderr, "final cost    = %.12e\n", chisq);
  fprintf(stderr, "final x       = (%.12e, %.12e)\n",
          gsl_vector_get(x, 0), gsl_vector_get(x, 1));
  fprintf(stderr, "final cond(J) = %.12e\n", 1.0 / rcond);

  printf("\n\n");

  gsl_multifit_nlinear_free(work);
```

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```
}

int
main (void)
{
  const size_t n = 2;
  const size_t p = 2;
  gsl_vector *f = gsl_vector_alloc(n);
  gsl_vector *x = gsl_vector_alloc(p);
  gsl_multifit_nlinear_fdf fdf;
  gsl_multifit_nlinear_parameters fdf_params =
    gsl_multifit_nlinear_default_parameters();

  /* print map of Phi(x1, x2) */
  {
    double x1, x2, chisq;
    double *f1 = gsl_vector_ptr(f, 0);
    double *f2 = gsl_vector_ptr(f, 1);

    for (x1 = -1.2; x1 < 1.3; x1 += 0.1)
      {
        for (x2 = -0.5; x2 < 2.1; x2 += 0.1)
          {
            gsl_vector_set(x, 0, x1);
            gsl_vector_set(x, 1, x2);
            func_f(x, NULL, f);

            chisq = (*f1) * (*f1) + (*f2) * (*f2);
            printf("%f %f %f\n", x1, x2, chisq);
          }
        printf("\n");
      }
    printf("\n\n");
  }

  /* define function to be minimized */
  fdf.f = func_f;
  fdf.df = func_df;
  fdf.fvv = func_fvv;
  fdf.n = n;
  fdf.p = p;
  fdf.params = NULL;

  /* starting point */
  gsl_vector_set(x, 0, -0.5);
  gsl_vector_set(x, 1, 1.75);

  fprintf(stderr, "=== Solving system without acceleration ===\n");
  fdf_params.trs = gsl_multifit_nlinear_trs_lm;
  solve_system(x, &fdf, &fdf_params);

  fprintf(stderr, "=== Solving system with acceleration ===\n");
```

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```
  fdf_params.trs = gsl_multifit_nlinear_trs_lmaccel;
  solve_system(x, &fdf, &fdf_params);

  gsl_vector_free(f);
  gsl_vector_free(x);

  return 0;
}
```

41.12.3 Geodesic Acceleration Example 2

The following example fits a set of data to a Gaussian model using the Levenberg-Marquardt method with geodesic acceleration. The cost function is

$$\Phi(x) = \frac{1}{2}\sum_i f_i^2$$
$$f_i = y_i - Y(a, b, c; t_i)$$

where y_i is the measured data point at time t_i, and the model is specified by

$$Y(a, b, c; t) = a \exp\left[-\frac{1}{2}\left(\frac{t-b}{c}\right)^2\right]$$

The parameters a, b, c represent the amplitude, mean, and width of the Gaussian respectively. The program below generates the y_i data on $[0, 1]$ using the values $a = 5$, $b = 0.4$, $c = 0.15$ and adding random noise. The i-th row of the Jacobian is

$$J_{i,:} = \left(\begin{array}{ccc} \frac{\partial f_i}{\partial a} & \frac{\partial f_i}{\partial b} & \frac{\partial f_i}{\partial c} \end{array} \right) = \left(\begin{array}{ccc} -e_i & -\frac{a}{c} z_i e_i & -\frac{a}{c} z_i^2 e_i \end{array} \right)$$

where

$$z_i = \frac{t_i - b}{c}$$
$$e_i = \exp\left(-\frac{1}{2} z_i^2\right)$$

In order to use geodesic acceleration, we need the second directional derivative of the residuals in the velocity direction, $D_v^2 f_i = \sum_{\alpha\beta} v_\alpha v_\beta \partial_\alpha \partial_\beta f_i$, where v is provided by the solver. To compute this, it is helpful to make a table of all second derivatives of the residuals f_i with respect to each combination of model parameters. This table is

$$\begin{array}{cccc} & \frac{\partial}{\partial a} & \frac{\partial}{\partial b} & \frac{\partial}{\partial c} \\ \frac{\partial}{\partial a} & 0 & -\frac{z_i}{c} e_i & -\frac{z_i^2}{c} e_i \\ \frac{\partial}{\partial b} & & \frac{a}{c^2}\left(1 - z_i^2\right) e_i & \frac{a}{c^2} z_i \left(2 - z_i^2\right) e_i \\ \frac{\partial}{\partial c} & & & \frac{a}{c^2} z_i^2 \left(3 - z_i^2\right) e_i \end{array}$$

The lower half of the table is omitted since it is symmetric. Then, the second directional derivative of f_i is

$$D_v^2 f_i = v_a^2 \partial_a^2 f_i + 2 v_a v_b \partial_a \partial_b f_i + 2 v_a v_c \partial_a \partial_c f_i + v_b^2 \partial_b^2 f_i + 2 v_b v_c \partial_b \partial_c f_i + v_c^2 \partial_c^2 f_i$$

The factors of 2 come from the symmetry of the mixed second partial derivatives. The iteration is started using the initial guess $a = 1, b = 0, c = 1$. The program output is shown below:

```
iter  0: a = 1.0000, b = 0.0000, c = 1.0000, |a|/|v| = 0.0000 cond(J) =      inf, |f(x)|␣
↪= 35.4785
iter  1: a = 1.5708, b = 0.5321, c = 0.5219, |a|/|v| = 0.3093 cond(J) =  29.0443, |f(x)|␣
↪= 31.1042
iter  2: a = 1.7387, b = 0.4040, c = 0.4568, |a|/|v| = 0.1199 cond(J) =   3.5256, |f(x)|␣
↪= 28.7217
iter  3: a = 2.2340, b = 0.3829, c = 0.3053, |a|/|v| = 0.3308 cond(J) =   4.5121, |f(x)|␣
↪= 23.8074
iter  4: a = 3.2275, b = 0.3952, c = 0.2243, |a|/|v| = 0.2784 cond(J) =   8.6499, |f(x)|␣
↪= 15.6003
iter  5: a = 4.3347, b = 0.3974, c = 0.1752, |a|/|v| = 0.2029 cond(J) =  15.1732, |f(x)|␣
↪= 7.5908
iter  6: a = 4.9352, b = 0.3992, c = 0.1536, |a|/|v| = 0.1001 cond(J) =  26.6621, |f(x)|␣
↪= 4.8402
iter  7: a = 5.0716, b = 0.3994, c = 0.1498, |a|/|v| = 0.0166 cond(J) =  34.6922, |f(x)|␣
↪= 4.7103
iter  8: a = 5.0828, b = 0.3994, c = 0.1495, |a|/|v| = 0.0012 cond(J) =  36.5422, |f(x)|␣
↪= 4.7095
iter  9: a = 5.0831, b = 0.3994, c = 0.1495, |a|/|v| = 0.0000 cond(J) =  36.6929, |f(x)|␣
↪= 4.7095
iter 10: a = 5.0831, b = 0.3994, c = 0.1495, |a|/|v| = 0.0000 cond(J) =  36.6975, |f(x)|␣
↪= 4.7095
iter 11: a = 5.0831, b = 0.3994, c = 0.1495, |a|/|v| = 0.0000 cond(J) =  36.6976, |f(x)|␣
↪= 4.7095
NITER         = 11
NFEV          = 18
NJEV          = 12
NAEV          = 17
initial cost  = 1.258724737288e+03
final cost    = 2.217977560180e+01
final x       = (5.083101559156e+00, 3.994484109594e-01, 1.494898e-01)
final cond(J) = 3.669757713403e+01
```

We see the method converges after 11 iterations. For comparison the standard Levenberg-Marquardt method requires 26 iterations and so the Gaussian fitting problem benefits substantially from the geodesic acceleration correction. The column marked `|a|/|v|` above shows the ratio of the acceleration term to the velocity term as the iteration progresses. Larger values of this ratio indicate that the geodesic acceleration correction term is contributing substantial information to the solver relative to the standard LM velocity step.

The data and fitted model are shown in Fig. 41.3.

The program is given below.

```
#include <stdlib.h>
#include <stdio.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_multifit_nlinear.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>

struct data
{
```

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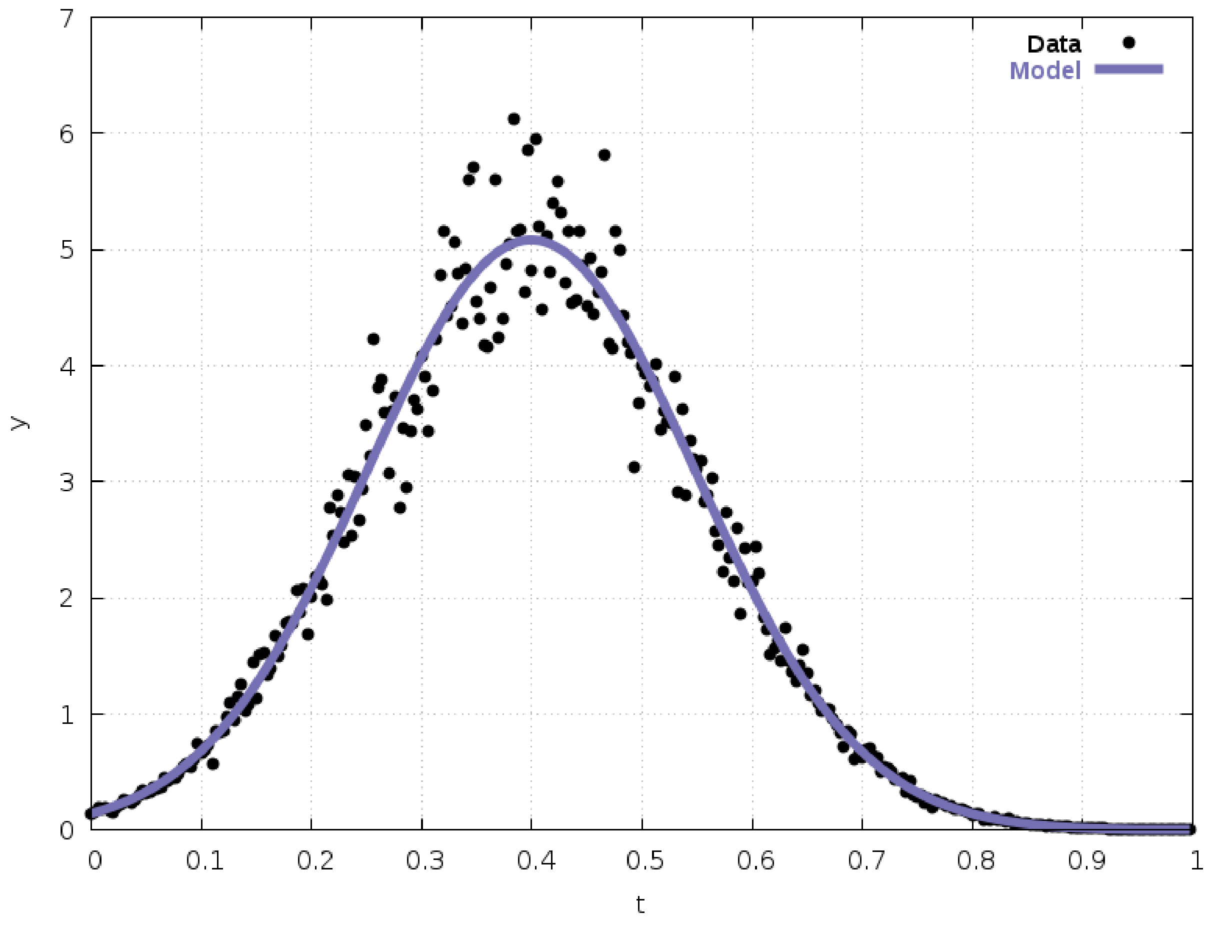

Fig. 41.3: Gaussian model fitted to data

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```
  double *t;
  double *y;
  size_t n;
};

/* model function: a * exp( -1/2 * [ (t - b) / c ]^2 ) */
double
gaussian(const double a, const double b, const double c, const double t)
{
  const double z = (t - b) / c;
  return (a * exp(-0.5 * z * z));
}

int
func_f (const gsl_vector * x, void *params, gsl_vector * f)
{
  struct data *d = (struct data *) params;
  double a = gsl_vector_get(x, 0);
  double b = gsl_vector_get(x, 1);
  double c = gsl_vector_get(x, 2);
  size_t i;

  for (i = 0; i < d->n; ++i)
    {
      double ti = d->t[i];
      double yi = d->y[i];
      double y = gaussian(a, b, c, ti);

      gsl_vector_set(f, i, yi - y);
    }

  return GSL_SUCCESS;
}

int
func_df (const gsl_vector * x, void *params, gsl_matrix * J)
{
  struct data *d = (struct data *) params;
  double a = gsl_vector_get(x, 0);
  double b = gsl_vector_get(x, 1);
  double c = gsl_vector_get(x, 2);
  size_t i;

  for (i = 0; i < d->n; ++i)
    {
      double ti = d->t[i];
      double zi = (ti - b) / c;
      double ei = exp(-0.5 * zi * zi);

      gsl_matrix_set(J, i, 0, -ei);
      gsl_matrix_set(J, i, 1, -(a / c) * ei * zi);
      gsl_matrix_set(J, i, 2, -(a / c) * ei * zi * zi);
```

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```
    }

  return GSL_SUCCESS;
}

int
func_fvv (const gsl_vector * x, const gsl_vector * v,
          void *params, gsl_vector * fvv)
{
  struct data *d = (struct data *) params;
  double a = gsl_vector_get(x, 0);
  double b = gsl_vector_get(x, 1);
  double c = gsl_vector_get(x, 2);
  double va = gsl_vector_get(v, 0);
  double vb = gsl_vector_get(v, 1);
  double vc = gsl_vector_get(v, 2);
  size_t i;

  for (i = 0; i < d->n; ++i)
    {
      double ti = d->t[i];
      double zi = (ti - b) / c;
      double ei = exp(-0.5 * zi * zi);
      double Dab = -zi * ei / c;
      double Dac = -zi * zi * ei / c;
      double Dbb = a * ei / (c * c) * (1.0 - zi*zi);
      double Dbc = a * zi * ei / (c * c) * (2.0 - zi*zi);
      double Dcc = a * zi * zi * ei / (c * c) * (3.0 - zi*zi);
      double sum;

      sum = 2.0 * va * vb * Dab +
            2.0 * va * vc * Dac +
                  vb * vb * Dbb +
            2.0 * vb * vc * Dbc +
                  vc * vc * Dcc;

      gsl_vector_set(fvv, i, sum);
    }

  return GSL_SUCCESS;
}

void
callback(const size_t iter, void *params,
         const gsl_multifit_nlinear_workspace *w)
{
  gsl_vector *f = gsl_multifit_nlinear_residual(w);
  gsl_vector *x = gsl_multifit_nlinear_position(w);
  double avratio = gsl_multifit_nlinear_avratio(w);
  double rcond;

  (void) params; /* not used */
```

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```
  /* compute reciprocal condition number of J(x) */
  gsl_multifit_nlinear_rcond(&rcond, w);

  fprintf(stderr, "iter %2zu: a = %.4f, b = %.4f, c = %.4f, |a|/|v| = %.4f cond(J) = %8.
↪4f, |f(x)| = %.4f\n",
          iter,
          gsl_vector_get(x, 0),
          gsl_vector_get(x, 1),
          gsl_vector_get(x, 2),
          avratio,
          1.0 / rcond,
          gsl_blas_dnrm2(f));
}

void
solve_system(gsl_vector *x, gsl_multifit_nlinear_fdf *fdf,
             gsl_multifit_nlinear_parameters *params)
{
  const gsl_multifit_nlinear_type *T = gsl_multifit_nlinear_trust;
  const size_t max_iter = 200;
  const double xtol = 1.0e-8;
  const double gtol = 1.0e-8;
  const double ftol = 1.0e-8;
  const size_t n = fdf->n;
  const size_t p = fdf->p;
  gsl_multifit_nlinear_workspace *work =
    gsl_multifit_nlinear_alloc(T, params, n, p);
  gsl_vector * f = gsl_multifit_nlinear_residual(work);
  gsl_vector * y = gsl_multifit_nlinear_position(work);
  int info;
  double chisq0, chisq, rcond;

  /* initialize solver */
  gsl_multifit_nlinear_init(x, fdf, work);

  /* store initial cost */
  gsl_blas_ddot(f, f, &chisq0);

  /* iterate until convergence */
  gsl_multifit_nlinear_driver(max_iter, xtol, gtol, ftol,
                              callback, NULL, &info, work);

  /* store final cost */
  gsl_blas_ddot(f, f, &chisq);

  /* store cond(J(x)) */
  gsl_multifit_nlinear_rcond(&rcond, work);

  gsl_vector_memcpy(x, y);

  /* print summary */
```

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```
  fprintf(stderr, "NITER         = %zu\n", gsl_multifit_nlinear_niter(work));
  fprintf(stderr, "NFEV          = %zu\n", fdf->nevalf);
  fprintf(stderr, "NJEV          = %zu\n", fdf->nevaldf);
  fprintf(stderr, "NAEV          = %zu\n", fdf->nevalfvv);
  fprintf(stderr, "initial cost  = %.12e\n", chisq0);
  fprintf(stderr, "final cost    = %.12e\n", chisq);
  fprintf(stderr, "final x       = (%.12e, %.12e, %12e)\n",
          gsl_vector_get(x, 0), gsl_vector_get(x, 1), gsl_vector_get(x, 2));
  fprintf(stderr, "final cond(J) = %.12e\n", 1.0 / rcond);

  gsl_multifit_nlinear_free(work);
}

int
main (void)
{
  const size_t n = 300;  /* number of data points to fit */
  const size_t p = 3;    /* number of model parameters */
  const double a = 5.0;  /* amplitude */
  const double b = 0.4;  /* center */
  const double c = 0.15; /* width */
  const gsl_rng_type * T = gsl_rng_default;
  gsl_vector *f = gsl_vector_alloc(n);
  gsl_vector *x = gsl_vector_alloc(p);
  gsl_multifit_nlinear_fdf fdf;
  gsl_multifit_nlinear_parameters fdf_params =
    gsl_multifit_nlinear_default_parameters();
  struct data fit_data;
  gsl_rng * r;
  size_t i;

  gsl_rng_env_setup ();
  r = gsl_rng_alloc (T);

  fit_data.t = malloc(n * sizeof(double));
  fit_data.y = malloc(n * sizeof(double));
  fit_data.n = n;

