GNU Scientific Library

Reference Manual
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The Texinfo source for this manual may be obtained from `ftp.gnu.org` in the directory `/gnu/gsl/`.

1 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	BLAS Support
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

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.

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 give away copies of any programs related to 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 related code which uses the GNU Scientific Library, you must give the recipients all the rights that you have. You must make sure that they, too, receive or can get the source code. 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 (see [GNU General Public License], page 419). Further information about this license is available from the GNU Project webpage *Frequently Asked Questions about the GNU GPL*,

```
http://www.gnu.org/copyleft/gpl-faq.html
```

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 compiles on most Unix platforms. It is also available for Microsoft Windows. Precompiled versions of the library can be purchased from commercial redistributors listed on the website.

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

```
To: gsl-announce-request@sources.redhat.com
Subject: subscribe
```

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

1.4 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,

```
J0(5) = -1.775967713143382920e-01
```

The steps needed to compile programs which use the library are described in the next chapter.

1.5 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. Consult the GNU General Public license for further details (see [GNU General Public License], page 419).

1.6 Further Information

Additional information, including online copies of this manual, links to related projects, and mailing list archives are available from the development website mentioned above. The developers of the library can be reached via the project's public mailing list,

```
gsl-discuss@sources.redhat.com
```

This mailing list can be used to ask questions not covered by this manual.

2 Using the library

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

2.1 ANSI C Compliance

The library is written in ANSI C and is intended to conform to the ANSI C standard. 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_`.

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 '`app.c`' with the GNU C compiler `gcc` is,

```
gcc -I/usr/local/include -c app.c
```

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

The library is installed as a single file, '`libgsl.a`'. A shared version of the library is also installed on systems that support shared libraries. The default location of these files is '`/usr/local/lib`'. 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 app.o -lgsl -lgslcblas -lm
```

The following command line shows how you would link the same application with an alternative blas library called '`libcblas`',

```
gcc app.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 app.o -lgsl -lcblas -latlas -lm
```

For more information see Chapter 12 [BLAS Support], page 114.

The program `gsl-config` provides information on the local version of the library. For example, the following command shows that the library has been installed under the directory '`/usr/local`',

```
bash$ gsl-config --prefix
/usr/local
```

Further information is available using the command `gsl-config --help`.

2.3 Shared Libraries

To run a program linked with the shared version of the library it may be necessary to define the shell variable `LD_LIBRARY_PATH` to include the directory where the library is installed. For example,

```
LD_LIBRARY_PATH=/usr/local/lib:$LD_LIBRARY_PATH ./app
```

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

```
gcc -static app.o -lgsl -lgslcblas -lm
```

2.4 Autoconf macros

For applications using `autoconf` the standard macro `AC_CHECK_LIB` can be used to link with the library 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.in`' file to perform these tests,

```
AC_CHECK_LIB(m,main)
AC_CHECK_LIB(gslcblas,main)
AC_CHECK_LIB(gsl,main)
```

Assuming the libraries are found the output during the configure stage looks like this,

```
checking for main in -lm... yes
checking for main in -lgslcblas... yes
checking for main 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:

```
AM_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,

```
libgsdv_la_LDFLAGS =    \
        $(GTK_LIBDIR) \
        $(GTK_LIBS) -lgsdvgsl $(GSL_LIBS) -lgslcblas
```

Note that the macro `AM_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++.

2.5 Inline functions

The `inline` keyword is not part of ANSI C and the library does not export any inline function definitions by default. However, the library provides optional inline versions of performance-critical functions by conditional compilation. The inline versions of these functions can be included by defining the macro `HAVE_INLINE` when compiling an application.

```
gcc -c -DHAVE_INLINE app.c
```

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

Note that the actual usage of the inline keyword is `extern inline`, which eliminates unnecessary function definitions in GCC. If the form `extern inline` causes problems with other compilers a stricter autoconf test can be used, see Appendix C [Autoconf Macros], page 403.

2.6 Long double

The extended numerical type `long double` is part of the ANSI C standard and should be available in every modern compiler. However, the precision of `long double` is platform dependent, and this should be considered when using it. The IEEE standard only specifies the minimum precision of extended precision numbers, while the precision of `double` is the same on all platforms.

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. The substitution 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.

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 alternate 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, or any other specific type, file 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
#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.

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 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.

3 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. Many of the error codes use the same base name as a corresponding error code in C library. Here are some of the most common error codes, `int` **GSL_EDOM** Macro

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** Macro

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** Macro

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** Macro

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*) Function

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`',

gsl_error_handler_t Data Type

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*) Function

This functions 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** () Function

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*) Macro

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*) Macro

This macro is the same as `GSL_ERROR` but returns a user-defined status 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
main (void)
{
  int status;

  gsl_set_error_handler_off();

  status = gsl_fft_complex_radix2_forward (data, 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);
    }

    exit (0);
  }
```

The function `gsl_fft_complex_radix2` 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.

4 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 Macro

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

GSL_NEGINF Macro

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

GSL_NAN Macro

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*) Function

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

`int` **gsl_isinf** (`const double` *x*) Function

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

`int` **gsl_finite** (`const double` *x*) Function

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 Section 2.7 [Portability functions], page 7).

`double` **gsl_log1p** (`const double` *x*) Function

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*) Function

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*) Function

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_acosh** (`const double` *x*) Function

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) Function

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

double **gsl_atanh** (const double x) Function

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) Function

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

double **gsl_frexp** (double x, int * e) Function

This function splits the number x into its normalized fraction f and exponent e, such that $x = f * 2^e$ and $0.5 \le f < 1$. Ihe 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 a 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) Function

This routine computes 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. 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) Function
double **gsl_pow_3** (const double x) Function
double **gsl_pow_4** (const double x) Function
double **gsl_pow_5** (const double x) Function
double **gsl_pow_6** (const double x) Function
double **gsl_pow_7** (const double x) Function
double **gsl_pow_8** (const double x) Function
double **gsl_pow_9** (const double x) Function

These functions can be used to compute small integer powers x^2, x^3, etc. efficiently. The functions will be inlined when possible 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*) Macro

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*) Macro

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*) Macro

This macro is the opposite of `GSL_IS_ODD(n)`. 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

GSL_MAX (*a*, *b*) Macro

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

GSL_MIN (*a*, *b*) Macro

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*) Function

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*) Function

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

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*) Function

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

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*) Function

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 maximimum 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.

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

5 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 in the *Handbook of Mathematical Functions*. 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)* (n.b. The second edition uses different definitions from the first edition) 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 Complex numbers

Complex numbers are represented using the type `gsl_complex`. The internal representation of this type may vary across platforms and should not be accessed directly. The functions and macros described below allow complex numbers to be manipulated in a portable way.