  /* generate synthetic data with noise */
  for (i = 0; i < n; ++i)
    {
      double t = (double)i / (double) n;
      double y0 = gaussian(a, b, c, t);
      double dy = gsl_ran_gaussian (r, 0.1 * y0);

      fit_data.t[i] = t;
      fit_data.y[i] = y0 + dy;
    }

  /* define function to be minimized */
  fdf.f = func_f;
```

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```
  fdf.df = func_df;
  fdf.fvv = func_fvv;
  fdf.n = n;
  fdf.p = p;
  fdf.params = &fit_data;

  /* starting point */
  gsl_vector_set(x, 0, 1.0);
  gsl_vector_set(x, 1, 0.0);
  gsl_vector_set(x, 2, 1.0);

  fdf_params.trs = gsl_multifit_nlinear_trs_lmaccel;
  solve_system(x, &fdf, &fdf_params);

  /* print data and model */
  {
    double A = gsl_vector_get(x, 0);
    double B = gsl_vector_get(x, 1);
    double C = gsl_vector_get(x, 2);

    for (i = 0; i < n; ++i)
      {
        double ti = fit_data.t[i];
        double yi = fit_data.y[i];
        double fi = gaussian(A, B, C, ti);

        printf("%f %f %f\n", ti, yi, fi);
      }
  }

  gsl_vector_free(f);
  gsl_vector_free(x);
  gsl_rng_free(r);

  return 0;
}
```

41.12.4 Comparing TRS Methods Example

The following program compares all available nonlinear least squares trust-region subproblem (TRS) methods on the Branin function, a common optimization test problem. The cost function is

$$\Phi(x) = \frac{1}{2}(f_1^2 + f_2^2)$$
$$f_1 = x_2 + a_1 x_1^2 + a_2 x_1 + a_3$$
$$f_2 = \sqrt{a_4}\sqrt{1 + (1 - a_5)\cos x_1}$$

with $a_1 = -\frac{5.1}{4\pi^2}, a_2 = \frac{5}{\pi}, a_3 = -6, a_4 = 10, a_5 = \frac{1}{8\pi}$. There are three minima of this function in the range $(x_1, x_2) \in [-5, 15] \times [-5, 15]$. The program below uses the starting point $(x_1, x_2) = (6, 14.5)$ and calculates the solution with all available nonlinear least squares TRS methods. The program output is shown below:

```
Method                      NITER  NFEV  NJEV  Initial Cost  Final cost   Final cond(J)␣
↪Final x
levenberg-marquardt         20     27    21    1.9874e+02    3.9789e-01   6.1399e+07    (-
↪3.14e+00, 1.23e+01)
levenberg-marquardt+accel   27     36    28    1.9874e+02    3.9789e-01   1.4465e+07    (3.
↪14e+00, 2.27e+00)
dogleg                      23     64    23    1.9874e+02    3.9789e-01   5.0692e+08    (3.
↪14e+00, 2.28e+00)
double-dogleg               24     69    24    1.9874e+02    3.9789e-01   3.4879e+07    (3.
↪14e+00, 2.27e+00)
2D-subspace                 23     54    24    1.9874e+02    3.9789e-01   2.5142e+07    (3.
↪14e+00, 2.27e+00)
```

The first row of output above corresponds to standard Levenberg-Marquardt, while the second row includes geodesic acceleration. We see that the standard LM method converges to the minimum at $(-\pi, 12.275)$ and also uses the least number of iterations and Jacobian evaluations. All other methods converge to the minimum $(\pi, 2.275)$ and perform similarly in terms of number of Jacobian evaluations. We see that J is fairly ill-conditioned at both minima, indicating that the QR (or SVD) solver is the best choice for this problem. Since there are only two parameters in this optimization problem, we can easily visualize the paths taken by each method, which are shown in Fig. 41.4. The figure shows contours of the cost function $\Phi(x_1, x_2)$ which exhibits three global minima in the range $[-5, 15] \times [-5, 15]$. The paths taken by each solver are shown as colored lines.

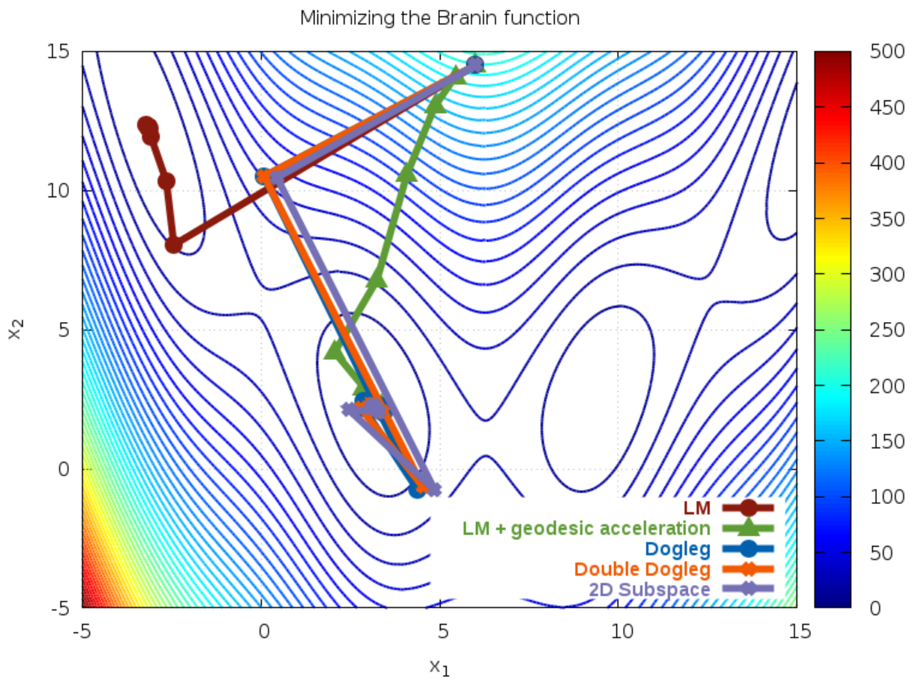

Fig. 41.4: Paths taken for different TRS methods for the Branin function

The program is given below.

```
#include <stdlib.h>
#include <stdio.h>
#include <gsl/gsl_vector.h>
```

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```
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_multifit_nlinear.h>

/* parameters to model */
struct model_params
{
  double a1;
  double a2;
  double a3;
  double a4;
  double a5;
};

/* Branin function */
int
func_f (const gsl_vector * x, void *params, gsl_vector * f)
{
  struct model_params *par = (struct model_params *) params;
  double x1 = gsl_vector_get(x, 0);
  double x2 = gsl_vector_get(x, 1);
  double f1 = x2 + par->a1 * x1 * x1 + par->a2 * x1 + par->a3;
  double f2 = sqrt(par->a4) * sqrt(1.0 + (1.0 - par->a5) * cos(x1));

  gsl_vector_set(f, 0, f1);
  gsl_vector_set(f, 1, f2);

  return GSL_SUCCESS;
}

int
func_df (const gsl_vector * x, void *params, gsl_matrix * J)
{
  struct model_params *par = (struct model_params *) params;
  double x1 = gsl_vector_get(x, 0);
  double f2 = sqrt(par->a4) * sqrt(1.0 + (1.0 - par->a5) * cos(x1));

  gsl_matrix_set(J, 0, 0, 2.0 * par->a1 * x1 + par->a2);
  gsl_matrix_set(J, 0, 1, 1.0);

  gsl_matrix_set(J, 1, 0, -0.5 * par->a4 / f2 * (1.0 - par->a5) * sin(x1));
  gsl_matrix_set(J, 1, 1, 0.0);

  return GSL_SUCCESS;
}

int
func_fvv (const gsl_vector * x, const gsl_vector * v,
          void *params, gsl_vector * fvv)
{
  struct model_params *par = (struct model_params *) params;
  double x1 = gsl_vector_get(x, 0);
```

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```
  double v1 = gsl_vector_get(v, 0);
  double c = cos(x1);
  double s = sin(x1);
  double f2 = sqrt(par->a4) * sqrt(1.0 + (1.0 - par->a5) * c);
  double t = 0.5 * par->a4 * (1.0 - par->a5) / f2;

  gsl_vector_set(fvv, 0, 2.0 * par->a1 * v1 * v1);
  gsl_vector_set(fvv, 1, -t * (c + s*s/f2) * v1 * v1);

  return GSL_SUCCESS;
}

void
callback(const size_t iter, void *params,
         const gsl_multifit_nlinear_workspace *w)
{
  gsl_vector * x = gsl_multifit_nlinear_position(w);
  double x1 = gsl_vector_get(x, 0);
  double x2 = gsl_vector_get(x, 1);

  /* print out current location */
  printf("%f %f\n", x1, x2);
}

void
solve_system(gsl_vector *x0, gsl_multifit_nlinear_fdf *fdf,
             gsl_multifit_nlinear_parameters *params)
{
  const gsl_multifit_nlinear_type *T = gsl_multifit_nlinear_trust;
  const size_t max_iter = 200;
  const double xtol = 1.0e-8;
  const double gtol = 1.0e-8;
  const double ftol = 1.0e-8;
  const size_t n = fdf->n;
  const size_t p = fdf->p;
  gsl_multifit_nlinear_workspace *work =
    gsl_multifit_nlinear_alloc(T, params, n, p);
  gsl_vector * f = gsl_multifit_nlinear_residual(work);
  gsl_vector * x = gsl_multifit_nlinear_position(work);
  int info;
  double chisq0, chisq, rcond;

  printf("# %s/%s\n",
         gsl_multifit_nlinear_name(work),
         gsl_multifit_nlinear_trs_name(work));

  /* initialize solver */
  gsl_multifit_nlinear_init(x0, fdf, work);

  /* store initial cost */
  gsl_blas_ddot(f, f, &chisq0);
```

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```
  /* iterate until convergence */
  gsl_multifit_nlinear_driver(max_iter, xtol, gtol, ftol,
                              callback, NULL, &info, work);

  /* store final cost */
  gsl_blas_ddot(f, f, &chisq);

  /* store cond(J(x)) */
  gsl_multifit_nlinear_rcond(&rcond, work);

  /* print summary */
  fprintf(stderr, "%-25s %-6zu %-5zu %-5zu %-13.4e %-12.4e %-13.4e (%.2e, %.2e)\n",
          gsl_multifit_nlinear_trs_name(work),
          gsl_multifit_nlinear_niter(work),
          fdf->nevalf,
          fdf->nevaldf,
          chisq0,
          chisq,
          1.0 / rcond,
          gsl_vector_get(x, 0),
          gsl_vector_get(x, 1));

  printf("\n\n");

  gsl_multifit_nlinear_free(work);
}

int
main (void)
{
  const size_t n = 2;
  const size_t p = 2;
  gsl_vector *f = gsl_vector_alloc(n);
  gsl_vector *x = gsl_vector_alloc(p);
  gsl_multifit_nlinear_fdf fdf;
  gsl_multifit_nlinear_parameters fdf_params =
    gsl_multifit_nlinear_default_parameters();
  struct model_params params;

  params.a1 = -5.1 / (4.0 * M_PI * M_PI);
  params.a2 = 5.0 / M_PI;
  params.a3 = -6.0;
  params.a4 = 10.0;
  params.a5 = 1.0 / (8.0 * M_PI);

  /* print map of Phi(x1, x2) */
  {
    double x1, x2, chisq;

    for (x1 = -5.0; x1 < 15.0; x1 += 0.1)
      {
        for (x2 = -5.0; x2 < 15.0; x2 += 0.1)
```

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```
          {
            gsl_vector_set(x, 0, x1);
            gsl_vector_set(x, 1, x2);
            func_f(x, &params, f);

            gsl_blas_ddot(f, f, &chisq);

            printf("%f %f %f\n", x1, x2, chisq);
          }
        printf("\n");
      }
    printf("\n\n");
  }

  /* define function to be minimized */
  fdf.f = func_f;
  fdf.df = func_df;
  fdf.fvv = func_fvv;
  fdf.n = n;
  fdf.p = p;
  fdf.params = &params;

  /* starting point */
  gsl_vector_set(x, 0, 6.0);
  gsl_vector_set(x, 1, 14.5);

  fprintf(stderr, "%-25s %-6s %-5s %-5s %-13s %-12s %-13s %-15s\n",
          "Method", "NITER", "NFEV", "NJEV", "Initial Cost",
          "Final cost", "Final cond(J)", "Final x");

  fdf_params.trs = gsl_multifit_nlinear_trs_lm;
  solve_system(x, &fdf, &fdf_params);

  fdf_params.trs = gsl_multifit_nlinear_trs_lmaccel;
  solve_system(x, &fdf, &fdf_params);

  fdf_params.trs = gsl_multifit_nlinear_trs_dogleg;
  solve_system(x, &fdf, &fdf_params);

  fdf_params.trs = gsl_multifit_nlinear_trs_ddogleg;
  solve_system(x, &fdf, &fdf_params);

  fdf_params.trs = gsl_multifit_nlinear_trs_subspace2D;
  solve_system(x, &fdf, &fdf_params);

  gsl_vector_free(f);
  gsl_vector_free(x);

  return 0;
}
```

41.12.5 Large Nonlinear Least Squares Example

The following program illustrates the large nonlinear least squares solvers on a system with significant sparse structure in the Jacobian. The cost function is

$$\begin{aligned}\Phi(x) &= \frac{1}{2}\sum_{i=1}^{p+1} f_i^2 \\ f_i &= \sqrt{\alpha}(x_i - 1), \quad 1 \le i \le p \\ f_{p+1} &= ||x||^2 - \frac{1}{4}\end{aligned}$$

with $\alpha = 10^{-5}$. The residual f_{p+1} imposes a constraint on the p parameters x, to ensure that $||x||^2 \approx \frac{1}{4}$. The $(p+1)$-by-p Jacobian for this system is

$$J(x) = \begin{pmatrix} \sqrt{\alpha} I_p \\ 2x^T \end{pmatrix}$$

and the normal equations matrix is

$$J^T J = \alpha I_p + 4xx^T$$

Finally, the second directional derivative of f for the geodesic acceleration method is

$$f_{vv} = D_v^2 f = \begin{pmatrix} 0 \\ 2||v||^2 \end{pmatrix}$$

Since the upper p-by-p block of J is diagonal, this sparse structure should be exploited in the nonlinear solver. For comparison, the following program solves the system for $p = 2000$ using the dense direct Cholesky solver based on the normal equations matrix $J^T J$, as well as the iterative Steihaug-Toint solver, based on sparse matrix-vector products Ju and $J^T u$. The program output is shown below:

```
Method                     NITER NFEV NJUEV NJTJEV NAEV Init Cost  Final cost cond(J)␣
↪Final |x|^2 Time (s)
levenberg-marquardt        25    31   26    26     0    7.1218e+18 1.9555e-02 447.50  2.
↪5044e-01  46.28
levenberg-marquardt+accel  22    23   45    23     22   7.1218e+18 1.9555e-02 447.64  2.
↪5044e-01  33.92
dogleg                     37    87   36    36     0    7.1218e+18 1.9555e-02 447.59  2.
↪5044e-01  56.05
double-dogleg              35    88   34    34     0    7.1218e+18 1.9555e-02 447.62  2.
↪5044e-01  52.65
2D-subspace                37    88   36    36     0    7.1218e+18 1.9555e-02 447.71  2.
↪5044e-01  59.75
steihaug-toint             35    88   345   0      0    7.1218e+18 1.9555e-02 inf     2.
↪5044e-01  0.09
```

The first five rows use methods based on factoring the dense $J^T J$ matrix while the last row uses the iterative Steihaug-Toint method. While the number of Jacobian matrix-vector products (NJUEV) is less for the dense methods, the added time to construct and factor the $J^T J$ matrix (NJTJEV) results in a much larger runtime than the iterative method (see last column).

The program is given below.

```
#include <stdlib.h>
#include <stdio.h>
```

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```
#include <sys/time.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_multilarge_nlinear.h>
#include <gsl/gsl_spblas.h>
#include <gsl/gsl_spmatrix.h>

/* parameters for functions */
struct model_params
{
  double alpha;
  gsl_spmatrix *J;
};

/* penalty function */
int
penalty_f (const gsl_vector * x, void *params, gsl_vector * f)
{
  struct model_params *par = (struct model_params *) params;
  const double sqrt_alpha = sqrt(par->alpha);
  const size_t p = x->size;
  size_t i;
  double sum = 0.0;

  for (i = 0; i < p; ++i)
    {
      double xi = gsl_vector_get(x, i);

      gsl_vector_set(f, i, sqrt_alpha*(xi - 1.0));

      sum += xi * xi;
    }

  gsl_vector_set(f, p, sum - 0.25);

  return GSL_SUCCESS;
}

int
penalty_df (CBLAS_TRANSPOSE_t TransJ, const gsl_vector * x,
            const gsl_vector * u, void * params, gsl_vector * v,
            gsl_matrix * JTJ)
{
  struct model_params *par = (struct model_params *) params;
  const size_t p = x->size;
  size_t j;

  /* store 2*x in last row of J */
  for (j = 0; j < p; ++j)
    {
      double xj = gsl_vector_get(x, j);
```

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```
      gsl_spmatrix_set(par->J, p, j, 2.0 * xj);
    }

  /* compute v = op(J) u */
  if (v)
    gsl_spblas_dgemv(TransJ, 1.0, par->J, u, 0.0, v);

  if (JTJ)
    {
      gsl_vector_view diag = gsl_matrix_diagonal(JTJ);

      /* compute J^T J = [ alpha*I_p + 4 x x^T ] */
      gsl_matrix_set_zero(JTJ);

      /* store 4 x x^T in lower half of JTJ */
      gsl_blas_dsyr(CblasLower, 4.0, x, JTJ);

      /* add alpha to diag(JTJ) */
      gsl_vector_add_constant(&diag.vector, par->alpha);
    }

  return GSL_SUCCESS;
}

int
penalty_fvv (const gsl_vector * x, const gsl_vector * v,
             void *params, gsl_vector * fvv)
{
  const size_t p = x->size;
  double normv = gsl_blas_dnrm2(v);

  gsl_vector_set_zero(fvv);
  gsl_vector_set(fvv, p, 2.0 * normv * normv);

  (void)params; /* avoid unused parameter warning */

  return GSL_SUCCESS;
}

void
solve_system(const gsl_vector *x0, gsl_multilarge_nlinear_fdf *fdf,
             gsl_multilarge_nlinear_parameters *params)
{
  const gsl_multilarge_nlinear_type *T = gsl_multilarge_nlinear_trust;
  const size_t max_iter = 200;
  const double xtol = 1.0e-8;
  const double gtol = 1.0e-8;
  const double ftol = 1.0e-8;
  const size_t n = fdf->n;
  const size_t p = fdf->p;
  gsl_multilarge_nlinear_workspace *work =
    gsl_multilarge_nlinear_alloc(T, params, n, p);
```

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```
  gsl_vector * f = gsl_multilarge_nlinear_residual(work);
  gsl_vector * x = gsl_multilarge_nlinear_position(work);
  int info;
  double chisq0, chisq, rcond, xsq;
  struct timeval tv0, tv1;

  gettimeofday(&tv0, NULL);

  /* initialize solver */
  gsl_multilarge_nlinear_init(x0, fdf, work);

  /* store initial cost */
  gsl_blas_ddot(f, f, &chisq0);

  /* iterate until convergence */
  gsl_multilarge_nlinear_driver(max_iter, xtol, gtol, ftol,
                                NULL, NULL, &info, work);

  gettimeofday(&tv1, NULL);

  /* store final cost */
  gsl_blas_ddot(f, f, &chisq);

  /* compute final ||x||^2 */
  gsl_blas_ddot(x, x, &xsq);

  /* store cond(J(x)) */
  gsl_multilarge_nlinear_rcond(&rcond, work);

  /* print summary */
  fprintf(stderr, "%-25s %-5zu %-4zu %-5zu %-6zu %-4zu %-10.4e %-10.4e %-7.2f %-11.4e %.
↪2f\n",
          gsl_multilarge_nlinear_trs_name(work),
          gsl_multilarge_nlinear_niter(work),
          fdf->nevalf,
          fdf->nevaldfu,
          fdf->nevaldf2,
          fdf->nevalfvv,
          chisq0,
          chisq,
          1.0 / rcond,
          xsq,
          (tv1.tv_sec - tv0.tv_sec) + 1.0e-6 * (tv1.tv_usec - tv0.tv_usec));

  gsl_multilarge_nlinear_free(work);
}

int
main (void)
{
  const size_t p = 2000;
  const size_t n = p + 1;
```

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```
  gsl_vector *f = gsl_vector_alloc(n);
  gsl_vector *x = gsl_vector_alloc(p);

  /* allocate sparse Jacobian matrix with 2*p non-zero elements in triplet format */
  gsl_spmatrix *J = gsl_spmatrix_alloc_nzmax(n, p, 2 * p, GSL_SPMATRIX_TRIPLET);

  gsl_multilarge_nlinear_fdf fdf;
  gsl_multilarge_nlinear_parameters fdf_params =
    gsl_multilarge_nlinear_default_parameters();
  struct model_params params;
  size_t i;

  params.alpha = 1.0e-5;
  params.J = J;

  /* define function to be minimized */
  fdf.f = penalty_f;
  fdf.df = penalty_df;
  fdf.fvv = penalty_fvv;
  fdf.n = n;
  fdf.p = p;
  fdf.params = &params;

  for (i = 0; i < p; ++i)
    {
      /* starting point */
      gsl_vector_set(x, i, i + 1.0);

      /* store sqrt(alpha)*I_p in upper p-by-p block of J */
      gsl_spmatrix_set(J, i, i, sqrt(params.alpha));
    }

  fprintf(stderr, "%-25s %-4s %-4s %-5s %-6s %-4s %-10s %-10s %-7s %-11s %-10s\n",
          "Method", "NITER", "NFEV", "NJUEV", "NJTJEV", "NAEV", "Init Cost",
          "Final cost", "cond(J)", "Final |x|^2", "Time (s)");

  fdf_params.scale = gsl_multilarge_nlinear_scale_levenberg;

  fdf_params.trs = gsl_multilarge_nlinear_trs_lm;
  solve_system(x, &fdf, &fdf_params);

  fdf_params.trs = gsl_multilarge_nlinear_trs_lmaccel;
  solve_system(x, &fdf, &fdf_params);

  fdf_params.trs = gsl_multilarge_nlinear_trs_dogleg;
  solve_system(x, &fdf, &fdf_params);

  fdf_params.trs = gsl_multilarge_nlinear_trs_ddogleg;
  solve_system(x, &fdf, &fdf_params);

  fdf_params.trs = gsl_multilarge_nlinear_trs_subspace2D;
  solve_system(x, &fdf, &fdf_params);
```

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```
  fdf_params.trs = gsl_multilarge_nlinear_trs_cgst;
  solve_system(x, &fdf, &fdf_params);

  gsl_vector_free(f);
  gsl_vector_free(x);
  gsl_spmatrix_free(J);

  return 0;
}
```

41.13 References and Further Reading

The following publications are relevant to the algorithms described in this section,

- J.J. Moré, *The Levenberg-Marquardt Algorithm: Implementation and Theory*, Lecture Notes in Mathematics, v630 (1978), ed G. Watson.
- H. B. Nielsen, "Damping Parameter in Marquardt's Method", IMM Department of Mathematical Modeling, DTU, Tech. Report IMM-REP-1999-05 (1999).
- K. Madsen and H. B. Nielsen, "Introduction to Optimization and Data Fitting", IMM Department of Mathematical Modeling, DTU, 2010.
- J. E. Dennis and R. B. Schnabel, Numerical Methods for Unconstrained Optimization and Nonlinear Equations, SIAM, 1996.
- M. K. Transtrum, B. B. Machta, and J. P. Sethna, Geometry of nonlinear least squares with applications to sloppy models and optimization, Phys. Rev. E 83, 036701, 2011.
- M. K. Transtrum and J. P. Sethna, Improvements to the Levenberg-Marquardt algorithm for nonlinear least-squares minimization, arXiv:1201.5885, 2012.
- J.J. Moré, B.S. Garbow, K.E. Hillstrom, "Testing Unconstrained Optimization Software", ACM Transactions on Mathematical Software, Vol 7, No 1 (1981), p 17–41.
- H. B. Nielsen, "UCTP Test Problems for Unconstrained Optimization", IMM Department of Mathematical Modeling, DTU, Tech. Report IMM-REP-2000-17 (2000).

CHAPTER

FORTYTWO

BASIS SPLINES

This chapter describes functions for the computation of smoothing basis splines (B-splines). A smoothing spline differs from an interpolating spline in that the resulting curve is not required to pass through each datapoint. For information about interpolating splines, see *Interpolation*.

The header file `gsl_bspline.h` contains the prototypes for the bspline functions and related declarations.

42.1 Overview

B-splines are commonly used as basis functions to fit smoothing curves to large data sets. To do this, the abscissa axis is broken up into some number of intervals, where the endpoints of each interval are called *breakpoints*. These breakpoints are then converted to *knots* by imposing various continuity and smoothness conditions at each interface. Given a nondecreasing knot vector

$$t = \{t_0, t_1, \dots, t_{n+k-1}\}$$

the n basis splines of order k are defined by

$$B_{i,1}(x) = \left\{ \begin{array}{ll} 1, & t_i \le x < t_{i+1} \\ 0, & else \end{array} \right.$$

$$B_{i,k}(x) = \frac{(x - t_i)}{(t_{i+k-1} - t_i)} B_{i,k-1}(x) + \frac{(t_{i+k} - x)}{(t_{i+k} - t_{i+1})} B_{i+1,k-1}(x)$$

for $i = 0, \dots, n-1$. The common case of cubic B-splines is given by $k = 4$. The above recurrence relation can be evaluated in a numerically stable way by the de Boor algorithm.

If we define appropriate knots on an interval $[a, b]$ then the B-spline basis functions form a complete set on that interval. Therefore we can expand a smoothing function as

$$f(x) = \sum_{i=0}^{n-1} c_i B_{i,k}(x)$$

given enough $(x_j, f(x_j))$ data pairs. The coefficients c_i can be readily obtained from a least-squares fit.

42.2 Initializing the B-splines solver

type **gsl_bspline_workspace**

The computation of B-spline functions requires a preallocated workspace.

gsl_bspline_workspace ***gsl_bspline_alloc**(const size_t k, const size_t nbreak)

This function allocates a workspace for computing B-splines of order `k`. The number of breakpoints is given by `nbreak`. This leads to $n = nbreak + k - 2$ basis functions. Cubic B-splines are specified by $k = 4$. The size of the workspace is $O(2k^2 + 5k + nbreak)$.

void **gsl_bspline_free**(*gsl_bspline_workspace* *w)

This function frees the memory associated with the workspace `w`.

42.3 Constructing the knots vector

int **gsl_bspline_knots**(const *gsl_vector* *breakpts, *gsl_bspline_workspace* *w)

This function computes the knots associated with the given breakpoints and stores them internally in `w->knots`.

int **gsl_bspline_knots_uniform**(const double a, const double b, *gsl_bspline_workspace* *w)

This function assumes uniformly spaced breakpoints on $[a, b]$ and constructs the corresponding knot vector using the previously specified `nbreak` parameter. The knots are stored in `w->knots`.

42.4 Evaluation of B-splines

int **gsl_bspline_eval**(const double x, *gsl_vector* *B, *gsl_bspline_workspace* *w)

This function evaluates all B-spline basis functions at the position `x` and stores them in the vector `B`, so that the i-th element is $B_i(x)$. The vector `B` must be of length $n = nbreak + k - 2$. This value may also be obtained by calling `gsl_bspline_ncoeffs()`. Computing all the basis functions at once is more efficient than computing them individually, due to the nature of the defining recurrence relation.

int **gsl_bspline_eval_nonzero**(const double x, *gsl_vector* *Bk, size_t *istart, size_t *iend, *gsl_bspline_workspace* *w)

This function evaluates all potentially nonzero B-spline basis functions at the position `x` and stores them in the vector `Bk`, so that the i-th element is $B_{(istart+i)}(x)$. The last element of `Bk` is $B_{iend}(x)$. The vector `Bk` must be of length k. By returning only the nonzero basis functions, this function allows quantities involving linear combinations of the $B_i(x)$ to be computed without unnecessary terms (such linear combinations occur, for example, when evaluating an interpolated function).

size_t **gsl_bspline_ncoeffs**(*gsl_bspline_workspace* *w)

This function returns the number of B-spline coefficients given by $n = nbreak + k - 2$.

42.5 Evaluation of B-spline derivatives

int **gsl_bspline_deriv_eval**(const double x, const size_t nderiv, *gsl_matrix* *dB, *gsl_bspline_workspace* *w)

This function evaluates all B-spline basis function derivatives of orders 0 through `nderiv` (inclusive) at the position `x` and stores them in the matrix `dB`. The (i, j)-th element of `dB` is $d^j B_i(x)/dx^j$. The matrix `dB` must be of size $n = nbreak + k - 2$ by $nderiv + 1$. The value n may also be obtained by calling `gsl_bspline_ncoeffs()`. Note that function evaluations are included as the zeroth order derivatives in `dB`. Computing all the basis function derivatives at once is more efficient than computing them individually, due to the nature of the defining recurrence relation.

int **gsl_bspline_deriv_eval_nonzero**(const double x, const size_t nderiv, *gsl_matrix* *dB, size_t *istart, size_t *iend, *gsl_bspline_workspace* *w)

This function evaluates all potentially nonzero B-spline basis function derivatives of orders 0 through `nderiv` (inclusive) at the position `x` and stores them in the matrix `dB`. The (i, j)-th element of `dB` is $d^j B_{(istart+i)}(x)/dx^j$. The last row of `dB` contains $d^j B_{iend}(x)/dx^j$. The matrix `dB` must be of size k by at least $nderiv + 1$. Note that function evaluations are included as the zeroth order derivatives in `dB`. By returning only the nonzero basis functions, this function allows quantities involving linear combinations of the $B_i(x)$ and their derivatives to be computed without unnecessary terms.

42.6 Working with the Greville abscissae

The Greville abscissae are defined to be the mean location of $k - 1$ consecutive knots in the knot vector for each basis spline function of order k. With the first and last knots in the `gsl_bspline_workspace` knot vector excluded, there are `gsl_bspline_ncoeffs()` Greville abscissae for any given B-spline basis. These values are often used in B-spline collocation applications and may also be called Marsden-Schoenberg points.

double **gsl_bspline_greville_abscissa**(size_t i, *gsl_bspline_workspace* *w)

Returns the location of the i-th Greville abscissa for the given B-spline basis. For the ill-defined case when $k = 1$, the implementation chooses to return breakpoint interval midpoints.

42.7 Examples

The following program computes a linear least squares fit to data using cubic B-spline basis functions with uniform breakpoints. The data is generated from the curve $y(x) = \cos(x) \exp(-x/10)$ on the interval $[0, 15]$ with Gaussian noise added.

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <gsl/gsl_bspline.h>
#include <gsl/gsl_multifit.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_statistics.h>

/* number of data points to fit */
#define N        200

/* number of fit coefficients */
#define NCOEFFS  12

/* nbreak = ncoeffs + 2 - k = ncoeffs - 2 since k = 4 */
#define NBREAK   (NCOEFFS - 2)

int
main (void)
{
  const size_t n = N;
  const size_t ncoeffs = NCOEFFS;
  const size_t nbreak = NBREAK;
```

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```
  size_t i, j;
  gsl_bspline_workspace *bw;
  gsl_vector *B;
  double dy;
  gsl_rng *r;
  gsl_vector *c, *w;
  gsl_vector *x, *y;
  gsl_matrix *X, *cov;
  gsl_multifit_linear_workspace *mw;
  double chisq, Rsq, dof, tss;

  gsl_rng_env_setup();
  r = gsl_rng_alloc(gsl_rng_default);

  /* allocate a cubic bspline workspace (k = 4) */
  bw = gsl_bspline_alloc(4, nbreak);
  B = gsl_vector_alloc(ncoeffs);

  x = gsl_vector_alloc(n);
  y = gsl_vector_alloc(n);
  X = gsl_matrix_alloc(n, ncoeffs);
  c = gsl_vector_alloc(ncoeffs);
  w = gsl_vector_alloc(n);
  cov = gsl_matrix_alloc(ncoeffs, ncoeffs);
  mw = gsl_multifit_linear_alloc(n, ncoeffs);

  /* this is the data to be fitted */
  for (i = 0; i < n; ++i)
    {
      double sigma;
      double xi = (15.0 / (N - 1)) * i;
      double yi = cos(xi) * exp(-0.1 * xi);

      sigma = 0.1 * yi;
      dy = gsl_ran_gaussian(r, sigma);
      yi += dy;

      gsl_vector_set(x, i, xi);
      gsl_vector_set(y, i, yi);
      gsl_vector_set(w, i, 1.0 / (sigma * sigma));

      printf("%f %f\n", xi, yi);
    }

  /* use uniform breakpoints on [0, 15] */
  gsl_bspline_knots_uniform(0.0, 15.0, bw);

  /* construct the fit matrix X */
  for (i = 0; i < n; ++i)
    {
      double xi = gsl_vector_get(x, i);
```

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```
      /* compute B_j(xi) for all j */
      gsl_bspline_eval(xi, B, bw);

      /* fill in row i of X */
      for (j = 0; j < ncoeffs; ++j)
        {
          double Bj = gsl_vector_get(B, j);
          gsl_matrix_set(X, i, j, Bj);
        }
    }

  /* do the fit */
  gsl_multifit_wlinear(X, w, y, c, cov, &chisq, mw);

  dof = n - ncoeffs;
  tss = gsl_stats_wtss(w->data, 1, y->data, 1, y->size);
  Rsq = 1.0 - chisq / tss;

  fprintf(stderr, "chisq/dof = %e, Rsq = %f\n",
                   chisq / dof, Rsq);

  printf("\n\n");

  /* output the smoothed curve */
  {
    double xi, yi, yerr;

    for (xi = 0.0; xi < 15.0; xi += 0.1)
      {
        gsl_bspline_eval(xi, B, bw);
        gsl_multifit_linear_est(B, c, cov, &yi, &yerr);
        printf("%f %f\n", xi, yi);
      }
  }

  gsl_rng_free(r);
  gsl_bspline_free(bw);
  gsl_vector_free(B);
  gsl_vector_free(x);
  gsl_vector_free(y);
  gsl_matrix_free(X);
  gsl_vector_free(c);
  gsl_vector_free(w);
  gsl_matrix_free(cov);
  gsl_multifit_linear_free(mw);

  return 0;
} /* main() */
```