For reference, the default form of the `gsl_complex` type is given by the following struct,

```
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.

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

This function uses the rectangular cartesian components (*x*,*y*) to return the complex number $z = x + iy$.

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

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

GSL_REAL (*z*) Macro
GSL_IMAG (*z*) Macro

These macros return the real and imaginary parts of the complex number *z*.

GSL_SET_COMPLEX (*zp*, *x*, *y*) Macro

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 $3 + 4i$.

GSL_SET_REAL (*zp,x*) Macro
GSL_SET_IMAG (*zp,y*) Macro

These macros allow the real and imaginary parts of the complex number pointed to by *zp* to be set independently.

5.2 Properties of complex numbers

`double` **gsl_complex_arg** (`gsl_complex` *z*) Function

This function returns the argument of the complex number z, $\arg(z)$, where $-\pi < \arg(z) \leq \pi$.

`double` **gsl_complex_abs** (`gsl_complex` *z*) Function

This function returns the magnitude of the complex number z, $|z|$.

`double` **gsl_complex_abs2** (`gsl_complex` *z*) Function

This function returns the squared magnitude of the complex number z, $|z|^2$.

`double` **gsl_complex_logabs** (`gsl_complex` *z*) Function

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.

5.3 Complex arithmetic operators

`gsl_complex` **gsl_complex_add** (`gsl_complex` *a*, `gsl_complex` *b*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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

`gsl_complex` **gsl_complex_inverse** (`gsl_complex` *z*) Function

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*) Function

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

5.4 Elementary Complex Functions

`gsl_complex` **gsl_complex_sqrt** (`gsl_complex` *z*) Function

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`) Function

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*) Function

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*) Function

This function returns the complex number z raised to the real power x, z^x.

gsl_complex **gsl_complex_exp** (gsl_complex *z*) Function

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

gsl_complex **gsl_complex_log** (gsl_complex *z*) Function

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*) Function

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*) Function

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

5.5 Complex Trigonometric Functions

gsl_complex **gsl_complex_sin** (gsl_complex *z*) Function

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*) Function

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*) Function

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*) Function

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

gsl_complex **gsl_complex_csc** (gsl_complex *z*) Function

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

gsl_complex **gsl_complex_cot** (gsl_complex *z*) Function

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

5.6 Inverse Complex Trigonometric Functions

gsl_complex **gsl_complex_arcsin** (gsl_complex z) Function

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) Function

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 $(-\pi, \pi]$. 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) Function

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) Function

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 $\pi/2$ 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) Function

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) Function

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) Function

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) Function

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) Function

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) Function

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

5.7 Complex Hyperbolic Functions

gsl_complex **gsl_complex_sinh** (gsl_complex z) Function

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) Function

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) Function

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) Function

This function returns the complex hyperbolic secant of the complex number z, $\operatorname{sech}(z) = 1/\cosh(z)$.

gsl_complex **gsl_complex_csch** (gsl_complex z) Function

This function returns the complex hyperbolic cosecant of the complex number z, $\operatorname{csch}(z) = 1/\sinh(z)$.

gsl_complex **gsl_complex_coth** (gsl_complex z) Function

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

5.8 Inverse Complex Hyperbolic Functions

gsl_complex **gsl_complex_arcsinh** (gsl_complex z) Function

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

gsl_complex **gsl_complex_arccosh** (gsl_complex z) Function

This function returns the complex hyperbolic arccosine of the complex number z, $\operatorname{arccosh}(z)$. The branch cut is on the real axis, less than 1.

gsl_complex **gsl_complex_arccosh_real** (double z) Function

This function returns the complex hyperbolic arccosine of the real number z, $\operatorname{arccosh}(z)$.

gsl_complex **gsl_complex_arctanh** (gsl_complex z) Function

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

gsl_complex **gsl_complex_arctanh_real** (double z) Function

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

gsl_complex **gsl_complex_arcsech** (gsl_complex z) Function

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) Function

This function returns the complex hyperbolic arccosecant of the complex number z, $\text{arccsch}(z) = \arcsin(1/z)$.

gsl_complex **gsl_complex_arccoth** (gsl_complex z) Function

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

5.9 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

6 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

`double` **gsl_poly_eval** (`const double c[], const int` *len*`, const double` *x*) Function

This function evaluates the polynomial $c[0] + c[1]x + c[2]x^2 + \ldots + c[len-1]x^{len-1}$ using Horner's method for stability. The function is inlined when possible.

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, 25.2.26.

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

This function computes a divided-difference representation of the interpolating polynomial for the points (*xa*, *ya*) 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*.

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

This function evaluates the polynomial stored in divided-difference form in the arrays *dd* and *xa* of length *size* at the point *x*.

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

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*.

6.3 Quadratic Equations

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

This function finds the real roots of the quadratic equation,

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

The number of real roots (either zero 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. 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*) Function

This function finds the complex roots of the quadratic equation,

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

The number of complex roots is returned (always 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.

6.4 Cubic Equations

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

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.

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

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.

`gsl_poly_complex_workspace *` **gsl_poly_complex_workspace_alloc** (`size_t` *n*) — Function

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*) — Function

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*) — Function

This function computes the roots of the general polynomial $P(x) = a_0 + a_1 x + a_2 x^2 + ... + a_{n-1} x^{n-1}$ 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 and `GSL_EFAILED` if the QR reduction does not converge.

6.6 Examples

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

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

int
main (void)
{
  int i;
  /* coefficient 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,

```
bash$ ./a.out
z0 = -0.809016994374947451 +0.587785252292473137
z1 = -0.809016994374947451 -0.587785252292473137
z2 = +0.309016994374947451 +0.951056516295153642
z3 = +0.309016994374947451 -0.951056516295153642
z4 = +1.000000000000000000 +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 is 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.