The output is shown below:

```
$ ./a.out > bspline.txt
```

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```
chisq/dof = 1.118217e+00, Rsq = 0.989771
```

The data and fitted model are shown in Fig. 42.1.

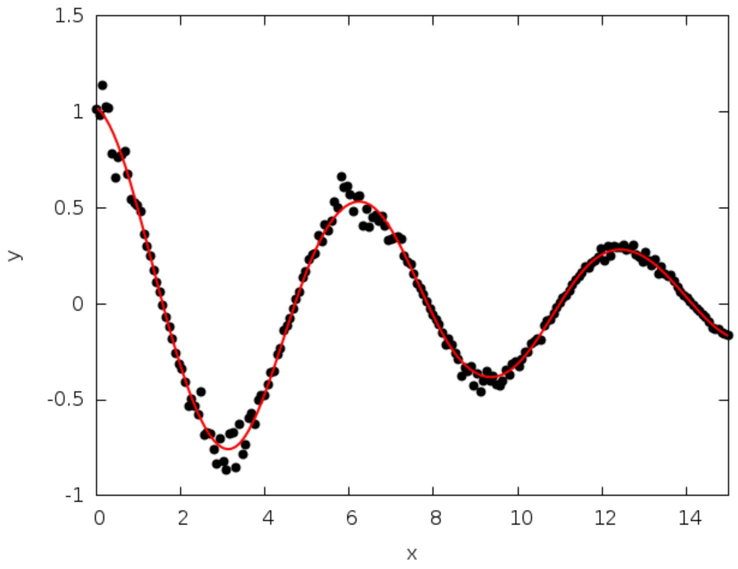

Fig. 42.1: Data (black) and fitted model (red)

42.8 References and Further Reading

Further information on the algorithms described in this section can be found in the following book,

- C. de Boor, *A Practical Guide to Splines* (1978), Springer-Verlag, ISBN 0-387-90356-9.

Further information of Greville abscissae and B-spline collocation can be found in the following paper,

- Richard W. Johnson, Higher order B-spline collocation at the Greville abscissae. *Applied Numerical Mathematics.* vol.: 52, 2005, 63–75.

A large collection of B-spline routines is available in the PPPACK library available at http://www.netlib.org/pppack, which is also part of SLATEC.

CHAPTER

FORTYTHREE

SPARSE MATRICES

This chapter describes functions for the construction and manipulation of sparse matrices, matrices which are populated primarily with zeros and contain only a few non-zero elements. Sparse matrices often appear in the solution of partial differential equations. It is beneficial to use specialized data structures and algorithms for storing and working with sparse matrices, since dense matrix algorithms and structures can be prohibitively slow and use huge amounts of memory when applied to sparse matrices.

The header file `gsl_spmatrix.h` contains the prototypes for the sparse matrix functions and related declarations.

43.1 Data types

All the functions are available for each of the standard data-types. The versions for `double` have the prefix `gsl_spmatrix`, Similarly the versions for single-precision `float` arrays have the prefix `gsl_spmatrix_float`. The full list of available types is given below,

Prefix	Type
gsl_spmatrix	double
gsl_spmatrix_float	float
gsl_spmatrix_long_double	long double
gsl_spmatrix_int	int
gsl_spmatrix_uint	unsigned int
gsl_spmatrix_long	long
gsl_spmatrix_ulong	unsigned long
gsl_spmatrix_short	short
gsl_spmatrix_ushort	unsigned short
gsl_spmatrix_char	char
gsl_spmatrix_uchar	unsigned char
gsl_spmatrix_complex	complex double
gsl_spmatrix_complex_float	complex float
gsl_spmatrix_complex_long_double	complex long double

43.2 Sparse Matrix Storage Formats

GSL currently supports three storage formats for sparse matrices: the coordinate (COO) representation, compressed sparse column (CSC) and compressed sparse row (CSR) formats. These are discussed in more detail below. In order to illustrate the different storage formats, the following sections will reference this M-by-N sparse matrix, with $M = 4$ and $N = 5$:

$$\begin{pmatrix} 9 & 0 & 0 & 0 & -3 \\ 4 & 7 & 0 & 0 & 0 \\ 0 & 8 & -1 & 8 & 0 \\ 4 & 0 & 5 & 6 & 0 \end{pmatrix}$$

The number of non-zero elements in the matrix, also abbreviated as `nnz` is equal to 10 in this case.

43.2.1 Coordinate Storage (COO)

The coordinate storage format, also known as *triplet format*, stores triplets (i, j, x) for each non-zero element of the matrix. This notation means that the (i, j) element of the matrix A is $A_{ij} = x$. The matrix is stored using three arrays of the same length, representing the row indices, column indices, and matrix data. For the reference matrix above, one possible storage format is:

data	9	7	4	8	-3	-1	8	5	6	4
row	0	1	1	2	0	2	2	3	3	3
col	0	1	0	1	4	2	3	2	3	0

Note that this representation is not unique - the coordinate triplets may appear in any ordering and would still represent the same sparse matrix. The length of the three arrays is equal to the number of non-zero elements in the matrix, `nnz`, which in this case is 10. The coordinate format is extremely convenient for sparse matrix *assembly*, the process of adding new elements, or changing existing elements, in a sparse matrix. However, it is generally not suitable for the efficient implementation of matrix-matrix products, or matrix factorization algorithms. For these applications it is better to use one of the compressed formats discussed below.

In order to faciliate efficient sparse matrix assembly, GSL stores the coordinate data in a balanced binary search tree, specifically an AVL tree, in addition to the three arrays discussed above. This allows GSL to efficiently determine whether an entry (i, j) already exists in the matrix, and to replace an existing matrix entry with a new value, without needing to search unsorted arrays.

43.2.2 Compressed Sparse Column (CSC)

Compressed sparse column storage stores each column of non-zero values in the sparse matrix in a continuous memory block, keeping pointers to the beginning of each column in that memory block, and storing the row indices of each non-zero element. For the reference matrix above, these arrays look like

data	9	4	4	7	8	-1	5	8	6	-3
row	0	1	3	1	2	2	3	2	3	0
col_ptr	0	3	5	7	9	10				

The `data` and `row` arrays are of length `nnz` and are the same as the COO storage format. The `col_ptr` array has length $N + 1$, and `col_ptr[j]` gives the index in `data` of the start of column `j`. Therefore, the j-th column of the matrix is stored in `data[col_ptr[j]]`, `data[col_ptr[j] + 1]`, …, `data[col_ptr[j+1] - 1]`. The last element of `col_ptr` is `nnz`.

43.2.3 Compressed Sparse Row (CSR)

Compressed row storage stores each row of non-zero values in a continuous memory block, keeping pointers to the beginning of each row in the block and storing the column indices of each non-zero element. For the reference matrix above, these arrays look like

data	9	-3	4	7	8	-1	8	4	5	6
col	0	4	0	1	1	2	3	0	2	3
row_ptr	0	2	4	7	10					

The `data` and `col` arrays are of length `nnz` and are the same as the COO storage format. The `row_ptr` array has length $M + 1$, and `row_ptr[i]` gives the index in `data` of the start of row `i`. Therefore, the i-th row of the matrix is stored in `data[row_ptr[i]]`, `data[row_ptr[i] + 1]`, ..., `data[row_ptr[i+1] - 1]`. The last element of `row_ptr` is `nnz`.

43.3 Overview

These routines provide support for constructing and manipulating sparse matrices in GSL, using an API similar to *gsl_matrix*. The basic structure is called *gsl_spmatrix*.

type **gsl_spmatrix**

This structure is defined as:

```
typedef struct
{
  size_t size1;
  size_t size2;
  int *i;
  double *data;
  int *p;
  size_t nzmax;
  size_t nz;
  [ ... variables for binary tree and memory management ... ]
  size_t sptype;
} gsl_spmatrix;
```

This defines a `size1`-by-`size2` sparse matrix. The number of non-zero elements currently in the matrix is given by `nz`. For the triplet representation, `i`, `p`, and `data` are arrays of size `nz` which contain the row indices, column indices, and element value, respectively. So if $data[k] = A(i, j)$, then $i = i[k]$ and $j = p[k]$.

For compressed column storage, `i` and `data` are arrays of size `nz` containing the row indices and element values, identical to the triplet case. `p` is an array of size `size2` + 1 where `p[j]` points to the index in `data` of the start of column `j`. Thus, if $data[k] = A(i, j)$, then $i = i[k]$ and $p[j] <= k < p[j + 1]$.

For compressed row storage, `i` and `data` are arrays of size `nz` containing the column indices and element values, identical to the triplet case. `p` is an array of size `size1` + 1 where `p[i]` points to the index in `data` of the start of row `i`. Thus, if $data[k] = A(i, j)$, then $j = i[k]$ and $p[i] <= k < p[i + 1]$.

There are additional variables in the *gsl_spmatrix* structure related to binary tree storage and memory management. The GSL implementation of sparse matrices uses balanced AVL trees to sort matrix elements in the triplet representation. This speeds up element searches and duplicate detection during the matrix assembly process. The *gsl_spmatrix* structure also contains additional workspace variables needed for various operations like converting from triplet to compressed storage. `sptype` indicates the type of storage format being used (COO, CSC or CSR).

The compressed storage format defined above makes it very simple to interface with sophisticated external linear solver libraries which accept compressed storage input. The user can simply pass the arrays `i`, `p`, and `data` as the inputs to external libraries.

43.4 Allocation

The functions for allocating memory for a sparse matrix follow the style of `malloc()` and `free()`. They also perform their own error checking. If there is insufficient memory available to allocate a matrix then the functions call the GSL error handler with an error code of *`GSL_ENOMEM`* in addition to returning a null pointer.

gsl_spmatrix ***gsl_spmatrix_alloc**(const size_t n1, const size_t n2)

This function allocates a sparse matrix of size *`n1`*-by-*`n2`* and initializes it to all zeros. If the size of the matrix is not known at allocation time, both *`n1`* and *`n2`* may be set to 1, and they will automatically grow as elements are added to the matrix. This function sets the matrix to the triplet representation, which is the easiest for adding and accessing matrix elements. This function tries to make a reasonable guess for the number of non-zero elements (`nzmax`) which will be added to the matrix by assuming a sparse density of 10%. The function *`gsl_spmatrix_alloc_nzmax()`* can be used if this number is known more accurately. The workspace is of size $O(nzmax)$.

gsl_spmatrix ***gsl_spmatrix_alloc_nzmax**(const size_t n1, const size_t n2, const size_t nzmax, const size_t sptype)

This function allocates a sparse matrix of size *`n1`*-by-*`n2`* and initializes it to all zeros. If the size of the matrix is not known at allocation time, both *`n1`* and *`n2`* may be set to 1, and they will automatically grow as elements are added to the matrix. The parameter *`nzmax`* specifies the maximum number of non-zero elements which will be added to the matrix. It does not need to be precisely known in advance, since storage space will automatically grow using *`gsl_spmatrix_realloc()`* if *`nzmax`* is not large enough. Accurate knowledge of this parameter reduces the number of reallocation calls required. The parameter *`sptype`* specifies the storage format of the sparse matrix. Possible values are

GSL_SPMATRIX_COO

This flag specifies coordinate (triplet) storage.

GSL_SPMATRIX_CSC

This flag specifies compressed sparse column storage.

GSL_SPMATRIX_CSR

This flag specifies compressed sparse row storage.

The allocated *`gsl_spmatrix`* structure is of size $O(nzmax)$.

int **gsl_spmatrix_realloc**(const size_t nzmax, *gsl_spmatrix* *m)

This function reallocates the storage space for *`m`* to accomodate *`nzmax`* non-zero elements. It is typically called internally by *`gsl_spmatrix_set()`* if the user wants to add more elements to the sparse matrix than the previously specified *`nzmax`*.

Input matrix formats supported: *COO*, *CSC*, *CSR*

void **gsl_spmatrix_free**(*gsl_spmatrix* *m)

This function frees the memory associated with the sparse matrix *`m`*.

Input matrix formats supported: *COO*, *CSC*, *CSR*

43.5 Accessing Matrix Elements

double **gsl_spmatrix_get**(const *gsl_spmatrix* *m, const size_t i, const size_t j)

This function returns element (*i*, *j*) of the matrix *m*.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_set**(*gsl_spmatrix* *m, const size_t i, const size_t j, const double x)

This function sets element (*i*, *j*) of the matrix *m* to the value *x*.

Input matrix formats supported: *COO*

double ***gsl_spmatrix_ptr**(*gsl_spmatrix* *m, const size_t i, const size_t j)

This function returns a pointer to the (*i*, *j*) element of the matrix *m*. If the (*i*, *j*) element is not explicitly stored in the matrix, a null pointer is returned.

Input matrix formats supported: *COO*, *CSC*, *CSR*

43.6 Initializing Matrix Elements

Since the sparse matrix format only stores the non-zero elements, it is automatically initialized to zero upon allocation. The function `gsl_spmatrix_set_zero()` may be used to re-initialize a matrix to zero after elements have been added to it.

int **gsl_spmatrix_set_zero**(*gsl_spmatrix* *m)

This function sets (or resets) all the elements of the matrix *m* to zero. For CSC and CSR matrices, the cost of this operation is $O(1)$. For COO matrices, the binary tree structure must be dismantled, so the cost is $O(nz)$.

Input matrix formats supported: *COO*, *CSC*, *CSR*

43.7 Reading and Writing Matrices

int **gsl_spmatrix_fwrite**(FILE *stream, const *gsl_spmatrix* *m)

This function writes the elements of the matrix *m* to the stream `stream` in binary format. The return value is 0 for success and `GSL_EFAILED` if there was a problem writing to the file. Since the data is written in the native binary format it may not be portable between different architectures.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_fread**(FILE *stream, *gsl_spmatrix* *m)

This function reads into the matrix *m* from the open stream `stream` in binary format. The matrix *m* must be preallocated with the correct storage format, dimensions and have a sufficiently large `nzmax` in order to read in all matrix elements, otherwise `GSL_EBADLEN` is returned. The return value is 0 for success and `GSL_EFAILED` if there was a problem reading from the file. The data is assumed to have been written in the native binary format on the same architecture.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_fprintf**(FILE *stream, const *gsl_spmatrix* *m, const char *format)

This function writes the elements of the matrix *m* line-by-line to the stream `stream` using the format specifier `format`, which should be one of the `%g`, `%e` or `%f` formats for floating point numbers. The function returns 0 for success and `GSL_EFAILED` if there was a problem writing to the file. The input matrix *m* may be in any storage format, and the output file will be written in MatrixMarket format.

Input matrix formats supported: *COO*, *CSC*, *CSR*

gsl_spmatrix ***gsl_spmatrix_fscanf**(FILE *stream)

This function reads sparse matrix data in the MatrixMarket format from the stream `stream` and stores it in a newly allocated matrix which is returned in *COO* format. The function returns 0 for success and `GSL_EFAILED` if there was a problem reading from the file. The user should free the returned matrix when it is no longer needed.

43.8 Copying Matrices

int **gsl_spmatrix_memcpy**(*gsl_spmatrix* *dest, const *gsl_spmatrix* *src)

This function copies the elements of the sparse matrix `src` into `dest`. The two matrices must have the same dimensions and be in the same storage format.

Input matrix formats supported: *COO*, *CSC*, *CSR*

43.9 Exchanging Rows and Columns

int **gsl_spmatrix_transpose_memcpy**(*gsl_spmatrix* *dest, const *gsl_spmatrix* *src)

This function copies the transpose of the sparse matrix `src` into `dest`. The dimensions of `dest` must match the transpose of the matrix `src`. Also, both matrices must use the same sparse storage format.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_transpose**(*gsl_spmatrix* *m)

This function replaces the matrix `m` by its transpose, but changes the storage format for compressed matrix inputs. Since compressed column storage is the transpose of compressed row storage, this function simply converts a CSC matrix to CSR and vice versa. This is the most efficient way to transpose a compressed storage matrix, but the user should note that the storage format of their compressed matrix will change on output. For COO matrix inputs, the output matrix is also in COO storage.

Input matrix formats supported: *COO*, *CSC*, *CSR*

43.10 Matrix Operations

int **gsl_spmatrix_scale**(*gsl_spmatrix* *m, const double x)

This function scales all elements of the matrix `m` by the constant factor `x`. The result $m(i,j) \leftarrow xm(i,j)$ is stored in `m`.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_scale_columns**(*gsl_spmatrix* *A, const *gsl_vector* *x)

This function scales the columns of the M-by-N sparse matrix `A` by the elements of the vector `x`, of length N. The j-th column of `A` is multiplied by `x[j]`. This is equivalent to forming

$$A \rightarrow AX$$

where $X = \text{diag}(x)$.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_scale_rows**(*gsl_spmatrix* *A, const *gsl_vector* *x)

This function scales the rows of the M-by-N sparse matrix `A` by the elements of the vector `x`, of length M. The i-th row of `A` is multiplied by `x[i]`. This is equivalent to forming

$$A \rightarrow XA$$

where $X = \mathrm{diag}(x)$.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_add**(*gsl_spmatrix* *c, const *gsl_spmatrix* *a, const *gsl_spmatrix* *b)

This function computes the sum $c = a + b$. The three matrices must have the same dimensions.

Input matrix formats supported: *CSC*, *CSR*

int **gsl_spmatrix_dense_add**(*gsl_matrix* *a, const *gsl_spmatrix* *b)

This function adds the elements of the sparse matrix `b` to the elements of the dense matrix `a`. The result $a(i, j) \leftarrow a(i, j) + b(i, j)$ is stored in `a` and `b` remains unchanged. The two matrices must have the same dimensions.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_dense_sub**(*gsl_matrix* *a, const *gsl_spmatrix* *b)

This function subtracts the elements of the sparse matrix `b` from the elements of the dense matrix `a`. The result $a(i, j) \leftarrow a(i, j) - b(i, j)$ is stored in `a` and `b` remains unchanged. The two matrices must have the same dimensions.

Input matrix formats supported: *COO*, *CSC*, *CSR*

43.11 Matrix Properties

const char ***gsl_spmatrix_type**(const *gsl_spmatrix* *m)

This function returns a string describing the sparse storage format of the matrix `m`. For example:

```
printf ("matrix is '%s' format.\n", gsl_spmatrix_type (m));
```

would print something like:

```
matrix is 'CSR' format.
```

Input matrix formats supported: *COO*, *CSC*, *CSR*

size_t **gsl_spmatrix_nnz**(const *gsl_spmatrix* *m)

This function returns the number of non-zero elements in `m`.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_equal**(const *gsl_spmatrix* *a, const *gsl_spmatrix* *b)

This function returns 1 if the matrices `a` and `b` are equal (by comparison of element values) and 0 otherwise. The matrices `a` and `b` must be in the same sparse storage format for comparison.

Input matrix formats supported: *COO*, *CSC*, *CSR*

double **gsl_spmatrix_norm1**(const *gsl_spmatrix* *A)

This function returns the 1-norm of the m-by-n matrix `A`, defined as the maximum column sum,

$$||A||_1 = \max_{1 \le j \le n} \sum_{i=1}^{m} |A_{ij}|$$

Input matrix formats supported: *COO*, *CSC*, *CSR*

43.12 Finding Maximum and Minimum Elements

int **gsl_spmatrix_minmax**(const *gsl_spmatrix* *m, double *min_out, double *max_out)

This function returns the minimum and maximum elements of the matrix `m`, storing them in `min_out` and `max_out`, and searching only the non-zero values.

Input matrix formats supported: *COO*, *CSC*, *CSR*

int **gsl_spmatrix_min_index**(const *gsl_spmatrix* *m, size_t *imin, size_t *jmin)

This function returns the indices of the minimum value in the matrix `m`, searching only the non-zero values, and storing them in `imin` and `jmin`. When there are several equal minimum elements then the first element found is returned.

Input matrix formats supported: *COO*, *CSC*, *CSR*

43.13 Compressed Format

These routines calculate a compressed matrix from a coordinate representation.

int **gsl_spmatrix_csc**(*gsl_spmatrix* *dest, const *gsl_spmatrix* *src)

This function creates a sparse matrix in *compressed sparse column* format from the input sparse matrix `src` which must be in COO format. The compressed matrix is stored in `dest`.

Input matrix formats supported: *COO*

int **gsl_spmatrix_csr**(*gsl_spmatrix* *dest, const *gsl_spmatrix* *src)

This function creates a sparse matrix in *compressed sparse row* format from the input sparse matrix `src` which must be in COO format. The compressed matrix is stored in `dest`.

Input matrix formats supported: *COO*

gsl_spmatrix ***gsl_spmatrix_compress**(const *gsl_spmatrix* *src, const int sptype)

This function allocates a new sparse matrix, and stores `src` into it using the format specified by `sptype`. The input `sptype` can be one of `GSL_SPMATRIX_COO`, `GSL_SPMATRIX_CSC`, or `GSL_SPMATRIX_CSR`. A pointer to the newly allocated matrix is returned, and must be freed by the caller when no longer needed.

43.14 Conversion Between Sparse and Dense Matrices

The `gsl_spmatrix` structure can be converted into the dense `gsl_matrix` format and vice versa with the following routines.

int **gsl_spmatrix_d2sp**(*gsl_spmatrix* *S, const *gsl_matrix* *A)

This function converts the dense matrix `A` into sparse COO format and stores the result in `S`.

Input matrix formats supported: *COO*

int **gsl_spmatrix_sp2d**(*gsl_matrix* *A, const *gsl_spmatrix* *S)

This function converts the sparse matrix `S` into a dense matrix and stores the result in `A`.

Input matrix formats supported: *COO*, *CSC*, *CSR*

43.15 Examples

The following example program builds a 5-by-4 sparse matrix and prints it in coordinate, compressed column, and compressed row format. The matrix which is constructed is

$$\begin{pmatrix} 0 & 0 & 3.1 & 4.6 \\ 1 & 0 & 7.2 & 0 \\ 0 & 0 & 0 & 0 \\ 2.1 & 2.9 & 0 & 8.5 \\ 4.1 & 0 & 0 & 0 \end{pmatrix}$$

The output of the program is:

```
printing all matrix elements:
A(0,0) = 0
A(0,1) = 0
A(0,2) = 3.1
A(0,3) = 4.6
A(1,0) = 1
.
.
.
A(4,0) = 4.1
A(4,1) = 0
A(4,2) = 0
A(4,3) = 0
matrix in triplet format (i,j,Aij):
(0, 2, 3.1)
(0, 3, 4.6)
(1, 0, 1.0)
(1, 2, 7.2)
(3, 0, 2.1)
(3, 1, 2.9)
(3, 3, 8.5)
(4, 0, 4.1)
matrix in compressed column format:
i = [ 1, 3, 4, 3, 0, 1, 0, 3, ]
p = [ 0, 3, 4, 6, 8, ]
d = [ 1, 2.1, 4.1, 2.9, 3.1, 7.2, 4.6, 8.5, ]
matrix in compressed row format:
i = [ 2, 3, 0, 2, 0, 1, 3, 0, ]
p = [ 0, 2, 4, 4, 7, 8, ]
d = [ 3.1, 4.6, 1, 7.2, 2.1, 2.9, 8.5, 4.1, ]
```

We see in the compressed column output, the data array stores each column contiguously, the array i stores the row index of the corresponding data element, and the array p stores the index of the start of each column in the data array. Similarly, for the compressed row output, the data array stores each row contiguously, the array i stores the column index of the corresponding data element, and the p array stores the index of the start of each row in the data array.

```
#include <stdio.h>
#include <stdlib.h>

#include <gsl/gsl_spmatrix.h>

```

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```
int
main()
{
  gsl_spmatrix *A = gsl_spmatrix_alloc(5, 4); /* triplet format */
  gsl_spmatrix *B, *C;
  size_t i, j;

  /* build the sparse matrix */
  gsl_spmatrix_set(A, 0, 2, 3.1);
  gsl_spmatrix_set(A, 0, 3, 4.6);
  gsl_spmatrix_set(A, 1, 0, 1.0);
  gsl_spmatrix_set(A, 1, 2, 7.2);
  gsl_spmatrix_set(A, 3, 0, 2.1);
  gsl_spmatrix_set(A, 3, 1, 2.9);
  gsl_spmatrix_set(A, 3, 3, 8.5);
  gsl_spmatrix_set(A, 4, 0, 4.1);

  printf("printing all matrix elements:\n");
  for (i = 0; i < 5; ++i)
    for (j = 0; j < 4; ++j)
      printf("A(%zu,%zu) = %g\n", i, j,
             gsl_spmatrix_get(A, i, j));

  /* print out elements in triplet format */
  printf("matrix in triplet format (i,j,Aij):\n");
  gsl_spmatrix_fprintf(stdout, A, "%.1f");

  /* convert to compressed column format */
  B = gsl_spmatrix_ccs(A);

  printf("matrix in compressed column format:\n");
  printf("i = [ ");
  for (i = 0; i < B->nz; ++i)
    printf("%d, ", B->i[i]);
  printf("]\n");

  printf("p = [ ");
  for (i = 0; i < B->size2 + 1; ++i)
    printf("%d, ", B->p[i]);
  printf("]\n");

  printf("d = [ ");
  for (i = 0; i < B->nz; ++i)
    printf("%g, ", B->data[i]);
  printf("]\n");

  /* convert to compressed row format */
  C = gsl_spmatrix_crs(A);

  printf("matrix in compressed row format:\n");
  printf("i = [ ");
  for (i = 0; i < C->nz; ++i)
```

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```
    printf("%d, ", C->i[i]);
  printf("]\n");

  printf("p = [ ");
  for (i = 0; i < C->size1 + 1; ++i)
    printf("%d, ", C->p[i]);
  printf("]\n");

  printf("d = [ ");
  for (i = 0; i < C->nz; ++i)
    printf("%g, ", C->data[i]);
  printf("]\n");

  gsl_spmatrix_free(A);
  gsl_spmatrix_free(B);
  gsl_spmatrix_free(C);

  return 0;
}
```

43.16 References and Further Reading

The algorithms used by these functions are described in the following sources,

- Davis, T. A., Direct Methods for Sparse Linear Systems, SIAM, 2006.
- CSparse software library, https://www.cise.ufl.edu/research/sparse/CSparse

CHAPTER

FORTYFOUR

SPARSE BLAS SUPPORT

The Sparse Basic Linear Algebra Subprograms (BLAS) define a set of fundamental operations on vectors and sparse matrices which can be used to create optimized higher-level linear algebra functionality. GSL supports a limited number of BLAS operations for sparse matrices.

The header file `gsl_spblas.h` contains the prototypes for the sparse BLAS functions and related declarations.

44.1 Sparse BLAS operations

int **gsl_spblas_dgemv**(const CBLAS_TRANSPOSE_t TransA, const double alpha, const *gsl_spmatrix* *A, const *gsl_vector* *x, const double beta, *gsl_vector* *y)

This function computes the matrix-vector product and sum $y \leftarrow \alpha op(A)x + \beta y$, where $op(A) = A, A^T$ for *TransA* = `CblasNoTrans`, `CblasTrans`. In-place computations are not supported, so *x* and *y* must be distinct vectors. The matrix *A* may be in triplet or compressed format.

int **gsl_spblas_dgemm**(const double alpha, const *gsl_spmatrix* *A, const *gsl_spmatrix* *B, *gsl_spmatrix* *C)

This function computes the sparse matrix-matrix product $C = \alpha AB$. The matrices must be in compressed format.

44.2 References and Further Reading

The algorithms used by these functions are described in the following sources:

- Davis, T. A., Direct Methods for Sparse Linear Systems, SIAM, 2006.
- CSparse software library, https://www.cise.ufl.edu/research/sparse/CSparse

CHAPTER

FORTYFIVE

SPARSE LINEAR ALGEBRA

This chapter describes functions for solving sparse linear systems of equations. The library provides linear algebra routines which operate directly on the *gsl_spmatrix* and *gsl_vector* objects.

The functions described in this chapter are declared in the header file `gsl_splinalg.h`.

45.1 Overview

This chapter is primarily concerned with the solution of the linear system

$$Ax = b$$

where A is a general square n-by-n non-singular sparse matrix, x is an unknown n-by-1 vector, and b is a given n-by-1 right hand side vector. There exist many methods for solving such sparse linear systems, which broadly fall into either direct or iterative categories. Direct methods include LU and QR decompositions, while iterative methods start with an initial guess for the vector x and update the guess through iteration until convergence. GSL does not currently provide any direct sparse solvers.

45.2 Sparse Iterative Solvers

45.2.1 Overview

Many practical iterative methods of solving large n-by-n sparse linear systems involve projecting an approximate solution for `x` onto a subspace of $\mathbf{R}^n$. If we define a m-dimensional subspace $\mathcal{K}$ as the subspace of approximations to the solution `x`, then m constraints must be imposed to determine the next approximation. These m constraints define another m-dimensional subspace denoted by $\mathcal{L}$. The subspace dimension m is typically chosen to be much smaller than n in order to reduce the computational effort needed to generate the next approximate solution vector. The many iterative algorithms which exist differ mainly in their choice of $\mathcal{K}$ and $\mathcal{L}$.

45.2.2 Types of Sparse Iterative Solvers

The sparse linear algebra library provides the following types of iterative solvers:

type **`gsl_splinalg_itersolve_type`**

gsl_splinalg_itersolve_type ***gsl_splinalg_itersolve_gmres**

This specifies the Generalized Minimum Residual Method (GMRES). This is a projection method using $\mathcal{K} = \mathcal{K}_m$ and $\mathcal{L} = A\mathcal{K}_m$ where $\mathcal{K}_m$ is the m-th Krylov subspace

$$\mathcal{K}_m = span \left\{ r_0, Ar_0, ..., A^{m-1} r_0 \right\}$$

and $r_0 = b - Ax_0$ is the residual vector of the initial guess x_0. If m is set equal to n, then the Krylov subspace is $\mathbf{R}^n$ and GMRES will provide the exact solution `x`. However, the goal is for the method to arrive at a very good approximation to `x` using a much smaller subspace $\mathcal{K}_m$. By default, the GMRES method selects $m = MIN(n, 10)$ but the user may specify a different value for m. The GMRES storage requirements grow as $O(n(m+1))$ and the number of flops grow as $O(4m^2n - 4m^3/3)$.

In the below function `gsl_splinalg_itersolve_iterate()`, one GMRES iteration is defined as projecting the approximate solution vector onto each Krylov subspace $\mathcal{K}_1, ..., \mathcal{K}_m$, and so m can be kept smaller by "restarting" the method and calling `gsl_splinalg_itersolve_iterate()` multiple times, providing the updated approximation `x` to each new call. If the method is not adequately converging, the user may try increasing the parameter m.

GMRES is considered a robust general purpose iterative solver, however there are cases where the method stagnates if the matrix is not positive-definite and fails to reduce the residual until the very last projection onto the subspace $\mathcal{K}_n = \mathbf{R}^n$. In these cases, preconditioning the linear system can help, but GSL does not currently provide any preconditioners.

45.2.3 Iterating the Sparse Linear System

The following functions are provided to allocate storage for the sparse linear solvers and iterate the system to a solution.

gsl_splinalg_itersolve ***gsl_splinalg_itersolve_alloc**(const *gsl_splinalg_itersolve_type* *T, const size_t n, const size_t m)

This function allocates a workspace for the iterative solution of `n`-by-`n` sparse matrix systems. The iterative solver type is specified by `T`. The argument `m` specifies the size of the solution candidate subspace $\mathcal{K}_m$. The dimension `m` may be set to 0 in which case a reasonable default value is used.

void **gsl_splinalg_itersolve_free**(gsl_splinalg_itersolve *w)

This function frees the memory associated with the workspace `w`.

const char ***gsl_splinalg_itersolve_name**(const gsl_splinalg_itersolve *w)

This function returns a string pointer to the name of the solver.

int **gsl_splinalg_itersolve_iterate**(const *gsl_spmatrix* *A, const *gsl_vector* *b, const double tol, *gsl_vector* *x, gsl_splinalg_itersolve *w)

This function performs one iteration of the iterative method for the sparse linear system specfied by the matrix `A`, right hand side vector `b` and solution vector `x`. On input, `x` must be set to an initial guess for the solution. On output, `x` is updated to give the current solution estimate. The parameter `tol` specifies the relative tolerance between the residual norm and norm of `b` in order to check for convergence. When the following condition is satisfied:

$$||Ax - b|| \leq tol \times ||b||$$

the method has converged, the function returns `GSL_SUCCESS` and the final solution is provided in `x`. Otherwise, the function returns `GSL_CONTINUE` to signal that more iterations are required. Here, $|| \cdot ||$ represents the Euclidean norm. The input matrix `A` may be in triplet or compressed format.

double **gsl_splinalg_itersolve_normr**(const gsl_splinalg_itersolve *w)

This function returns the current residual norm $||r|| = ||Ax - b||$, which is updated after each call to `gsl_splinalg_itersolve_iterate()`.

45.3 Examples

This example program demonstrates the sparse linear algebra routines on the solution of a simple 1D Poisson equation on $[0, 1]$:

$$\frac{d^2u(x)}{dx^2} = f(x) = -\pi^2 \sin(\pi x)$$

with boundary conditions $u(0) = u(1) = 0$. The analytic solution of this simple problem is $u(x) = \sin \pi x$. We will solve this problem by finite differencing the left hand side to give

$$\frac{1}{h^2}(u_{i+1} - 2u_i + u_{i-1}) = f_i$$

Defining a grid of N points, $h = 1/(N-1)$. In the finite difference equation above, $u_0 = u_{N-1} = 0$ are known from the boundary conditions, so we will only put the equations for $i = 1, ..., N-2$ into the matrix system. The resulting $(N-2) \times (N-2)$ matrix equation is

$$\frac{1}{h^2}\begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \dots & 1 & -2 & 1 \\ 0 & \dots & \dots & \dots & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-3} \\ u_{N-2} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{N-3} \\ f_{N-2} \end{pmatrix}$$

An example program which constructs and solves this system is given below. The system is solved using the iterative GMRES solver. Here is the output of the program:

```
iter 0 residual = 4.297275996844e-11
Converged
```

showing that the method converged in a single iteration. The calculated solution is shown in Fig. 45.1.

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_spmatrix.h>
#include <gsl/gsl_splinalg.h>

int
main()
{
  const size_t N = 100;                       /* number of grid points */
  const size_t n = N - 2;                     /* subtract 2 to exclude boundaries */
  const double h = 1.0 / (N - 1.0);           /* grid spacing */
  gsl_spmatrix *A = gsl_spmatrix_alloc(n ,n); /* triplet format */
  gsl_spmatrix *C;                            /* compressed format */
  gsl_vector *f = gsl_vector_alloc(n);        /* right hand side vector */
  gsl_vector *u = gsl_vector_alloc(n);        /* solution vector */
  size_t i;
```

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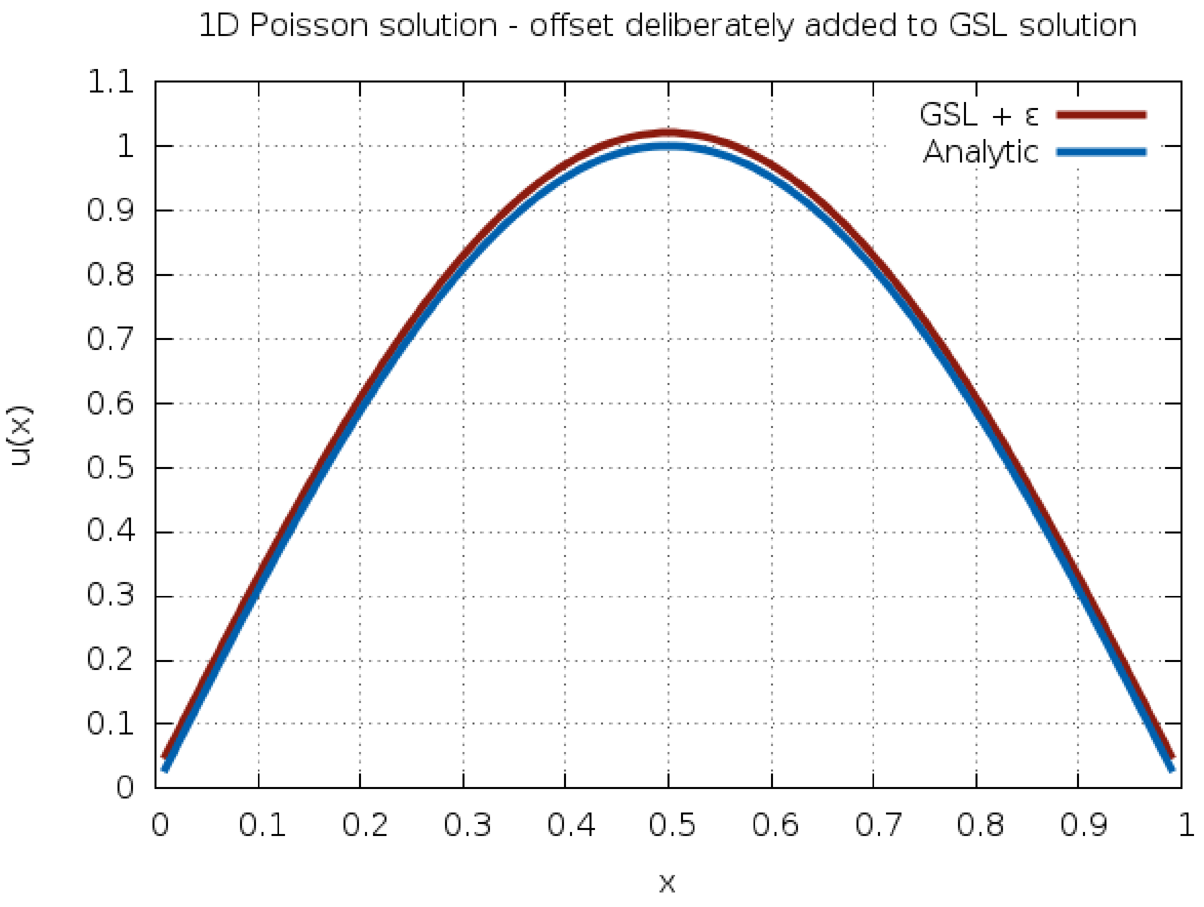

Fig. 45.1: Solution of PDE

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```
/* construct the sparse matrix for the finite difference equation */

/* construct first row */
gsl_spmatrix_set(A, 0, 0, -2.0);
gsl_spmatrix_set(A, 0, 1, 1.0);

/* construct rows [1:n-2] */
for (i = 1; i < n - 1; ++i)
  {
    gsl_spmatrix_set(A, i, i + 1, 1.0);
    gsl_spmatrix_set(A, i, i, -2.0);
    gsl_spmatrix_set(A, i, i - 1, 1.0);
  }

/* construct last row */
gsl_spmatrix_set(A, n - 1, n - 1, -2.0);
gsl_spmatrix_set(A, n - 1, n - 2, 1.0);

/* scale by h^2 */
gsl_spmatrix_scale(A, 1.0 / (h * h));

/* construct right hand side vector */
for (i = 0; i < n; ++i)
  {
    double xi = (i + 1) * h;
    double fi = -M_PI * M_PI * sin(M_PI * xi);
    gsl_vector_set(f, i, fi);
  }

/* convert to compressed column format */
C = gsl_spmatrix_ccs(A);

/* now solve the system with the GMRES iterative solver */
{
  const double tol = 1.0e-6;  /* solution relative tolerance */
  const size_t max_iter = 10; /* maximum iterations */
  const gsl_splinalg_itersolve_type *T = gsl_splinalg_itersolve_gmres;
  gsl_splinalg_itersolve *work =
    gsl_splinalg_itersolve_alloc(T, n, 0);
  size_t iter = 0;
  double residual;
  int status;

  /* initial guess u = 0 */
  gsl_vector_set_zero(u);

  /* solve the system A u = f */
  do
    {
      status = gsl_splinalg_itersolve_iterate(C, f, tol, u, work);

      /* print out residual norm ||A*u - f|| */
```

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```
        residual = gsl_splinalg_itersolve_normr(work);
        fprintf(stderr, "iter %zu residual = %.12e\n", iter, residual);

        if (status == GSL_SUCCESS)
          fprintf(stderr, "Converged\n");
      }
    while (status == GSL_CONTINUE && ++iter < max_iter);

    /* output solution */
    for (i = 0; i < n; ++i)
      {
        double xi = (i + 1) * h;
        double u_exact = sin(M_PI * xi);
        double u_gsl = gsl_vector_get(u, i);

        printf("%f %.12e %.12e\n", xi, u_gsl, u_exact);
      }

    gsl_splinalg_itersolve_free(work);
  }

  gsl_spmatrix_free(A);
  gsl_spmatrix_free(C);
  gsl_vector_free(f);
  gsl_vector_free(u);

  return 0;
} /* main() */
```

45.4 References and Further Reading

The implementation of the GMRES iterative solver closely follows the publications

- H. F. Walker, Implementation of the GMRES method using Householder transformations, SIAM J. Sci. Stat. Comput. 9(1), 1988.
- Y. Saad, Iterative methods for sparse linear systems, 2nd edition, SIAM, 2003.