7 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, 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 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 `gsl_sf_result` struct contains value and error fields.

```
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 `gsl_sf_result_e10` struct contains value and error fields as well as an exponent field such that the actual result is obtained as `result * 10^(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 allows the accuracy of the function to be reduced in order to improve performance. The following precision levels are available for the mode argument,

`GSL_PREC_DOUBLE`
: Double-precision, a relative accuracy of approximately 2×10^{-16}.

`GSL_PREC_SINGLE`
: Single-precision, a relative accuracy of approximately 1×10^{-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,

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

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

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*) Function

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

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

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

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

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

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

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

These routines compute the derivative of the scaled Airy function $S_A(x)Ai(x)$.

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

These routines compute the derivative of the scaled Airy function $S_B(x)Bi(x)$.

7.4.3 Zeros of Airy Functions

double **gsl_sf_airy_zero_Ai** (unsigned int *s*) Function
int **gsl_sf_airy_zero_Ai_e** (unsigned int *s*, gsl_sf_result * *result*) Function

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

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

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

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

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

double **gsl_sf_bessel_J1** (double *x*) Function
int **gsl_sf_bessel_J1_e** (double *x*, gsl_sf_result * *result*) Function

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

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

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*[]) Function

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

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

double **gsl_sf_bessel_Y1** (double *x*) Function
int **gsl_sf_bessel_Y1_e** (double *x*, gsl_sf_result * *result*) Function

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

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*[]) Function

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

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

double **gsl_sf_bessel_I1** (double *x*) Function
int **gsl_sf_bessel_I1_e** (double *x*, gsl_sf_result * *result*) Function

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

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

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*[]) Function

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

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

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

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*[]) Function

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

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

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

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*[]) Function

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

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

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

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*[]) Function

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

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

`double` **gsl_sf_bessel_j1** (`double` *x*) Function
`int` **gsl_sf_bessel_j1_e** (`double` *x*, `gsl_sf_result *` *result*) Function

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

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

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*[]) Function

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 * *jl_x_array*) Function

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

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

double **gsl_sf_bessel_y1** (double *x*) Function
int **gsl_sf_bessel_y1_e** (double *x*, gsl_sf_result * *result*) Function

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

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

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

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*[]) Function

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

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

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

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

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*[]) Function

This routine computes the values of the scaled regular modified cylindrical 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*) Function
`int` **gsl_sf_bessel_k0_scaled_e** (`double` *x*, `gsl_sf_result *` *result*) Function

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*) Function
`int` **gsl_sf_bessel_k1_scaled_e** (`double` *x*, `gsl_sf_result *` *result*) Function

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*) Function
`int` **gsl_sf_bessel_k2_scaled_e** (`double` *x*, `gsl_sf_result *` *result*) Function

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*) Function
`int` **gsl_sf_bessel_kl_scaled_e** (`int` *l*, `double` *x*, `gsl_sf_result *` *result*) Function

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*[]) Function

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*) Function
`int` **gsl_sf_bessel_Jnu_e** (`double` *nu*, `double` *x*, `gsl_sf_result *` *result*) Function

These routines compute the regular cylindrical Bessel function of fractional order *nu*, $J_\nu(x)$.

`int` **gsl_sf_bessel_sequence_Jnu_e** (`double` *nu*, `gsl_mode_t` *mode*, `size_t` *size*, `double` *v*[]) Function

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 overwritten 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*) Function
`int` **gsl_sf_bessel_Ynu_e** (`double` *nu*, `double` *x*, `gsl_sf_result *` *result*) Function

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

7.5.11 Regular Modified Bessel Functions - Fractional Order

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

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

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

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

7.5.12 Irregular Modified Bessel Functions - Fractional Order

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

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

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

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

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

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

7.5.13 Zeros of Regular Bessel Functions

double **gsl_sf_bessel_zero_J0** (unsigned int *s*) Function
int **gsl_sf_bessel_zero_J0_e** (unsigned int *s*, gsl_sf_result * *result*) Function

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

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

These routines compute the location of the s-th positive zero of the Bessel function $J_\nu(x)$.

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 $Cl_2(\theta) = \mathrm{Im} Li_2(\exp(i\theta))$. The Clausen functions are declared in the header file 'gsl_sf_clausen.h'.

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

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

7.7 Coulomb Functions

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

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

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

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

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*) Function

This function computes the coulomb wave functions $F_L(\eta, x)$, $G_{L-k}(\eta, x)$ and their derivatives with respect to x, $F'_L(\eta, x)$ $G'_{L-k}(\eta, x)$. 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*) Function

This function computes the function $F_L(eta, x)$ for $L = Lmin \ldots Lmin{+}kmax$ 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*) Function

This function computes the functions $F_L(\eta, x)$, $G_L(\eta, x)$ for $L = Lmin \ldots Lmin + kmax$ 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*) Function

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 $L = Lmin \ldots Lmin + kmax$ 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*[]) Function

This function computes the Coulomb wave function divided by the argument $F_L(\eta, x)/x$ for $L = Lmin \ldots Lmin + kmax$, 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*) Function

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*[]) Function

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

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*) Function

`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*) Function

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*) Function

`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*) Function

These routines compute the Wigner 6-j coefficient,

$$\left\{ \begin{matrix} ja & jb & jc \\ jd & je & jf \end{matrix} \right\}$$

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*) Function

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*) Function

These routines compute the Wigner 9-j coefficient,

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

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*) Function

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

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

7.10 Debye Functions

The Debye functions are defined by the integral $D_n(x) = n/x^n \int_0^x dt (t^n/(e^t - 1))$. 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*) Function

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

These routines compute the first-order Debye function $D_1(x) = (1/x) \int_0^x dt (t/(e^t - 1))$.

double **gsl_sf_debye_2** (double *x*) Function

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

These routines compute the second-order Debye function $D_2(x) = (2/x^2) \int_0^x dt (t^2/(e^t - 1))$.

double **gsl_sf_debye_3** (double *x*) Function
int **gsl_sf_debye_3_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the third-order Debye function $D_3(x) = (3/x^3) \int_0^x dt(t^3/(e^t - 1))$.

double **gsl_sf_debye_4** (double *x*) Function
int **gsl_sf_debye_4_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the fourth-order Debye function $D_4(x) = (4/x^4) \int_0^x dt(t^4/(e^t - 1))$.

7.11 Dilogarithm

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

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 $Li_2(x) = -\mathrm{Re} \int_0^x ds \log(1-s)/s$. Note that $\mathrm{Im}(Li_2(x)) = 0$ for $x \le 1$, and $-\pi \log(x)$ for $x > 1$.

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*) Function

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'.

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

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*) Function

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`'.

7.13.1 Definition of Legendre Forms

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

$$F(\phi, k) = \int_0^\phi dt \frac{1}{\sqrt{(1 - k^2 \sin^2(t))}}$$

$$E(\phi, k) = \int_0^\phi dt \sqrt{(1 - k^2 \sin^2(t))}$$

$$P(\phi, k, n) = \int_0^\phi dt \frac{1}{(1 + n \sin^2(t))\sqrt{1 - k^2 \sin^2(t)}}$$