CHAPTER

FORTYSIX

PHYSICAL CONSTANTS

This chapter describes macros for the values of physical constants, such as the speed of light, c, and gravitational constant, G. The values are available in different unit systems, including the standard MKSA system (meters, kilograms, seconds, amperes) and the CGSM system (centimeters, grams, seconds, gauss), which is commonly used in Astronomy.

The definitions of constants in the MKSA system are available in the file `gsl_const_mksa.h`. The constants in the CGSM system are defined in `gsl_const_cgsm.h`. Dimensionless constants, such as the fine structure constant, which are pure numbers are defined in `gsl_const_num.h`.

The full list of constants is described briefly below. Consult the header files themselves for the values of the constants used in the library.

46.1 Fundamental Constants

GSL_CONST_MKSA_SPEED_OF_LIGHT
The speed of light in vacuum, c.

GSL_CONST_MKSA_VACUUM_PERMEABILITY
The permeability of free space, μ_0. This constant is defined in the MKSA system only.

GSL_CONST_MKSA_VACUUM_PERMITTIVITY
The permittivity of free space, ϵ_0. This constant is defined in the MKSA system only.

GSL_CONST_MKSA_PLANCKS_CONSTANT_H
Planck's constant, h.

GSL_CONST_MKSA_PLANCKS_CONSTANT_HBAR
Planck's constant divided by 2π, $\hbar$.

GSL_CONST_NUM_AVOGADRO
Avogadro's number, N_a.

GSL_CONST_MKSA_FARADAY
The molar charge of 1 Faraday.

GSL_CONST_MKSA_BOLTZMANN
The Boltzmann constant, k.

GSL_CONST_MKSA_MOLAR_GAS
The molar gas constant, R_0.

GSL_CONST_MKSA_STANDARD_GAS_VOLUME
The standard gas volume, V_0.

GSL_CONST_MKSA_STEFAN_BOLTZMANN_CONSTANT
The Stefan-Boltzmann radiation constant, σ.

GSL_CONST_MKSA_GAUSS
The magnetic field of 1 Gauss.

46.2 Astronomy and Astrophysics

GSL_CONST_MKSA_ASTRONOMICAL_UNIT
The length of 1 astronomical unit (mean earth-sun distance), au.

GSL_CONST_MKSA_GRAVITATIONAL_CONSTANT
The gravitational constant, G.

GSL_CONST_MKSA_LIGHT_YEAR
The distance of 1 light-year, ly.

GSL_CONST_MKSA_PARSEC
The distance of 1 parsec, pc.

GSL_CONST_MKSA_GRAV_ACCEL
The standard gravitational acceleration on Earth, g.

GSL_CONST_MKSA_SOLAR_MASS
The mass of the Sun.

46.3 Atomic and Nuclear Physics

GSL_CONST_MKSA_ELECTRON_CHARGE
The charge of the electron, e.

GSL_CONST_MKSA_ELECTRON_VOLT
The energy of 1 electron volt, eV.

GSL_CONST_MKSA_UNIFIED_ATOMIC_MASS
The unified atomic mass, amu.

GSL_CONST_MKSA_MASS_ELECTRON
The mass of the electron, m_e.

GSL_CONST_MKSA_MASS_MUON
The mass of the muon, m_μ.

GSL_CONST_MKSA_MASS_PROTON
The mass of the proton, m_p.

GSL_CONST_MKSA_MASS_NEUTRON
The mass of the neutron, m_n.

GSL_CONST_NUM_FINE_STRUCTURE
The electromagnetic fine structure constant α.

GSL_CONST_MKSA_RYDBERG
The Rydberg constant, Ry, in units of energy. This is related to the Rydberg inverse wavelength R_∞ by $Ry = hcR_\infty$.

GSL_CONST_MKSA_BOHR_RADIUS
The Bohr radius, a_0.

GSL_CONST_MKSA_ANGSTROM
The length of 1 angstrom.

GSL_CONST_MKSA_BARN
The area of 1 barn.

GSL_CONST_MKSA_BOHR_MAGNETON
The Bohr Magneton, μ_B.

GSL_CONST_MKSA_NUCLEAR_MAGNETON
The Nuclear Magneton, μ_N.

GSL_CONST_MKSA_ELECTRON_MAGNETIC_MOMENT
The absolute value of the magnetic moment of the electron, μ_e. The physical magnetic moment of the electron is negative.

GSL_CONST_MKSA_PROTON_MAGNETIC_MOMENT
The magnetic moment of the proton, μ_p.

GSL_CONST_MKSA_THOMSON_CROSS_SECTION
The Thomson cross section, σ_T.

GSL_CONST_MKSA_DEBYE
The electric dipole moment of 1 Debye, D.

46.4 Measurement of Time

GSL_CONST_MKSA_MINUTE
The number of seconds in 1 minute.

GSL_CONST_MKSA_HOUR
The number of seconds in 1 hour.

GSL_CONST_MKSA_DAY
The number of seconds in 1 day.

GSL_CONST_MKSA_WEEK
The number of seconds in 1 week.

46.5 Imperial Units

GSL_CONST_MKSA_INCH
The length of 1 inch.

GSL_CONST_MKSA_FOOT
The length of 1 foot.

GSL_CONST_MKSA_YARD
The length of 1 yard.

GSL_CONST_MKSA_MILE
The length of 1 mile.

GSL_CONST_MKSA_MIL
The length of 1 mil (1/1000th of an inch).

46.6 Speed and Nautical Units

`GSL_CONST_MKSA_KILOMETERS_PER_HOUR`
The speed of 1 kilometer per hour.

`GSL_CONST_MKSA_MILES_PER_HOUR`
The speed of 1 mile per hour.

`GSL_CONST_MKSA_NAUTICAL_MILE`
The length of 1 nautical mile.

`GSL_CONST_MKSA_FATHOM`
The length of 1 fathom.

`GSL_CONST_MKSA_KNOT`
The speed of 1 knot.

46.7 Printers Units

`GSL_CONST_MKSA_POINT`
The length of 1 printer's point (1/72 inch).

`GSL_CONST_MKSA_TEXPOINT`
The length of 1 TeX point (1/72.27 inch).

46.8 Volume, Area and Length

`GSL_CONST_MKSA_MICRON`
The length of 1 micron.

`GSL_CONST_MKSA_HECTARE`
The area of 1 hectare.

`GSL_CONST_MKSA_ACRE`
The area of 1 acre.

`GSL_CONST_MKSA_LITER`
The volume of 1 liter.

`GSL_CONST_MKSA_US_GALLON`
The volume of 1 US gallon.

`GSL_CONST_MKSA_CANADIAN_GALLON`
The volume of 1 Canadian gallon.

`GSL_CONST_MKSA_UK_GALLON`
The volume of 1 UK gallon.

`GSL_CONST_MKSA_QUART`
The volume of 1 quart.

`GSL_CONST_MKSA_PINT`
The volume of 1 pint.

46.9 Mass and Weight

GSL_CONST_MKSA_POUND_MASS
The mass of 1 pound.

GSL_CONST_MKSA_OUNCE_MASS
The mass of 1 ounce.

GSL_CONST_MKSA_TON
The mass of 1 ton.

GSL_CONST_MKSA_METRIC_TON
The mass of 1 metric ton (1000 kg).

GSL_CONST_MKSA_UK_TON
The mass of 1 UK ton.

GSL_CONST_MKSA_TROY_OUNCE
The mass of 1 troy ounce.

GSL_CONST_MKSA_CARAT
The mass of 1 carat.

GSL_CONST_MKSA_GRAM_FORCE
The force of 1 gram weight.

GSL_CONST_MKSA_POUND_FORCE
The force of 1 pound weight.

GSL_CONST_MKSA_KILOPOUND_FORCE
The force of 1 kilopound weight.

GSL_CONST_MKSA_POUNDAL
The force of 1 poundal.

46.10 Thermal Energy and Power

GSL_CONST_MKSA_CALORIE
The energy of 1 calorie.

GSL_CONST_MKSA_BTU
The energy of 1 British Thermal Unit, btu.

GSL_CONST_MKSA_THERM
The energy of 1 Therm.

GSL_CONST_MKSA_HORSEPOWER
The power of 1 horsepower.

46.11 Pressure

`GSL_CONST_MKSA_BAR`
The pressure of 1 bar.

`GSL_CONST_MKSA_STD_ATMOSPHERE`
The pressure of 1 standard atmosphere.

`GSL_CONST_MKSA_TORR`
The pressure of 1 torr.

`GSL_CONST_MKSA_METER_OF_MERCURY`
The pressure of 1 meter of mercury.

`GSL_CONST_MKSA_INCH_OF_MERCURY`
The pressure of 1 inch of mercury.

`GSL_CONST_MKSA_INCH_OF_WATER`
The pressure of 1 inch of water.

`GSL_CONST_MKSA_PSI`
The pressure of 1 pound per square inch.

46.12 Viscosity

`GSL_CONST_MKSA_POISE`
The dynamic viscosity of 1 poise.

`GSL_CONST_MKSA_STOKES`
The kinematic viscosity of 1 stokes.

46.13 Light and Illumination

`GSL_CONST_MKSA_STILB`
The luminance of 1 stilb.

`GSL_CONST_MKSA_LUMEN`
The luminous flux of 1 lumen.

`GSL_CONST_MKSA_LUX`
The illuminance of 1 lux.

`GSL_CONST_MKSA_PHOT`
The illuminance of 1 phot.

`GSL_CONST_MKSA_FOOTCANDLE`
The illuminance of 1 footcandle.

`GSL_CONST_MKSA_LAMBERT`
The luminance of 1 lambert.

`GSL_CONST_MKSA_FOOTLAMBERT`
The luminance of 1 footlambert.

46.14 Radioactivity

`GSL_CONST_MKSA_CURIE`
The activity of 1 curie.

`GSL_CONST_MKSA_ROENTGEN`
The exposure of 1 roentgen.

`GSL_CONST_MKSA_RAD`
The absorbed dose of 1 rad.

46.15 Force and Energy

`GSL_CONST_MKSA_NEWTON`
The SI unit of force, 1 Newton.

`GSL_CONST_MKSA_DYNE`
The force of 1 Dyne = 10^{-5} Newton.

`GSL_CONST_MKSA_JOULE`
The SI unit of energy, 1 Joule.

`GSL_CONST_MKSA_ERG`
The energy 1 erg = 10^{-7} Joule.

46.16 Prefixes

These constants are dimensionless scaling factors.

`GSL_CONST_NUM_YOTTA`
10^{24}

`GSL_CONST_NUM_ZETTA`
10^{21}

`GSL_CONST_NUM_EXA`
10^{18}

`GSL_CONST_NUM_PETA`
10^{15}

`GSL_CONST_NUM_TERA`
10^{12}

`GSL_CONST_NUM_GIGA`
10^{9}

`GSL_CONST_NUM_MEGA`
10^{6}

`GSL_CONST_NUM_KILO`
10^{3}

`GSL_CONST_NUM_MILLI`
10^{-3}

GSL_CONST_NUM_MICRO
10^{-6}

GSL_CONST_NUM_NANO
10^{-9}

GSL_CONST_NUM_PICO
10^{-12}

GSL_CONST_NUM_FEMTO
10^{-15}

GSL_CONST_NUM_ATTO
10^{-18}

GSL_CONST_NUM_ZEPTO
10^{-21}

GSL_CONST_NUM_YOCTO
10^{-24}

46.17 Examples

The following program demonstrates the use of the physical constants in a calculation. In this case, the goal is to calculate the range of light-travel times from Earth to Mars.

The required data is the average distance of each planet from the Sun in astronomical units (the eccentricities and inclinations of the orbits will be neglected for the purposes of this calculation). The average radius of the orbit of Mars is 1.52 astronomical units, and for the orbit of Earth it is 1 astronomical unit (by definition). These values are combined with the MKSA values of the constants for the speed of light and the length of an astronomical unit to produce a result for the shortest and longest light-travel times in seconds. The figures are converted into minutes before being displayed.

```
#include <stdio.h>
#include <gsl/gsl_const_mksa.h>

int
main (void)
{
  double c  = GSL_CONST_MKSA_SPEED_OF_LIGHT;
  double au = GSL_CONST_MKSA_ASTRONOMICAL_UNIT;
  double minutes = GSL_CONST_MKSA_MINUTE;

  /* distance stored in meters */
  double r_earth = 1.00 * au;
  double r_mars  = 1.52 * au;

  double t_min, t_max;

  t_min = (r_mars - r_earth) / c;
  t_max = (r_mars + r_earth) / c;

  printf ("light travel time from Earth to Mars:\n");
  printf ("minimum = %.1f minutes\n", t_min / minutes);
  printf ("maximum = %.1f minutes\n", t_max / minutes);
```

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```
  return 0;
}
```

Here is the output from the program,

```
light travel time from Earth to Mars:
minimum = 4.3 minutes
maximum = 21.0 minutes
```

46.18 References and Further Reading

The authoritative sources for physical constants are the 2006 CODATA recommended values, published in the article below. Further information on the values of physical constants is also available from the NIST website.

- P.J. Mohr, B.N. Taylor, D.B. Newell, "CODATA Recommended Values of the Fundamental Physical Constants: 2006", Reviews of Modern Physics, 80(2), pp. 633–730 (2008).
- http://www.physics.nist.gov/cuu/Constants/index.html
- http://physics.nist.gov/Pubs/SP811/appenB9.html

CHAPTER

FORTYSEVEN

IEEE FLOATING-POINT ARITHMETIC

This chapter describes functions for examining the representation of floating point numbers and controlling the floating point environment of your program. The functions described in this chapter are declared in the header file `gsl_ieee_utils.h`.

47.1 Representation of floating point numbers

The IEEE Standard for Binary Floating-Point Arithmetic defines binary formats for single and double precision numbers. Each number is composed of three parts: a *sign bit* (s), an *exponent* (E) and a *fraction* (f). The numerical value of the combination (s, E, f) is given by the following formula,

$$(-1)^s(1 \cdot fffff \dots)2^E$$

The sign bit is either zero or one. The exponent ranges from a minimum value E_{min} to a maximum value E_{max} depending on the precision. The exponent is converted to an unsigned number e, known as the *biased exponent*, for storage by adding a *bias* parameter,

$$e = E + bias$$

The sequence $fffff$... represents the digits of the binary fraction f. The binary digits are stored in *normalized form*, by adjusting the exponent to give a leading digit of 1. Since the leading digit is always 1 for normalized numbers it is assumed implicitly and does not have to be stored. Numbers smaller than $2^{E_{min}}$ are be stored in *denormalized form* with a leading zero,

$$(-1)^s(0 \cdot fffff \dots)2^{E_{min}}$$

This allows gradual underflow down to $2^{E_{min}-p}$ for p bits of precision. A zero is encoded with the special exponent of $2^{E_{min}-1}$ and infinities with the exponent of $2^{E_{max}+1}$.

The format for single precision numbers uses 32 bits divided in the following way:

```
seeeeeeeefffffffffffffffffffffff

s = sign bit, 1 bit
e = exponent, 8 bits  (E_min=-126, E_max=127, bias=127)
f = fraction, 23 bits
```

The format for double precision numbers uses 64 bits divided in the following way:

```
seeeeeeeeeeeffffffffffffffffffffffffffffffffffffffffffffffffffff

s = sign bit, 1 bit
e = exponent, 11 bits  (E_min=-1022, E_max=1023, bias=1023)
f = fraction, 52 bits
```

It is often useful to be able to investigate the behavior of a calculation at the bit-level and the library provides functions for printing the IEEE representations in a human-readable form.

void **gsl_ieee_fprintf_float**(FILE *stream, const float *x)

void **gsl_ieee_fprintf_double**(FILE *stream, const double *x)

These functions output a formatted version of the IEEE floating-point number pointed to by *x* to the stream *stream*. A pointer is used to pass the number indirectly, to avoid any undesired promotion from `float` to `double`. The output takes one of the following forms,

`NaN`

the Not-a-Number symbol

`Inf, -Inf`

positive or negative infinity

`1.fffff...*2^E, -1.fffff...*2^E`

a normalized floating point number

`0.fffff...*2^E, -0.fffff...*2^E`

a denormalized floating point number

`0, -0`

positive or negative zero

The output can be used directly in GNU Emacs Calc mode by preceding it with `2#` to indicate binary.

void **gsl_ieee_printf_float**(const float *x)

void **gsl_ieee_printf_double**(const double *x)

These functions output a formatted version of the IEEE floating-point number pointed to by *x* to the stream `stdout`.

The following program demonstrates the use of the functions by printing the single and double precision representations of the fraction $1/3$. For comparison the representation of the value promoted from single to double precision is also printed.

```
#include <stdio.h>
#include <gsl/gsl_ieee_utils.h>

int
main (void)
{
  float f = 1.0/3.0;
  double d = 1.0/3.0;

  double fd = f; /* promote from float to double */

```

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```
  printf (" f="); gsl_ieee_printf_float(&f);
  printf ("\n");

  printf ("fd="); gsl_ieee_printf_double(&fd);
  printf ("\n");

  printf (" d="); gsl_ieee_printf_double(&d);
  printf ("\n");

  return 0;
}
```

The binary representation of $1/3$ is $0.01010101...$. The output below shows that the IEEE format normalizes this fraction to give a leading digit of 1:

```
 f= 1.01010101010101010101011*2^-2
fd= 1.0101010101010101010101100000000000000000000000000000*2^-2
 d= 1.0101010101010101010101010101010101010101010101010101*2^-2
```

The output also shows that a single-precision number is promoted to double-precision by adding zeros in the binary representation.

47.2 Setting up your IEEE environment

The IEEE standard defines several *modes* for controlling the behavior of floating point operations. These modes specify the important properties of computer arithmetic: the direction used for rounding (e.g. whether numbers should be rounded up, down or to the nearest number), the rounding precision and how the program should handle arithmetic exceptions, such as division by zero.