The complete Legendre forms are denoted by $K(k) = F(\pi/2, k)$ and $E(k) = E(\pi/2, k)$. Further information on the Legendre forms of elliptic integrals can be found in Abramowitz & Stegun, Chapter 17. The notation used here is based on Carlson, *Numerische Mathematik* 33 (1979) 1 and differs slightly from that used by Abramowitz & Stegun.

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,

$$RC(x, y) = 1/2 \int_0^\infty dt (t + x)^{-1/2} (t + y)^{-1}$$

$$RD(x, y, z) = 3/2 \int_0^\infty dt (t + x)^{-1/2} (t + y)^{-1/2} (t + z)^{-3/2}$$

$$RF(x, y, z) = 1/2 \int_0^\infty dt (t + x)^{-1/2} (t + y)^{-1/2} (t + z)^{-1/2}$$

$$RJ(x, y, z, p) = 3/2 \int_0^\infty dt (t + x)^{-1/2} (t + y)^{-1/2} (t + z)^{-1/2} (t + p)^{-1}$$

7.13.3 Legendre Form of Complete Elliptic Integrals

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

These routines compute the complete elliptic integral $K(k)$ to the accuracy specified by the mode variable *mode*.

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

These routines compute the complete elliptic integral $E(k)$ to the accuracy specified by the mode variable *mode*.

7.13.4 Legendre Form of Incomplete Elliptic Integrals

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

These routines compute the incomplete elliptic integral $F(\phi, k)$ to the accuracy specified by the mode variable *mode*.

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

These routines compute the incomplete elliptic integral $E(\phi, k)$ to the accuracy specified by the mode variable *mode*.

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

These routines compute the incomplete elliptic integral $P(\phi, k, n)$ to the accuracy specified by the mode variable *mode*.

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

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

$$D(\phi, k, n) = RD(1 - \sin^2(\phi), 1 - k^2 \sin^2(\phi), 1).$$

7.13.5 Carlson Forms

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

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

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*) Function

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

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*) Function

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

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*) Function

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*) Function

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

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

7.15.2 Complementary Error Function

double **gsl_sf_erfc** (double *x*) Function

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

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

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

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

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

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

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

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*) Function

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

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*) Function

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

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

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

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

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

These routines compute the N-relative exponential, which is the n-th generalization of the functions `gsl_sf_exprel` and `gsl_sf_exprel2`. 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*) Function

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*) Function

This functions exponentiate 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*) Function

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*) — Function

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

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

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

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

7.17.2 Ei(x)

double **gsl_sf_expint_Ei** (double *x*) — Function
int **gsl_sf_expint_Ei_e** (double *x*, gsl_sf_result * *result*) — Function

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

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

where PV denotes the principal value of the integral.

7.17.3 Hyperbolic Integrals

double **gsl_sf_Shi** (double *x*) — Function
int **gsl_sf_Shi_e** (double *x*, gsl_sf_result * *result*) — Function

These routines compute the integral $Shi(x) = \int_0^x dt \sinh(t)/t$.

double **gsl_sf_Chi** (double *x*) — Function
int **gsl_sf_Chi_e** (double *x*, gsl_sf_result * *result*) — Function

These routines compute the integral $Chi(x) := Re[\gamma_E + \log(x) + \int_0^x dt (\cosh[t] - 1)/t]$, 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*) Function
int **gsl_sf_expint_3_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the exponential integral $Ei_3(x) = \int_0^x dt \exp(-t^3)$ for $x \geq 0$.

7.17.5 Trigonometric Integrals

double **gsl_sf_Si** (const double *x*) Function
int **gsl_sf_Si_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the Sine integral $Si(x) = \int_0^x dt \sin(t)/t$.

double **gsl_sf_Ci** (const double *x*) Function
int **gsl_sf_Ci_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the Cosine integral $Ci(x) = -\int_x^\infty dt \cos(t)/t$ for $x > 0$.

7.17.6 Arctangent Integral

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

These routines compute the Arctangent integral $AtanInt(x) = \int_0^x dt \arctan(t)/t$.

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,

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

double **gsl_sf_fermi_dirac_m1** (double *x*) Function
int **gsl_sf_fermi_dirac_m1_e** (double *x*, gsl_sf_result * *result*) Function

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

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

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

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

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

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

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

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

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

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,

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

double **gsl_sf_fermi_dirac_inc_0** (double *x*, double *b*) Function
int **gsl_sf_fermi_dirac_inc_0_e** (double *x*, double *b*, gsl_sf_result * *result*) Function

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 Function

The Gamma function is defined by the following integral,

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

Further information on the Gamma function can be found in Abramowitz & Stegun, Chapter 6. The functions described in this section are declared in the header file '`gsl_sf_gamma.h`'.

`double` **gsl_sf_gamma** (`double` *x*) Function
`int` **gsl_sf_gamma_e** (`double` *x*, `gsl_sf_result *` *result*) Function

These routines compute the Gamma function $\Gamma(x)$, subject to x not being a negative integer. 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*) Function
`int` **gsl_sf_lngamma_e** (`double` *x*, `gsl_sf_result *` *result*) Function

These routines compute the logarithm of the Gamma function, $\log(\Gamma(x))$, subject to x not a being negative integer. 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*) Function

This routine computes the sign of the gamma function and the logarithm its magnitude, subject to x not being a negative integer. The function is computed using the real Lanczos method. The value of the gamma function can be reconstructed using the relation $\Gamma(x) = sgn * \exp(resultlg)$.

`double` **gsl_sf_gammastar** (`double` *x*) Function
`int` **gsl_sf_gammastar_e** (`double` *x*, `gsl_sf_result *` *result*) Function

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

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

and is a useful suggestion of Temme.

`double` **gsl_sf_gammainv** (`double` *x*) Function
`int` **gsl_sf_gammainv_e** (`double` *x*, `gsl_sf_result *` *result*) Function

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*) Function

This routine computes $\log(\Gamma(z))$ for complex $z = z_r + i z_i$ and z not a negative integer, 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.

`double` **gsl_sf_taylorcoeff** (`int` *n*, `double` *x*) Function
`int` **gsl_sf_taylorcoeff_e** (`int` *n*, `double` *x*, `gsl_sf_result *` *result*) Function

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

`double` **gsl_sf_fact** (`unsigned int` *n*) Function
`int` **gsl_sf_fact_e** (`unsigned int` *n*, `gsl_sf_result *` *result*) Function

These routines compute the factorial $n!$. The factorial is related to the Gamma function by $n! = \Gamma(n+1)$.

`double` **gsl_sf_doublefact** (`unsigned int` *n*) Function
`int` **gsl_sf_doublefact_e** (`unsigned int` *n*, `gsl_sf_result *` *result*) Function

These routines compute the double factorial $n!! = n(n-2)(n-4)\dots$.

`double` **gsl_sf_lnfact** (`unsigned int` *n*) Function
`int` **gsl_sf_lnfact_e** (`unsigned int` *n*, `gsl_sf_result *` *result*) Function

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

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

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

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

`double` **gsl_sf_lnchoose** (`unsigned int` *n*, `unsigned int` *m*) Function
`int` **gsl_sf_lnchoose_e** (`unsigned int` *n*, `unsigned int` *m*, `gsl_sf_result *` *result*) Function

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_poch** (`double` *a*, `double` *x*) Function
`int` **gsl_sf_poch_e** (`double` *a*, `double` *x*, `gsl_sf_result *` *result*) Function

These routines compute the Pochhammer symbol $(a)_x := \Gamma(a+x)/\Gamma(x)$, subject to a and $a+x$ not being negative integers. The Pochhammer symbol is also known as the Apell symbol.

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

These routines compute the logarithm of the Pochhammer symbol, $\log((a)_x) = \log(\Gamma(a+x)/\Gamma(a))$ for $a > 0$, $a + x > 0$.

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

These routines compute the sign of the Pochhammer symbol and the logarithm of its magnitude. The computed parameters are $result = \log(|(a)_x|)$ and $sgn = sgn((a)_x)$ where $(a)_x := \Gamma(a+x)/\Gamma(a)$, subject to a, $a+x$ not being negative integers.

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

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

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

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

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

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

double **gsl_sf_beta** (double *a*, double *b*) Function
int **gsl_sf_beta_e** (double *a*, double *b*, gsl_sf_result * *result*) Function

These routines compute the Beta Function, $B(a,b) = \Gamma(a)\Gamma(b)/\Gamma(a+b)$ for $a > 0$, $b > 0$.

double **gsl_sf_lnbeta** (double *a*, double *b*) Function
int **gsl_sf_lnbeta_e** (double *a*, double *b*, gsl_sf_result * *result*) Function

These routines compute the logarithm of the Beta Function, $\log(B(a,b))$ for $a > 0$, $b > 0$.

double **gsl_sf_beta_inc** (double *a*, double *b*, double *x*) Function
int **gsl_sf_beta_inc_e** (double *a*, double *b*, double *x*, gsl_sf_result * *result*) Function

These routines compute the normalize incomplete Beta function $B_x(a,b)/B(a,b)$ for $a > 0$, $b > 0$, and $0 \leq x \leq 1$.

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*) Function
double **gsl_sf_gegenpoly_2** (double *lambda*, double *x*) Function
double **gsl_sf_gegenpoly_3** (double *lambda*, double *x*) Function
int **gsl_sf_gegenpoly_1_e** (double *lambda*, double *x*, gsl_sf_result * *result*) Function