Many of these features can now be controlled via standard functions such as `fpsetround()`, which should be used whenever they are available. Unfortunately in the past there has been no universal API for controlling their behavior—each system has had its own low-level way of accessing them. To help you write portable programs GSL allows you to specify modes in a platform-independent way using the environment variable *GSL_IEEE_MODE*. The library then takes care of all the necessary machine-specific initializations for you when you call the function *gsl_ieee_env_setup()*.

GSL_IEEE_MODE

Environment variable which specifies IEEE mode.

void **gsl_ieee_env_setup**()

This function reads the environment variable *GSL_IEEE_MODE* and attempts to set up the corresponding specified IEEE modes. The environment variable should be a list of keywords, separated by commas, like this:

```
GSL_IEEE_MODE = "keyword, keyword, ..."
```

where `keyword` is one of the following mode-names:

```
single-precision
double-precision
extended-precision
round-to-nearest
round-down
```

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```
round-up
round-to-zero
mask-all
mask-invalid
mask-denormalized
mask-division-by-zero
mask-overflow
mask-underflow
trap-inexact
trap-common
```

If *GSL_IEEE_MODE* is empty or undefined then the function returns immediately and no attempt is made to change the system's IEEE mode. When the modes from *GSL_IEEE_MODE* are turned on the function prints a short message showing the new settings to remind you that the results of the program will be affected.

If the requested modes are not supported by the platform being used then the function calls the error handler and returns an error code of `GSL_EUNSUP`.

When options are specified using this method, the resulting mode is based on a default setting of the highest available precision (double precision or extended precision, depending on the platform) in round-to-nearest mode, with all exceptions enabled apart from the INEXACT exception. The INEXACT exception is generated whenever rounding occurs, so it must generally be disabled in typical scientific calculations. All other floating-point exceptions are enabled by default, including underflows and the use of denormalized numbers, for safety. They can be disabled with the individual `mask-` settings or together using `mask-all`.

The following adjusted combination of modes is convenient for many purposes:

```
GSL_IEEE_MODE="double-precision,"\
                "mask-underflow,"\
                  "mask-denormalized"
```

This choice ignores any errors relating to small numbers (either denormalized, or underflowing to zero) but traps overflows, division by zero and invalid operations.

Note that on the x86 series of processors this function sets both the original x87 mode and the newer MXCSR mode, which controls SSE floating-point operations. The SSE floating-point units do not have a precision-control bit, and always work in double-precision. The single-precision and extended-precision keywords have no effect in this case.

To demonstrate the effects of different rounding modes consider the following program which computes e, the base of natural logarithms, by summing a rapidly-decreasing series,

$$\begin{aligned} e &= \frac{1}{0!} + \frac{1}{1!} + \frac{1}{2!} + \frac{1}{3!} + \frac{1}{4!} + \dots \\ &= 2.71828182846... \end{aligned}$$

```
#include <stdio.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_ieee_utils.h>

int
main (void)
{
  double x = 1, oldsum = 0, sum = 0;
```

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```
  int i = 0;

  gsl_ieee_env_setup (); /* read GSL_IEEE_MODE */

  do
    {
      i++;

      oldsum = sum;
      sum += x;
      x = x / i;

      printf ("i=%2d sum=%.18f error=%g\n",
              i, sum, sum - M_E);

      if (i > 30)
         break;
    }
  while (sum != oldsum);

  return 0;
}
```

Here are the results of running the program in `round-to-nearest` mode. This is the IEEE default so it isn't really necessary to specify it here:

```
$ GSL_IEEE_MODE="round-to-nearest" ./a.out
i= 1 sum=1.000000000000000000 error=-1.71828
i= 2 sum=2.000000000000000000 error=-0.718282
....
i=18 sum=2.718281828459045535 error=4.44089e-16
i=19 sum=2.718281828459045535 error=4.44089e-16
```

After nineteen terms the sum converges to within 4×10^{-16} of the correct value. If we now change the rounding mode to `round-down` the final result is less accurate:

```
$ GSL_IEEE_MODE="round-down" ./a.out
i= 1 sum=1.000000000000000000 error=-1.71828
....
i=19 sum=2.718281828459041094 error=-3.9968e-15
```

The result is about 4×10^{-15} below the correct value, an order of magnitude worse than the result obtained in the `round-to-nearest` mode.

If we change to rounding mode to `round-up` then the final result is higher than the correct value (when we add each term to the sum the final result is always rounded up, which increases the sum by at least one tick until the added term underflows to zero). To avoid this problem we would need to use a safer converge criterion, such as `while (fabs(sum - oldsum) > epsilon)`, with a suitably chosen value of epsilon.

Finally we can see the effect of computing the sum using single-precision rounding, in the default `round-to-nearest` mode. In this case the program thinks it is still using double precision numbers but the CPU rounds the result of each floating point operation to single-precision accuracy. This simulates the effect of writing the program using single-precision `float` variables instead of `double` variables. The iteration stops after about half the number of iterations and the final result is much less accurate:

```
$ GSL_IEEE_MODE="single-precision" ./a.out
....
i=12 sum=2.718281984329223633 error=1.5587e-07
```

with an error of $O(10^{-7})$, which corresponds to single precision accuracy (about 1 part in 10^7). Continuing the iterations further does not decrease the error because all the subsequent results are rounded to the same value.

47.3 References and Further Reading

The reference for the IEEE standard is,

- ANSI/IEEE Std 754-1985, IEEE Standard for Binary Floating-Point Arithmetic.

A more pedagogical introduction to the standard can be found in the following paper,

- David Goldberg: What Every Computer Scientist Should Know About Floating-Point Arithmetic. *ACM Computing Surveys*, Vol.: 23, No.: 1 (March 1991), pages 5–48.
- Corrigendum: *ACM Computing Surveys*, Vol.: 23, No.: 3 (September 1991), page 413. and see also the sections by B. A. Wichmann and Charles B. Dunham in Surveyor's Forum: "What Every Computer Scientist Should Know About Floating-Point Arithmetic". *ACM Computing Surveys*, Vol.: 24, No.: 3 (September 1992), page 319.

A detailed textbook on IEEE arithmetic and its practical use is available from SIAM Press,

- Michael L. Overton, *Numerical Computing with IEEE Floating Point Arithmetic*, SIAM Press, ISBN 0898715717.

CHAPTER

FORTYEIGHT

DEBUGGING NUMERICAL PROGRAMS

This chapter describes some tips and tricks for debugging numerical programs which use GSL.

48.1 Using gdb

Any errors reported by the library are passed to the function `gsl_error()`. By running your programs under gdb and setting a breakpoint in this function you can automatically catch any library errors. You can add a breakpoint for every session by putting:

```
break gsl_error
```

into your `.gdbinit` file in the directory where your program is started.

If the breakpoint catches an error then you can use a backtrace (`bt`) to see the call-tree, and the arguments which possibly caused the error. By moving up into the calling function you can investigate the values of variables at that point. Here is an example from the program `fft/test_trap`, which contains the following line:

```
status = gsl_fft_complex_wavetable_alloc (0, &complex_wavetable);
```

The function *gsl_fft_complex_wavetable_alloc()* takes the length of an FFT as its first argument. When this line is executed an error will be generated because the length of an FFT is not allowed to be zero.

To debug this problem we start `gdb`, using the file `.gdbinit` to define a breakpoint in `gsl_error()`:

```
$ gdb test_trap

GDB is free software and you are welcome to distribute copies
of it under certain conditions; type "show copying" to see
the conditions.  There is absolutely no warranty for GDB;
type "show warranty" for details.  GDB 4.16 (i586-debian-linux),
Copyright 1996 Free Software Foundation, Inc.

Breakpoint 1 at 0x8050b1e: file error.c, line 14.
```

When we run the program this breakpoint catches the error and shows the reason for it:

```
(gdb) run
Starting program: test_trap

Breakpoint 1, gsl_error (reason=0x8052b0d
    "length n must be positive integer",
```

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```
    file=0x8052b04 "c_init.c", line=108, gsl_errno=1)
    at error.c:14
14        if (gsl_error_handler)
```

The first argument of `gsl_error()` is always a string describing the error. Now we can look at the backtrace to see what caused the problem:

```
(gdb) bt
#0  gsl_error (reason=0x8052b0d
    "length n must be positive integer",
    file=0x8052b04 "c_init.c", line=108, gsl_errno=1)
    at error.c:14
#1  0x8049376 in gsl_fft_complex_wavetable_alloc (n=0,
    wavetable=0xbffff778) at c_init.c:108
#2  0x8048a00 in main (argc=1, argv=0xbffff9bc)
    at test_trap.c:94
#3  0x80488be in ___crt_dummy__ ()
```

We can see that the error was generated in the function *gsl_fft_complex_wavetable_alloc()* when it was called with an argument of `n = 0`. The original call came from line 94 in the file `test_trap.c`.

By moving up to the level of the original call we can find the line that caused the error:

```
(gdb) up
#1  0x8049376 in gsl_fft_complex_wavetable_alloc (n=0,
    wavetable=0xbffff778) at c_init.c:108
108   GSL_ERROR ("length n must be positive integer", GSL_EDOM);
(gdb) up
#2  0x8048a00 in main (argc=1, argv=0xbffff9bc)
  at test_trap.c:94
94    status = gsl_fft_complex_wavetable_alloc (0,
        &complex_wavetable);
```

Thus we have found the line that caused the problem. From this point we could also print out the values of other variables such as `complex_wavetable`.

48.2 Examining floating point registers

The contents of floating point registers can be examined using the command `info float` (on supported platforms):

```
(gdb) info float
     st0: 0xc4018b895aa17a945000  Valid Normal -7.838871e+308
     st1: 0x3ff9ea3f50e4d7275000  Valid Normal 0.0285946
     st2: 0x3fe790c64ce27dad4800  Valid Normal 6.7415931e-08
     st3: 0x3ffaa3ef0df6607d7800  Spec  Normal 0.0400229
     st4: 0x3c028000000000000000  Valid Normal 4.4501477e-308
     st5: 0x3ffef5412c22219d9000  Zero  Normal 0.9580257
     st6: 0x3fff8000000000000000  Valid Normal 1
     st7: 0xc4028b65a1f6d243c800  Valid Normal -1.566206e+309
   fctrl: 0x0272 53 bit; NEAR; mask DENOR UNDER LOS;
   fstat: 0xb9ba flags 0001; top 7; excep DENOR OVERF UNDER LOS
```

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```
    ftag: 0x3fff
     fip: 0x08048b5c
     fcs: 0x051a0023
  fopoff: 0x08086820
  fopsel: 0x002b
```

Individual registers can be examined using the variables `$reg`, where `reg` is the register name:

```
(gdb) p $st1
$1 = 0.02859464454261210347719
```

48.3 Handling floating point exceptions

It is possible to stop the program whenever a `SIGFPE` floating point exception occurs. This can be useful for finding the cause of an unexpected infinity or `NaN`. The current handler settings can be shown with the command `info signal SIGFPE`:

```
(gdb) info signal SIGFPE
Signal  Stop  Print  Pass to program Description
SIGFPE  Yes   Yes    Yes             Arithmetic exception
```

Unless the program uses a signal handler the default setting should be changed so that SIGFPE is not passed to the program, as this would cause it to exit. The command `handle SIGFPE stop nopass` prevents this:

```
(gdb) handle SIGFPE stop nopass
Signal  Stop  Print  Pass to program Description
SIGFPE  Yes   Yes    No              Arithmetic exception
```

Depending on the platform it may be necessary to instruct the kernel to generate signals for floating point exceptions. For programs using GSL this can be achieved using the *`GSL_IEEE_MODE`* environment variable in conjunction with the function *`gsl_ieee_env_setup()`* as described in *IEEE floating-point arithmetic*:

```
(gdb) set env GSL_IEEE_MODE=double-precision
```

48.4 GCC warning options for numerical programs

Writing reliable numerical programs in C requires great care. The following GCC warning options are recommended when compiling numerical programs:

```
gcc -ansi -pedantic -Werror -Wall -W
  -Wmissing-prototypes -Wstrict-prototypes
  -Wconversion -Wshadow -Wpointer-arith
  -Wcast-qual -Wcast-align
  -Wwrite-strings -Wnested-externs
  -fshort-enums -fno-common -Dinline= -g -O2
```

For details of each option consult the manual *Using and Porting GCC*. The following table gives a brief explanation of what types of errors these options catch.

`-ansi -pedantic`

Use ANSI C, and reject any non-ANSI extensions. These flags help in writing portable programs that will compile on other systems.

`-Werror`

Consider warnings to be errors, so that compilation stops. This prevents warnings from scrolling off the top of the screen and being lost. You won't be able to compile the program until it is completely warning-free.

`-Wall`

This turns on a set of warnings for common programming problems. You need `-Wall`, but it is not enough on its own.

`-O2`

Turn on optimization. The warnings for uninitialized variables in `-Wall` rely on the optimizer to analyze the code. If there is no optimization then these warnings aren't generated.

`-W`

This turns on some extra warnings not included in `-Wall`, such as missing return values and comparisons between signed and unsigned integers.

`-Wmissing-prototypes -Wstrict-prototypes`

Warn if there are any missing or inconsistent prototypes. Without prototypes it is harder to detect problems with incorrect arguments.

`-Wconversion`

The main use of this option is to warn about conversions from signed to unsigned integers. For example, `unsigned int x = -1`. If you need to perform such a conversion you can use an explicit cast.

`-Wshadow`

This warns whenever a local variable shadows another local variable. If two variables have the same name then it is a potential source of confusion.

`-Wpointer-arith -Wcast-qual -Wcast-align`

These options warn if you try to do pointer arithmetic for types which don't have a size, such as `void`, if you remove a `const` cast from a pointer, or if you cast a pointer to a type which has a different size, causing an invalid alignment.

`-Wwrite-strings`

This option gives string constants a `const` qualifier so that it will be a compile-time error to attempt to overwrite them.

`-fshort-enums`

This option makes the type of `enum` as short as possible. Normally this makes an `enum` different from an `int`. Consequently any attempts to assign a pointer-to-int to a pointer-to-enum will generate a cast-alignment warning.

`-fno-common`

This option prevents global variables being simultaneously defined in different object files (you get an error at link time). Such a variable should be defined in one file and referred to in other files with an `extern` declaration.

`-Wnested-externs`

This warns if an `extern` declaration is encountered within a function.

`-Dinline=`

The `inline` keyword is not part of ANSI C. Thus if you want to use `-ansi` with a program which uses inline functions you can use this preprocessor definition to remove the `inline` keywords.

`-g`

It always makes sense to put debugging symbols in the executable so that you can debug it using `gdb`. The only effect of debugging symbols is to increase the size of the file, and you can use the `strip` command to remove them later if necessary.

48.5 References and Further Reading

The following books are essential reading for anyone writing and debugging numerical programs with `gcc` and `gdb`.

- R.M. Stallman, *Using and Porting GNU CC*, Free Software Foundation, ISBN 1882114388
- R.M. Stallman, R.H. Pesch, *Debugging with GDB: The GNU Source-Level Debugger*, Free Software Foundation, ISBN 1882114779

For a tutorial introduction to the GNU C Compiler and related programs, see

- B.J. Gough, http://www.network-theory.co.uk/gcc/intro/,' *An Introduction to GCC*, Network Theory Ltd, ISBN 0954161793

CHAPTER

FORTYNINE

CONTRIBUTORS TO GSL

(See the AUTHORS file in the distribution for up-to-date information.)

Mark Galassi

Conceived GSL (with James Theiler) and wrote the design document. Wrote the simulated annealing package and the relevant chapter in the manual.

James Theiler

Conceived GSL (with Mark Galassi). Wrote the random number generators and the relevant chapter in this manual.

Jim Davies

Wrote the statistical routines and the relevant chapter in this manual.

Brian Gough

FFTs, numerical integration, random number generators and distributions, root finding, minimization and fitting, polynomial solvers, complex numbers, physical constants, permutations, vector and matrix functions, histograms, statistics, ieee-utils, revised CBLAS Level 2 & 3, matrix decompositions, eigensystems, cumulative distribution functions, testing, documentation and releases.

Reid Priedhorsky

Wrote and documented the initial version of the root finding routines while at Los Alamos National Laboratory, Mathematical Modeling and Analysis Group.

Gerard Jungman

Special Functions, Series acceleration, ODEs, BLAS, Linear Algebra, Eigensystems, Hankel Transforms.

Patrick Alken

Implementation of nonsymmetric and generalized eigensystems, B-splines, linear and nonlinear least squares, matrix decompositions, associated Legendre functions, running statistics, sparse matrices, and sparse linear algebra.

Mike Booth

Wrote the Monte Carlo library.

Jorma Olavi Tähtinen

Wrote the initial complex arithmetic functions.

Thomas Walter

Wrote the initial heapsort routines and Cholesky decomposition.

Fabrice Rossi

Multidimensional minimization.

Carlo Perassi

Implementation of the random number generators in Knuth's *Seminumerical Algorithms*, 3rd Ed.

Szymon Jaroszewicz

Wrote the routines for generating combinations.

Nicolas Darnis

Wrote the cyclic functions and the initial functions for canonical permutations.

Jason H. Stover

Wrote the major cumulative distribution functions.

Ivo Alxneit

Wrote the routines for wavelet transforms.

Tuomo Keskitalo

Improved the implementation of the ODE solvers and wrote the ode-initval2 routines.

Lowell Johnson

Implementation of the Mathieu functions.

Rhys Ulerich

Wrote the multiset routines.

Pavel Holoborodko

Wrote the fixed order Gauss-Legendre quadrature routines.

Pedro Gonnet

Wrote the CQUAD integration routines.

Thanks to Nigel Lowry for help in proofreading the manual.

The non-symmetric eigensystems routines contain code based on the LAPACK linear algebra library. LAPACK is distributed under the following license:

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CHAPTER

FIFTY

AUTOCONF MACROS

For applications using `autoconf` the standard macro `AC_CHECK_LIB` can be used to link with GSL automatically from a `configure` script. The library itself depends on the presence of a CBLAS and math library as well, so these must also be located before linking with the main `libgsl` file. The following commands should be placed in the `configure.ac` file to perform these tests:

```
AC_CHECK_LIB([m],[cos])
AC_CHECK_LIB([gslcblas],[cblas_dgemm])
AC_CHECK_LIB([gsl],[gsl_blas_dgemm])
```

It is important to check for `libm` and `libgslcblas` before `libgsl`, otherwise the tests will fail. Assuming the libraries are found the output during the configure stage looks like this:

```
checking for cos in -lm... yes
checking for cblas_dgemm in -lgslcblas... yes
checking for gsl_blas_dgemm in -lgsl... yes
```

If the library is found then the tests will define the macros `HAVE_LIBGSL`, `HAVE_LIBGSLCBLAS`, `HAVE_LIBM` and add the options `-lgsl -lgslcblas -lm` to the variable `LIBS`.