int **gsl_sf_gegenpoly_2_e** (double *lambda*, double *x*, gsl_sf_result * *result*) Function
int **gsl_sf_gegenpoly_3_e** (double *lambda*, double *x*, gsl_sf_result * *result*) Function

These functions evaluate the Gegenbauer polynomials $C^{(\lambda)}_n(x)$ using explicit representations for $n = 1, 2, 3$.

double **gsl_sf_gegenpoly_n** (int *n*, double *lambda*, double *x*) Function
int **gsl_sf_gegenpoly_n_e** (int *n*, double *lambda*, double *x*, gsl_sf_result * *result*) Function

These functions evaluate the Gegenbauer polynomial $C^{(\lambda)}_n(x)$ 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*[]) Function

This function computes an array of Gegenbauer polynomials $C^{(\lambda)}_n(x)$ for $n = 0, 1, 2, \ldots, nmax$, subject to $\lambda > -1/2$, $nmax \geq 0$.

7.21 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*) Function
int **gsl_sf_hyperg_0F1_e** (double *c*, double *x*, gsl_sf_result * *result*) Function

These routines compute the hypergeometric function ${}_0F_1(c, x)$.

double **gsl_sf_hyperg_1F1_int** (int *m*, int *n*, double *x*) Function
int **gsl_sf_hyperg_1F1_int_e** (int *m*, int *n*, double *x*, gsl_sf_result * *result*) Function

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*) Function
`int` **gsl_sf_hyperg_1F1_e** (`double` *a*, `double` *b*, `double` *x*, `gsl_sf_result *` *result*) Function

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*) Function
`int` **gsl_sf_hyperg_U_int_e** (`int` *m*, `int` *n*, `double` *x*, `gsl_sf_result *` *result*) Function

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*) Function

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*) Function
`int` **gsl_sf_hyperg_U_e** (`double` *a*, `double` *b*, `double` *x*) Function

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*) Function

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*) Function
`int` **gsl_sf_hyperg_2F1_e** (`double` *a*, `double` *b*, `double` *c*, `double` *x*, `gsl_sf_result *` *result*) Function

These routines compute the Gauss hypergeometric function ${}_2F_1(a, b, c, x)$ 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*) Function
`int` **gsl_sf_hyperg_2F1_conj_e** (`double` *aR*, `double` *aI*, `double` *c*, `double` *x*, `gsl_sf_result *` *result*) Function

These routines compute the Gauss hypergeometric function ${}_2F_1(a_R + ia_I, aR - iaI, c, x)$ with complex parameters for $|x| < 1$. exceptions:

double **gsl_sf_hyperg_2F1_renorm** (double *a*, double *b*, double *c*, double *x*) Function

int **gsl_sf_hyperg_2F1_renorm_e** (double *a*, double *b*, double *c*, double *x*, gsl_sf_result * *result*) Function

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*) Function

int **gsl_sf_hyperg_2F1_conj_renorm_e** (double *aR*, double *aI*, double *c*, double *x*, gsl_sf_result * *result*) Function

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*) Function

int **gsl_sf_hyperg_2F0_e** (double *a*, double *b*, double *x*, gsl_sf_result * *result*) Function

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 ${}_2F_0(a, b, x) = (-1/x)^a U(a, 1 + a - b, -1/x)$

7.22 Laguerre Functions

The Laguerre polynomials are defined in terms of confluent hypergeometric functions as $L^a_n(x) = ((a + 1)_n/n!)_1F_1(-n, a + 1, x)$. These functions are declared in the header file 'gsl_sf_laguerre.h'.

double **gsl_sf_laguerre_1** (double *a*, double *x*) Function

double **gsl_sf_laguerre_2** (double *a*, double *x*) Function

double **gsl_sf_laguerre_3** (double *a*, double *x*) Function

int **gsl_sf_laguerre_1_e** (double *a*, double *x*, gsl_sf_result * *result*) Function

int **gsl_sf_laguerre_2_e** (double *a*, double *x*, gsl_sf_result * *result*) Function

int **gsl_sf_laguerre_3_e** (double *a*, double *x*, gsl_sf_result * *result*) Function

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*) Function

int **gsl_sf_laguerre_n_e** (int *n*, double *a*, double *x*, gsl_sf_result * *result*) Function

Thse routines evaluate the generalized Laguerre polynomials $L^a_n(x)$ for $a > -1$, $n \geq 0$.

7.23 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*) Function
int **gsl_sf_lambert_W0_e** (double *x*, gsl_sf_result * *result*) Function

These compute the principal branch of the Lambert W function, $W_0(x)$.

double **gsl_sf_lambert_Wm1** (double *x*) Function
int **gsl_sf_lambert_Wm1_e** (double *x*, gsl_sf_result * *result*) Function

These compute the secondary real-valued branch of the Lambert W function, $W_{-1}(x)$.

7.24 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'.

7.24.1 Legendre Polynomials

double **gsl_sf_legendre_P1** (double *x*) Function
double **gsl_sf_legendre_P2** (double *x*) Function
double **gsl_sf_legendre_P3** (double *x*) Function
int **gsl_sf_legendre_P1_e** (double *x*, gsl_sf_result * *result*) Function
int **gsl_sf_legendre_P2_e** (double *x*, gsl_sf_result * *result*) Function
int **gsl_sf_legendre_P3_e** (double *x*, gsl_sf_result * *result*) Function

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*) Function
int **gsl_sf_legendre_Pl_e** (int *l*, double *x*, gsl_sf_result * *result*) Function

These functions evaluate the Legendre polynomial $P_l(x)$ for a specific value of l, x subject to $l \geq 0$, $|x| \leq 1$

int **gsl_sf_legendre_Pl_array** (int *lmax*, double *x*, double *result_array*[]) Function

This function computes an array of Legendre polynomials $P_l(x)$ for $l = 0, \dots, lmax$, $|x| \leq 1$

double **gsl_sf_legendre_Q0** (double *x*) Function
int **gsl_sf_legendre_Q0_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the Legendre function $Q_0(x)$ for $x > -1$, $x \neq 1$.

double **gsl_sf_legendre_Q1** (double *x*) Function
int **gsl_sf_legendre_Q1_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the Legendre function $Q_1(x)$ for $x > -1$, $x \neq 1$.

double **gsl_sf_legendre_Ql** (int *l*, double *x*) Function
int **gsl_sf_legendre_Ql_e** (int *l*, double *x*, gsl_sf_result * *result*) Function

These routines compute the Legendre function $Q_l(x)$ for $x > -1$, $x \neq 1$ and $l \geq 0$.

7.24.2 Associated Legendre Polynomials and Spherical Harmonics

The following functions compute the associated Legendre Polynomials $P_l^m(x)$. Note that this function grows combinatorially with l and can overflow for l larger than about 150. There is no trouble for small m, but overflow occurs when m and l are both large. Rather than allow overflows, these functions refuse to calculate $P_l^m(x)$ and return `GSL_EOVRFLW` when they can sense that l and m are too big.

If you want to calculate a spherical harmonic, then *do not* use these functions. Instead use `gsl_sf_legendre_sphPlm()` below, which uses a similar recursion, but with the normalized functions.

double **gsl_sf_legendre_Plm** (int *l*, int *m*, double *x*) Function
int **gsl_sf_legendre_Plm_e** (int *l*, int *m*, double *x*, gsl_sf_result * *result*) Function

These routines compute the associated Legendre polynomial $P_l^m(x)$ for $m \geq 0$, $l \geq m$, $|x| \leq 1$.

int **gsl_sf_legendre_Plm_array** (int *lmax*, int *m*, double *x*, double *result_array*[]) Function

This function computes an array of Legendre polynomials $P_l^m(x)$ for $m \geq 0$, $l = |m|, \ldots, lmax$, $|x| \leq 1$.

double **gsl_sf_legendre_sphPlm** (int *l*, int *m*, double *x*) Function
int **gsl_sf_legendre_sphPlm_e** (int *l*, int *m*, double *x*, gsl_sf_result * *result*) Function

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 $m \geq 0$, $l \geq m$, $|x| \leq 1$. Theses routines avoid the overflows that occur for the standard normalization of $P_l^m(x)$.

int **gsl_sf_legendre_sphPlm_array** (int *lmax*, int *m*, double *x*, double *result_array*[]) Function

This function computes an array of normalized associated Legendre functions $\sqrt{(2l+1)/(4\pi)}\sqrt{(l-m)!/(l+m)!}P_l^m(x)$ for $m \geq 0$, $l = |m|, \ldots, lmax$, $|x| \leq 1$

int **gsl_sf_legendre_array_size** (const int *lmax*, const int *m*) Function

This functions returns the size of *result_array*[] needed for the array versions of $P_l^m(x)$, *lmax* - *m* + 1.

7.24.3 Conical Functions

The Conical Functions $P^{\mu}_{-(1/2)+i\lambda}(x)$, $Q^{\mu}_{-(1/2)+i\lambda}$ are described in Abramowitz & Stegun, Section 8.12.

`double` **gsl_sf_conicalP_half** (`double` *lambda*, `double` *x*) Function
`int` **gsl_sf_conicalP_half_e** (`double` *lambda*, `double` *x*, `gsl_sf_result *` *result*) Function

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*) Function
`int` **gsl_sf_conicalP_mhalf_e** (`double` *lambda*, `double` *x*, `gsl_sf_result *` *result*) Function

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*) Function
`int` **gsl_sf_conicalP_0_e** (`double` *lambda*, `double` *x*, `gsl_sf_result *` *result*) Function

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*) Function
`int` **gsl_sf_conicalP_1_e** (`double` *lambda*, `double` *x*, `gsl_sf_result *` *result*) Function

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*) Function
`int` **gsl_sf_conicalP_sph_reg_e** (`int` *l*, `double` *lambda*, `double` *x*, `gsl_sf_result *` *result*) Function

These routines compute the Regular Spherical Conical Function $P^{-1/2-l}_{-1/2+i\lambda}(x)$ for $x > -1$, $l \geq -1$.

`double` **gsl_sf_conicalP_cyl_reg** (`int` *m*, `double` *lambda*, `double` *x*) Function
`int` **gsl_sf_conicalP_cyl_reg_e** (`int` *m*, `double` *lambda*, `double` *x*, `gsl_sf_result *` *result*) Function

These routines compute the Regular Cylindrical Conical Function $P^{-m}_{-1/2+i\lambda}(x)$ for $x > -1$, $m \geq -1$.

7.24.4 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 $H3d$. 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*) Function
int **gsl_sf_legendre_H3d_0_e** (double *lambda*, double *eta*, gsl_sf_result * *result*) Function

These routines compute the zeroth radial eigenfunction of the Laplacian on the 3-dimensional hyperbolic space, $L^{H3d}_0(\lambda,\eta) := \sin(\lambda\eta)/(\lambda\sinh(\eta))$ 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*) Function
int **gsl_sf_legendre_H3d_1_e** (double *lambda*, double *eta*, gsl_sf_result * *result*) Function

These routines compute the first radial eigenfunction of the Laplacian on the 3-dimensional hyperbolic space, $L^{H3d}_1(\lambda,\eta) := 1/\sqrt{\lambda^2+1}\sin(\lambda\eta)/(\lambda\sinh(\eta))(\coth(\eta) - \lambda\cot(\lambda\eta))$ 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*) Function
int **gsl_sf_legendre_H3d_e** (int *l*, double *lambda*, double *eta*, gsl_sf_result * *result*) Function

These routines compute the l'th radial eigenfunction of the Laplacian on the 3-dimensional hyperbolic space $\eta \geq 0$, $l \geq 0$. 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*[]) Function

This function computes an array of radial eigenfunctions $L^{H3d}_l(\lambda,\eta)$ for $0 \leq l \leq lmax$.

7.25 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*) Function
int **gsl_sf_log_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the logarithm of x, $\log(x)$, for $x > 0$.

double **gsl_sf_log_abs** (double *x*) Function
int **gsl_sf_log_abs_e** (double *x*, gsl_sf_result * *result*) Function

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*) Function

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*) Function
int **gsl_sf_log_1plusx_e** (double *x*, gsl_sf_result * *result*) Function

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*) Function
int **gsl_sf_log_1plusx_mx_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute $\log(1+x)-x$ for $x > -1$ using an algorithm that is accurate for small x.

7.26 Power Function

The following functions are equivalent to the function `gsl_pow_int` (see Section 4.4 [Small integer powers], page 18) 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*) Function
int **gsl_sf_pow_int_e** (double *x*, int *n*, gsl_sf_result * *result*) Function

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.

```
#include <gsl/gsl_sf_pow_int.h>
/* compute 3.0**12 */
double y = gsl_sf_pow_int(3.0, 12);
```

7.27 Psi (Digamma) Function

The polygamma functions of order m defined by $\psi^{(m)}(x) = (d/dx)^m \psi(x) = (d/dx)^{m+1} \log(\Gamma(x))$, 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`'.

7.27.1 Digamma Function

double **gsl_sf_psi_int** (int *n*) Function
int **gsl_sf_psi_int_e** (int *n*, gsl_sf_result * *result*) Function

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*) Function
int **gsl_sf_psi_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the digamma function $\psi(x)$ for general x, $x \neq 0$.

double **gsl_sf_psi_1piy** (double *y*) Function
int **gsl_sf_psi_1piy_e** (double *y*, gsl_sf_result * *result*) Function

These routines compute the real part of the digamma function on the line $1 + iy$, $Re[\psi(1+iy)]$.

7.27.2 Trigamma Function

double **gsl_sf_psi_1_int** (int *n*) Function
int **gsl_sf_psi_1_int_e** (int *n*, gsl_sf_result * *result*) Function

These routines compute the Trigamma function $\psi'(n)$ for positive integer n.

7.27.3 Polygamma Function

double **gsl_sf_psi_n** (int *m*, double *x*) Function
int **gsl_sf_psi_n_e** (int *m*, double *x*, gsl_sf_result * *result*) Function

These routines compute the polygamma function $\psi^{(m)}(x)$ for $c \geq 0$, $x > 0$.

7.28 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*) Function
int **gsl_sf_synchrotron_1_e** (double *x*, gsl_sf_result * *result*) Function

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*) Function
int **gsl_sf_synchrotron_2_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the second synchrotron function $x K_{2/3}(x)$ for $x \geq 0$.

7.29 Transport Functions

The transport functions $J(n,x)$ are defined by the integral representations $J(n,x) := \int_0^x dt\, t^n e^t/(e^t-1)^2$. They are declared in the header file 'gsl_sf_transport.h'.

double **gsl_sf_transport_2** (double *x*) Function
int **gsl_sf_transport_2_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the transport function $J(2,x)$.

double **gsl_sf_transport_3** (double *x*) Function
int **gsl_sf_transport_3_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the transport function $J(3,x)$.

double **gsl_sf_transport_4** (double *x*) Function
int **gsl_sf_transport_4_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the transport function $J(4,x)$.

double **gsl_sf_transport_5** (double *x*) Function
int **gsl_sf_transport_5_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the transport function $J(5,x)$.

7.30 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'.

7.30.1 Circular Trigonometric Functions

double **gsl_sf_sin** (double *x*) Function
int **gsl_sf_sin_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the sine function $\sin(x)$.

double **gsl_sf_cos** (double *x*) Function
int **gsl_sf_cos_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute the cosine function $\cos(x)$.

double **gsl_sf_hypot** (double *x*, double *y*) Function
int **gsl_sf_hypot_e** (double *x*, double *y*, gsl_sf_result * *result*) Function

These routines compute the hypotenuse function $\sqrt{x^2 + y^2}$ avoiding overflow and underflow.

double **gsl_sf_sinc** (double *x*) Function
int **gsl_sf_sinc_e** (double *x*, gsl_sf_result * *result*) Function

These routines compute $\mathrm{sinc}(x) = \sin(\pi x)/(\pi x)$ for any value of *x*.

7.30.2 Trigonometric Functions for Complex Arguments

int **gsl_sf_complex_sin_e** (double *zr*, double *zi*, gsl_sf_result * *szr*, gsl_sf_result * *szi*) Function

This function computes the complex sine, $\sin(z_r + i z_i)$ 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*) Function

This function computes the complex cosine, $\cos(z_r + i z_i)$ storing the real and imaginary parts in *szr*, *szi*.

int **gsl_sf_complex_logsin_e** (double *zr*, double *zi*, gsl_sf_result * *lszr*, gsl_sf_result * *lszi*) Function

This function computes the logarithm of the complex sine, $\log(\sin(z_r + i z_i))$ storing the real and imaginary parts in *szr*, *szi*.

7.30.3 Hyperbolic Trigonometric Functions

`double` **gsl_sf_lnsinh** (`double` *x*) Function
`int` **gsl_sf_lnsinh_e** (`double` *x*, `gsl_sf_result *` *result*) Function

These routines compute $\log(\sinh(x))$ for $x > 0$.

`double` **gsl_sf_lncosh** (`double` *x*) Function
`int` **gsl_sf_lncosh_e** (`double` *x*, `gsl_sf_result *` *result*) Function

These routines compute $\log(\cosh(x))$ for any x.

7.30.4 Conversion Functions

`int` **gsl_sf_polar_to_rect** (`double` *r*, `double` *theta*, `gsl_sf_result *` *x*, `gsl_sf_result *` *y*); Function

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*) Function

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 $[-\pi, \pi]$.

7.30.5 Restriction Functions

`double` **gsl_sf_angle_restrict_symm** (`double` *theta*) Function
`int` **gsl_sf_angle_restrict_symm_e** (`double *` *theta*) Function

These routines force the angle *theta* to lie in the range $(-\pi, \pi]$.

`double` **gsl_sf_angle_restrict_pos** (`double` *theta*) Function
`int` **gsl_sf_angle_restrict_pos_e** (`double *` *theta*) Function

These routines force the angle *theta* to lie in the range $[0, 2\pi)$.

7.30.6 Trigonometric Functions With Error Estimates

`double` **gsl_sf_sin_err** (`double` *x*, `double` *dx*) Function
`int` **gsl_sf_sin_err_e** (`double` *x*, `double` *dx*, `gsl_sf_result *` *result*) Function

These routines compute the sine of an angle *x* with an associated absolute error *dx*, $\sin(x \pm dx)$.

`double` **gsl_sf_cos_err** (`double` *x*, `double` *dx*) Function
`int` **gsl_sf_cos_err_e** (`double` *x*, `double` *dx*, `gsl_sf_result *` *result*) Function

These routines compute the cosine of an angle *x* with an associated absolute error *dx*, $\cos(x \pm dx)$.

7.31 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'.

7.31.1 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*) Function
int **gsl_sf_zeta_int_e** (int *n*, gsl_sf_result * *result*) Function

These routines compute the Riemann zeta function $\zeta(n)$ for integer n, $n \neq 1$.

double **gsl_sf_zeta** (double *s*) Function
int **gsl_sf_zeta_e** (double *s*, gsl_sf_result * *result*) Function

These routines compute the Riemann zeta function $\zeta(s)$ for arbitrary s, $s \neq 1$.

7.31.2 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*) Function
int **gsl_sf_hzeta_e** (double *s*, double *q*, gsl_sf_result * *result*) Function

These routines compute the Hurwitz zeta function $\zeta(s,q)$ for $s > 1$, $q > 0$.

7.31.3 Eta Function

The eta function is defined by $\eta(s) = (1 - 2^{1-s})\zeta(s)$.

double **gsl_sf_eta_int** (int *n*) Function
int **gsl_sf_eta_int_e** (int *n*, gsl_sf_result * *result*) Function

These routines compute the eta function $\eta(n)$ for integer n.

double **gsl_sf_eta** (double *s*) Function
int **gsl_sf_eta_e** (double *s*, gsl_sf_result * *result*) Function

These routines compute the eta function $\eta(s)$ for arbitrary s.

7.32 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_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,