The tests above will find any version of the library. They are suitable for general use, where the versions of the functions are not important. An alternative macro is available in the file `gsl.m4` to test for a specific version of the library. To use this macro simply add the following line to your `configure.in` file instead of the tests above:

```
AX_PATH_GSL(GSL_VERSION,
           [action-if-found],
           [action-if-not-found])
```

The argument `GSL_VERSION` should be the two or three digit `major.minor` or `major.minor.micro` version number of the release you require. A suitable choice for `action-if-not-found` is:

```
AC_MSG_ERROR(could not find required version of GSL)
```

Then you can add the variables `GSL_LIBS` and `GSL_CFLAGS` to your Makefile.am files to obtain the correct compiler flags. `GSL_LIBS` is equal to the output of the `gsl-config --libs` command and `GSL_CFLAGS` is equal to `gsl-config --cflags` command. For example:

```
libfoo_la_LDFLAGS = -lfoo $(GSL_LIBS) -lgslcblas
```

Note that the macro `AX_PATH_GSL` needs to use the C compiler so it should appear in the `configure.in` file before the macro `AC_LANG_CPLUSPLUS` for programs that use C++.

To test for `inline` the following test should be placed in your `configure.in` file:

```
AC_C_INLINE

if test "$ac_cv_c_inline" != no ; then
  AC_DEFINE(HAVE_INLINE,1)
  AC_SUBST(HAVE_INLINE)
fi
```

and the macro will then be defined in the compilation flags or by including the file `config.h` before any library headers.

The following autoconf test will check for `extern inline`:

```
dnl Check for "extern inline", using a modified version
dnl of the test for AC_C_INLINE from acspecific.mt
dnl
AC_CACHE_CHECK([for extern inline], ac_cv_c_extern_inline,
[ac_cv_c_extern_inline=no
AC_TRY_COMPILE([extern $ac_cv_c_inline double foo(double x);
extern $ac_cv_c_inline double foo(double x) { return x+1.0; };
double foo (double x) { return x + 1.0; };],
[  foo(1.0)  ],
[ac_cv_c_extern_inline="yes"])
])

if test "$ac_cv_c_extern_inline" != no ; then
  AC_DEFINE(HAVE_INLINE,1)
  AC_SUBST(HAVE_INLINE)
fi
```

The substitution of portability functions can be made automatically if you use `autoconf`. For example, to test whether the BSD function `hypot()` is available you can include the following line in the configure file `configure.in` for your application:

```
AC_CHECK_FUNCS(hypot)
```

and place the following macro definitions in the file `config.h.in`:

```
/* Substitute gsl_hypot for missing system hypot */

#ifndef HAVE_HYPOT
#define hypot gsl_hypot
#endif
```

The application source files can then use the include command `#include <config.h>` to substitute *`gsl_hypot()`* for each occurrence of `hypot()` when `hypot()` is not available.

CHAPTER

FIFTYONE

GSL CBLAS LIBRARY

The prototypes for the low-level CBLAS functions are declared in the file `gsl_cblas.h`. For the definition of the functions consult the documentation available from Netlib (*see BLAS References and Further Reading*).

51.1 Level 1

float **cblas_sdsdot**(const int N, const float alpha, const float *x, const int incx, const float *y, const int incy)

double **cblas_dsdot**(const int N, const float *x, const int incx, const float *y, const int incy)

float **cblas_sdot**(const int N, const float *x, const int incx, const float *y, const int incy)

double **cblas_ddot**(const int N, const double *x, const int incx, const double *y, const int incy)

void **cblas_cdotu_sub**(const int N, const void *x, const int incx, const void *y, const int incy, void *dotu)

void **cblas_cdotc_sub**(const int N, const void *x, const int incx, const void *y, const int incy, void *dotc)

void **cblas_zdotu_sub**(const int N, const void *x, const int incx, const void *y, const int incy, void *dotu)

void **cblas_zdotc_sub**(const int N, const void *x, const int incx, const void *y, const int incy, void *dotc)

float **cblas_snrm2**(const int N, const float *x, const int incx)

float **cblas_sasum**(const int N, const float *x, const int incx)

double **cblas_dnrm2**(const int N, const double *x, const int incx)

double **cblas_dasum**(const int N, const double *x, const int incx)

float **cblas_scnrm2**(const int N, const void *x, const int incx)

float **cblas_scasum**(const int N, const void *x, const int incx) double **cblas_dznrm2**(const int N, const void *x, const int incx)

double **cblas_dzasum**(const int N, const void *x, const int incx)

CBLAS_INDEX **cblas_isamax**(const int N, const float *x, const int incx)

CBLAS_INDEX **cblas_idamax**(const int N, const double *x, const int incx)

CBLAS_INDEX **cblas_icamax**(const int N, const void *x, const int incx)

CBLAS_INDEX **cblas_izamax**(const int N, const void *x, const int incx)

void **cblas_sswap**(const int N, float *x, const int incx, float *y, const int incy)

void **cblas_scopy**(const int N, const float *x, const int incx, float *y, const int incy)

void **cblas_saxpy**(const int N, const float alpha, const float *x, const int incx, float *y, const int incy)

void **cblas_dswap**(const int N, double *x, const int incx, double *y, const int incy)

void **cblas_dcopy**(const int N, const double *x, const int incx, double *y, const int incy)

void **cblas_daxpy**(const int N, const double alpha, const double *x, const int incx, double *y, const int incy)

void **cblas_cswap**(const int N, void *x, const int incx, void *y, const int incy)

void **cblas_ccopy**(const int N, const void *x, const int incx, void *y, const int incy)

void **cblas_caxpy**(const int N, const void *alpha, const void *x, const int incx, void *y, const int incy)

void **cblas_zswap**(const int N, void *x, const int incx, void *y, const int incy)

void **cblas_zcopy**(const int N, const void *x, const int incx, void *y, const int incy)

void **cblas_zaxpy**(const int N, const void *alpha, const void *x, const int incx, void *y, const int incy)

void **cblas_srotg**(float *a, float *b, float *c, float *s)

void **cblas_srotmg**(float *d1, float *d2, float *b1, const float b2, float *P)

void **cblas_srot**(const int N, float *x, const int incx, float *y, const int incy, const float c, const float s) void **cblas_srotm**(const int N, float *x, const int incx, float *y, const int incy, const float *P)

void **cblas_drotg**(double *a, double *b, double *c, double *s)

void **cblas_drotmg**(double *d1, double *d2, double *b1, const double b2, double *P)

void **cblas_drot**(const int N, double *x, const int incx, double *y, const int incy, const double c, const double s)

void **cblas_drotm**(const int N, double *x, const int incx, double *y, const int incy, const double *P)

void **cblas_sscal**(const int N, const float alpha, float *x, const int incx)

void **cblas_dscal**(const int N, const double alpha, double *x, const int incx)

void **cblas_cscal**(const int N, const void *alpha, void *x, const int incx)

void **cblas_zscal**(const int N, const void *alpha, void *x, const int incx)

void **cblas_csscal**(const int N, const float alpha, void *x, const int incx)

void **cblas_zdscal**(const int N, const double alpha, void *x, const int incx)

51.2 Level 2

void **cblas_sgemv**(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const float alpha, const float *A, const int lda, const float *x, const int incx, const float beta, float *y, const int incy)

void **cblas_sgbmv**(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const int KL, const int KU, const float alpha, const float *A, const int lda, const float *x, const int incx, const float beta, float *y, const int incy)

void **cblas_strmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const float *A, const int lda, float *x, const int incx)

void **cblas_stbmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const float *A, const int lda, float *x, const int incx)

void **cblas_stpmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const float *Ap, float *x, const int incx) void `cblas_strsv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const float *A, const int lda, float *x, const int incx)

void `cblas_stbsv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const float *A, const int lda, float *x, const int incx)

void `cblas_stpsv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const float *Ap, float *x, const int incx)

void `cblas_dgemv`(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const double alpha, const double *A, const int lda, const double *x, const int incx, const double beta, double *y, const int incy)

void `cblas_dgbmv`(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const int KL, const int KU, const double alpha, const double *A, const int lda, const double *x, const int incx, const double beta, double *y, const int incy)

void `cblas_dtrmv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const double *A, const int lda, double *x, const int incx)

void `cblas_dtbmv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const double *A, const int lda, double *x, const int incx)

void `cblas_dtpmv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const double *Ap, double *x, const int incx)

void `cblas_dtrsv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const double *A, const int lda, double *x, const int incx)

void `cblas_dtbsv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const double *A, const int lda, double *x, const int incx)

void `cblas_dtpsv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const double *Ap, double *x, const int incx)

void `cblas_cgemv`(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const void *alpha, const void *A, const int lda, const void *x, const int incx, const void *beta, void *y, const int incy) void `cblas_cgbmv`(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const int KL, const int KU, const void *alpha, const void *A, const int lda, const void *x, const int incx, const void *beta, void *y, const int incy)

void `cblas_ctrmv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const void *A, const int lda, void *x, const int incx)

void `cblas_ctbmv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const void *A, const int lda, void *x, const int incx)

void `cblas_ctpmv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const void *Ap, void *x, const int incx)

void `cblas_ctrsv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const void *A, const int lda, void *x, const int incx)

void `cblas_ctbsv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const void *A, const int lda, void *x, const int incx)

void `cblas_ctpsv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const void *Ap, void *x, const int incx)

void `cblas_zgemv`(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const void *alpha, const void *A, const int lda, const void *x, const int incx, const void *beta, void *y, const int incy)

void `cblas_zgbmv`(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const int KL, const int KU, const void *alpha, const void *A, const int lda, const void *x, const int incx, const void *beta, void *y, const int incy)

void `cblas_ztrmv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const void *A, const int lda, void *x, const int incx)

void `cblas_ztbmv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const void *A, const int lda, void *x, const int incx)

void `cblas_ztpmv`(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const void *Ap, void *x, const int incx) void **cblas_ztrsv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const void *A, const int lda, void *x, const int incx)

void **cblas_ztbsv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const void *A, const int lda, void *x, const int incx)

void **cblas_ztpsv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const void *Ap, void *x, const int incx)

void **cblas_ssymv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *A, const int lda, const float *x, const int incx, const float beta, float *y, const int incy)

void **cblas_ssbmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const int K, const float alpha, const float *A, const int lda, const float *x, const int incx, const float beta, float *y, const int incy)

void **cblas_sspmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *Ap, const float *x, const int incx, const float beta, float *y, const int incy)

void **cblas_sger**(const enum CBLAS_ORDER order, const int M, const int N, const float alpha, const float *x, const int incx, const float *y, const int incy, float *A, const int lda)

void **cblas_ssyr**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *x, const int incx, float *A, const int lda)

void **cblas_sspr**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *x, const int incx, float *Ap)

void **cblas_ssyr2**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *x, const int incx, const float *y, const int incy, float *A, const int lda)

void **cblas_sspr2**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *x, const int incx, const float *y, const int incy, float *A)

void **cblas_dsymv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *A, const int lda, const double *x, const int incx, const double beta, double *y, const int incy)

void **cblas_dsbmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const int K, const double alpha, const double *A, const int lda, const double *x, const int incx, const double beta, double *y, const int incy) void **cblas_dspmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *Ap, const double *x, const int incx, const double beta, double *y, const int incy)

void **cblas_dger**(const enum CBLAS_ORDER order, const int M, const int N, const double alpha, const double *x, const int incx, const double *y, const int incy, double *A, const int lda)

void **cblas_dsyr**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *x, const int incx, double *A, const int lda)

void **cblas_dspr**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *x, const int incx, double *Ap)

void **cblas_dsyr2**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *x, const int incx, const double *y, const int incy, double *A, const int lda)

void **cblas_dspr2**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *x, const int incx, const double *y, const int incy, double *A)

void **cblas_chemv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *A, const int lda, const void *x, const int incx, const void *beta, void *y, const int incy)

void **cblas_chbmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const int K, const void *alpha, const void *A, const int lda, const void *x, const int incx, const void *beta, void *y, const int incy)

void **cblas_chpmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *Ap, const void *x, const int incx, const void *beta, void *y, const int incy)

void **cblas_cgeru**(const enum CBLAS_ORDER order, const int M, const int N, const void *alpha, const void *x, const int incx, const void *y, const int incy, void *A, const int lda)

void **cblas_cgerc**(const enum CBLAS_ORDER order, const int M, const int N, const void *alpha, const void *x, const int incx, const void *y, const int incy, void *A, const int lda)

void **cblas_cher**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const void *x, const int incx, void *A, const int lda)

void **cblas_chpr**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const void *x, const int incx, void *A)

void **cblas_cher2**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *x, const int incx, const void *y, const int incy, void *A, const int lda) void **cblas_chpr2**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *x, const int incx, const void *y, const int incy, void *Ap)

void **cblas_zhemv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *A, const int lda, const void *x, const int incx, const void *beta, void *y, const int incy)

void **cblas_zhbmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const int K, const void *alpha, const void *A, const int lda, const void *x, const int incx, const void *beta, void *y, const int incy)

void **cblas_zhpmv**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *Ap, const void *x, const int incx, const void *beta, void *y, const int incy)

void **cblas_zgeru**(const enum CBLAS_ORDER order, const int M, const int N, const void *alpha, const void *x, const int incx, const void *y, const int incy, void *A, const int lda)

void **cblas_zgerc**(const enum CBLAS_ORDER order, const int M, const int N, const void *alpha, const void *x, const int incx, const void *y, const int incy, void *A, const int lda)

void **cblas_zher**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const void *x, const int incx, void *A, const int lda)

void **cblas_zhpr**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const void *x, const int incx, void *A)

void **cblas_zher2**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *x, const int incx, const void *y, const int incy, void *A, const int lda)

void **cblas_zhpr2**(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *x, const int incx, const void *y, const int incy, void *Ap)

51.3 Level 3

void **cblas_sgemm**(const enum CBLAS_ORDER Order, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_TRANSPOSE TransB, const int M, const int N, const int K, const float alpha, const float *A, const int lda, const float *B, const int ldb, const float beta, float *C, const int ldc)

void **cblas_ssymm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const float alpha, const float *A, const int lda, const float *B, const int ldb, const float beta, float *C, const int ldc)

void **cblas_ssyrk**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const float alpha, const float *A, const int lda, const float beta, float *C, const int ldc) void **cblas_ssyr2k**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const float alpha, const float *A, const int lda, const float *B, const int ldb, const float beta, float *C, const int ldc)

void **cblas_strmm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const float alpha, const float *A, const int lda, float *B, const int ldb)

void **cblas_strsm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const float alpha, const float *A, const int lda, float *B, const int ldb)

void **cblas_dgemm**(const enum CBLAS_ORDER Order, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_TRANSPOSE TransB, const int M, const int N, const int K, const double alpha, const double *A, const int lda, const double *B, const int ldb, const double beta, double *C, const int ldc)

void **cblas_dsymm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const double alpha, const double *A, const int lda, const double *B, const int ldb, const double beta, double *C, const int ldc)

void **cblas_dsyrk**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const double alpha, const double *A, const int lda, const double beta, double *C, const int ldc)

void **cblas_dsyr2k**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const double alpha, const double *A, const int lda, const double *B, const int ldb, const double beta, double *C, const int ldc)

void **cblas_dtrmm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const double alpha, const double *A, const int lda, double *B, const int ldb)

void **cblas_dtrsm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const double alpha, const double *A, const int lda, double *B, const int ldb)

void **cblas_cgemm**(const enum CBLAS_ORDER Order, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_TRANSPOSE TransB, const int M, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc)

void **cblas_csymm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc) void **cblas_csyrk**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *beta, void *C, const int ldc)

void **cblas_csyr2k**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc)

void **cblas_ctrmm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const void *alpha, const void *A, const int lda, void *B, const int ldb)

void **cblas_ctrsm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const void *alpha, const void *A, const int lda, void *B, const int ldb)

void **cblas_zgemm**(const enum CBLAS_ORDER Order, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_TRANSPOSE TransB, const int M, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc)

void **cblas_zsymm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc)

void **cblas_zsyrk**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *beta, void *C, const int ldc)

void **cblas_zsyr2k**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc)

void **cblas_ztrmm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const void *alpha, const void *A, const int lda, void *B, const int ldb)

void **cblas_ztrsm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const void *alpha, const void *A, const int lda, void *B, const int ldb)

void **cblas_chemm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc) void **cblas_cherk**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const float alpha, const void *A, const int lda, const float beta, void *C, const int ldc)

void **cblas_cher2k**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const float beta, void *C, const int ldc)

void **cblas_zhemm**(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc)

void **cblas_zherk**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const double alpha, const void *A, const int lda, const double beta, void *C, const int ldc)

void **cblas_zher2k**(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const double beta, void *C, const int ldc)

void **cblas_xerbla**(int p, const char *rout, const char *form, ...)

51.4 Examples

The following program computes the product of two matrices using the Level-3 BLAS function SGEMM,

$$\begin{pmatrix} 0.11 & 0.12 & 0.13 \\ 0.21 & 0.22 & 0.23 \end{pmatrix} \begin{pmatrix} 1011 & 1012 \\ 1021 & 1022 \\ 1031 & 1032 \end{pmatrix} = \begin{pmatrix} 367.76 & 368.12 \\ 674.06 & 674.72 \end{pmatrix}$$

The matrices are stored in row major order but could be stored in column major order if the first argument of the call to *cblas_sgemm()* was changed to `CblasColMajor`.

```
#include <stdio.h>
#include <gsl/gsl_cblas.h>

int
main (void)
{
  int lda = 3;

  float A[] = { 0.11, 0.12, 0.13,
                0.21, 0.22, 0.23 };

  int ldb = 2;

  float B[] = { 1011, 1012,
                1021, 1022,
                1031, 1032 };
```

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```
  int ldc = 2;

  float C[] = { 0.00, 0.00,
                0.00, 0.00 };

  /* Compute C = A B */

  cblas_sgemm (CblasRowMajor,
               CblasNoTrans, CblasNoTrans, 2, 2, 3,
               1.0, A, lda, B, ldb, 0.0, C, ldc);

  printf ("[ %g, %g\n", C[0], C[1]);
  printf ("  %g, %g ]\n", C[2], C[3]);

  return 0;
}
```

To compile the program use the following command line:

```
$ gcc -Wall demo.c -lgslcblas
```

There is no need to link with the main library `-lgsl` in this case as the CBLAS library is an independent unit. Here is the output from the program,

```
[ 367.76, 368.12
  674.06, 674.72 ]
```

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