```
$ ./a.out
status  = success
J0(5.0) = -0.177596771314338292
      +/-  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,

```
$ ./a.out
J0(5.0) = -0.177596771314338292
exact   = -0.177596771314338292
```

7.33 References and Further Reading

The library follows the conventions of *Abramowitz & Stegun* where possible,

Abramowitz & Stegun (eds.), *Handbook of Mathematical Functions*

The following papers contain information on the algorithms used to compute the special functions,

MISCFUN: A software package to compute uncommon special functions. *ACM Trans. Math. Soft.*, vol. 22, 1996, 288-301

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)

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).

8 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,

```
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,

```
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*) Function

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.

A null pointer is returned if insufficient memory is available to create the block.

`gsl_block *` **gsl_block_calloc** (`size_t` *n*) Function

This function allocates memory for a block and initializes all the elements of the block to zero.

`void` **gsl_block_free** (`gsl_block *` *b*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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 = %u\n", b->size);
  printf("block data address = %#x\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,

```
typedef struct
{
  size_t size;
  size_t stride;
  double * data;
  gsl_block * block;
  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.

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*) Function

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.

`gsl_vector *` **gsl_vector_calloc** (`size_t` *n*) Function

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*) Function

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. Range checking is available in the GNU C Compiler extension `checkergcc` but it is not available on every platform. 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. 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.

double **gsl_vector_get** (const gsl_vector * *v*, size_t *i*) Function

This function returns the *i*-th element of a vector *v*. If *i* lies outside the allowed range of 0 to *n-1* then the error handler is invoked and 0 is returned.

void **gsl_vector_set** (gsl_vector * *v*, size_t *i*, double *x*) Function

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 *n-1* then the error handler is invoked.

double * **gsl_vector_ptr** (gsl_vector * *v*, size_t *i*) Function

const double * **gsl_vector_ptr** (const gsl_vector * *v*, size_t *i*) Function

These functions return a pointer to the *i*-th element of a vector *v*. If *i* lies outside the allowed range of 0 to *n-1* then the error handler is invoked and a null pointer is returned.

8.3.3 Initializing vector elements

void **gsl_vector_set_all** (gsl_vector * *v*, double *x*) Function

This function sets all the elements of the vector *v* to the value *x*.

void **gsl_vector_set_zero** (gsl_vector * *v*) Function

This function sets all the elements of the vector *v* to zero.

int **gsl_vector_set_basis** (gsl_vector * *v*, size_t *i*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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.

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.

gsl_vector_view **gsl_vector_subvector** (gsl_vector **v*, size_t *offset*, size_t *n*) Function

gsl_vector_const_view **gsl_vector_const_subvector** (const gsl_vector * *v*, size_t *offset*, size_t *n*) Function

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` **gsl_vector_subvector_with_stride** (`gsl_vector` **v*, `size_t` *offset*, `size_t` *stride*, `size_t` *n*) — Function

`gsl_vector_const_view` **gsl_vector_const_subvector_with_stride** (`const gsl_vector *` *v*, `size_t` *offset*, `size_t` *stride*, `size_t` *n*) — Function

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 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*) — Function

`gsl_vector_const_view` **gsl_vector_complex_const_real** (`const gsl_vector_complex` **v*) — Function

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*) — Function

`gsl_vector_const_view` **gsl_vector_complex_const_imag** (`const gsl_vector_complex` **v*) — Function

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*) — Function

`gsl_vector_const_view` **gsl_vector_const_view_array** (`const double` **base*, `size_t` *n*) — Function

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*) — Function

`gsl_vector_const_view` **gsl_vector_const_view_array_with_stride** (`const double *` *base*, `size_t` *stride*, `size_t` *n*) — Function

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 Chapter 12 [BLAS Support], page 114). 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*) — Function

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*) Function

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 function 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) Function

This function exchanges the *i*-th and *j*-th elements of the vector *v* in-place.

int **gsl_vector_reverse** (gsl_vector * *v*) Function

This function reverses the order of the elements of the vector *v*.

8.3.8 Vector operations

The following operations are only defined for real vectors.

int **gsl_vector_add** (gsl_vector * *a*, const gsl_vector * *b*) Function

This function adds the elements of vector *b* to the elements of vector *a*, $a'_i = a_i + b_i$. The two vectors must have the same length.

int **gsl_vector_sub** (gsl_vector * *a*, const gsl_vector * *b*) Function

This function subtracts the elements of vector *b* from the elements of vector *a*, $a'_i = a_i - b_i$. The two vectors must have the same length.

int **gsl_vector_mul** (gsl_vector * *a*, const gsl_vector * *b*) Function

This function multiplies the elements of vector *a* by the elements of vector *b*, $a'_i = a_i * b_i$. The two vectors must have the same length.

int **gsl_vector_div** (gsl_vector * *a*, const gsl_vector * *b*) Function

This function divides the elements of vector *a* by the elements of vector *b*, $a'_i = a_i / b_i$. The two vectors must have the same length.

int **gsl_vector_scale** (gsl_vector * *a*, const double *x*) Function

This function multiplies the elements of vector *a* by the constant factor *x*, $a'_i = x a_i$.

int **gsl_vector_add_constant** (gsl_vector * *a*, const double *x*) Function

This function adds the constant value *x* to the elements of the vector *a*, $a'_i = a_i + x$.

8.3.9 Finding maximum and minimum elements of vectors

double **gsl_vector_max** (const gsl_vector * *v*) Function

This function returns the maximum value in the vector *v*.

double **gsl_vector_min** (const gsl_vector * *v*) Function

This function returns the minimum value in the vector *v*.

void **gsl_vector_minmax** (const gsl_vector * *v*, double * *min_out*, double * *max_out*) Function

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*) Function

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*) Function

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*) Function

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

int **gsl_vector_isnull** (const gsl_vector * *v*) Function

This function returns 1 if all the elements of the vector *v* are zero, 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++)
    {
      printf("v_%d = %g\n", i, gsl_vector_get (v, i));
    }

  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`.

```
v_0 = 1.23
v_1 = 2.23
v_2 = 3.23
gsl: vector_source.c:12: ERROR: index out of range
IOT trap/Abort (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);
    }

  {
     FILE * f = fopen("test.dat", "w");
     gsl_vector_fprintf (f, v, "%.5g");
     fclose (f);
  }
  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));
    }

  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.

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 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_matrix *` **gsl_matrix_alloc** (`size_t` *n1*, `size_t` *n2*) Function

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.

`gsl_matrix *` **gsl_matrix_calloc** (`size_t` *n1*, `size_t` *n2*) Function

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*) Function

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 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*, size_t *i*, size_t *j*) Function

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.

void **gsl_matrix_set** (gsl_matrix * *m*, size_t *i*, size_t *j*, double *x*) Function

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.

double * **gsl_matrix_ptr** (gsl_matrix * *m*, size_t *i*, size_t *j*) Function
const double * **gsl_matrix_ptr** (const gsl_matrix * *m*, size_t *i*, size_t *j*) Function

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.

8.4.3 Initializing matrix elements

void **gsl_matrix_set_all** (gsl_matrix * *m*, double *x*) Function

This function sets all the elements of the matrix *m* to the value *x*.

void **gsl_matrix_set_zero** (gsl_matrix * *m*) Function

This function sets all the elements of the matrix *m* to zero.

void **gsl_matrix_set_identity** (gsl_matrix * *m*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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

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*) Function

gsl_matrix_const_view **gsl_matrix_const_submatrix** (const gsl_matrix * *m*, size_t *k1*, size_t *k2*, size_t *n1*, size_t *n2*) Function

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 + k1) + 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*) — Function

`gsl_matrix_const_view` **gsl_matrix_const_view_array** (`const double *` *base*, `size_t` *n1*, `size_t` *n2*) — Function

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*) — Function

`gsl_matrix_const_view` **gsl_matrix_const_view_array_with_tda** (`const double *` *base*, `size_t` *n1*, `size_t` *n2*, `size_t` *tda*) — Function

These functions return a matrix view of the array *base* with a physical number of columns *tda* which may differ from corresponding the 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*) — Function

`gsl_matrix_const_view` **gsl_matrix_const_view_vector** (`const gsl_vector *` *v*, `size_t` *n1*, `size_t` *n2*) — Function

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`) Function

`gsl_matrix_const_view` **gsl_matrix_const_view_vector_with_tda** (`const gsl_vector * v, size_t n1, size_t n2, size_t tda`) Function

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`) Function

`gsl_vector_const_view` **gsl_matrix_const_row** (`const gsl_matrix * m, size_t i`) Function

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_vector_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*) Function
`gsl_vector_const_view` **gsl_matrix_const_column** (`const gsl_matrix *` *m*, `size_t` *j*) Function

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_vector_const_column` equivalent to `gsl_matrix_column` but can be used for matrices which are declared `const`.

`gsl_vector_view` **gsl_matrix_diagonal** (`gsl_matrix *` *m*) Function
`gsl_vector_const_view` **gsl_matrix_const_diagonal** (`const gsl_matrix *` *m*) Function

These functions returns 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*) Function
`gsl_vector_const_view` **gsl_matrix_const_subdiagonal** (`const gsl_matrix *` *m*, `size_t` *k*) Function

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*) Function
`gsl_vector_const_view` **gsl_matrix_const_superdiagonal** (`const gsl_matrix *` *m*, `size_t` *k*) Function

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*) Function

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*, `const gsl_matrix *` *m2*) Function

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*) — Function

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*) — Function

This function copies the elements of the *i*-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*) — Function

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*) — Function

This function copies the elements of the vector *v* into the *i*-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*) — Function

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*) — Function

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*) — Function

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*, gsl_matrix * *src*) — Function

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*) Function

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.

8.4.10 Matrix operations

The following operations are only defined for real matrices.

int **gsl_matrix_add** (gsl_matrix * *a*, const gsl_matrix * *b*) Function

This function adds the elements of matrix *b* to the elements of matrix *a*, $a'(i,j) = a(i,j) + b(i,j)$. The two matrices must have the same dimensions.

int **gsl_matrix_sub** (gsl_matrix * *a*, const gsl_matrix * *b*) Function

This function subtracts the elements of matrix *b* from the elements of matrix *a*, $a'(i,j) = a(i,j) - b(i,j)$. The two matrices must have the same dimensions.

int **gsl_matrix_mul_elements** (gsl_matrix * *a*, const gsl_matrix * *b*) Function

This function multiplies the elements of matrix *a* by the elements of matrix *b*, $a'(i,j) = a(i,j) * b(i,j)$. The two matrices must have the same dimensions.

int **gsl_matrix_div_elements** (gsl_matrix * *a*, const gsl_matrix * *b*) Function

This function divides the elements of matrix *a* by the elements of matrix *b*, $a'(i,j) = a(i,j)/b(i,j)$. The two matrices must have the same dimensions.

int **gsl_matrix_scale** (gsl_matrix * *a*, const double *x*) Function

This function multiplies the elements of matrix *a* by the constant factor *x*, $a'(i,j) = xa(i,j)$.

int **gsl_matrix_add_constant** (gsl_matrix * *a*, const double *x*) Function

This function adds the constant value *x* to the elements of the matrix *a*, $a'(i,j) = a(i,j) + x$.

8.4.11 Finding maximum and minimum elements of matrices

double **gsl_matrix_max** (const gsl_matrix * *m*) Function

This function returns the maximum value in the matrix *m*.

double **gsl_matrix_min** (const gsl_matrix * *m*) Function

This function returns the minimum value in the matrix *m*.

void **gsl_matrix_minmax** (const gsl_matrix * *m*, double * *min_out*, double * *max_out*) Function

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*) Function

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.

void **gsl_matrix_min_index** (const gsl_matrix * *m*, size_t * *imax*, size_t * *jmax*) Function

This function returns the indices of the minimum value in the matrix *m*, storing them in *imax* and *jmax*. When there are several equal minimum elements then the first element found is returned.

void **gsl_matrix_minmax_index** (const gsl_matrix * *m*, size_t * *imin*, size_t * *imax*) Function

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.

8.4.12 Matrix properties

int **gsl_matrix_isnull** (const gsl_matrix * *m*) Function

This function returns 1 if all the elements of the matrix *m* are zero, and 0 otherwise.

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++)
    for (j = 0; j < 3; j++)
      printf("m(%d,%d) = %g\n", i, j,
             gsl_matrix_get (m, i, j));

  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.

```
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
IOT trap/Abort (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", "w");
     gsl_matrix_fwrite (f, m);
     fclose (f);
  }

  {
     FILE * f = fopen("test.dat", "r");
     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++;
      }

  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)
{
  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 %d, norm = %g\n", j, d);
    }

  gsl_matrix_free (m);
}
```

Here is the output of the program, which can be confirmed using GNU OCTAVE,

```
$ ./a.out
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
```

```
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
```

8.5 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.

9 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 .. $n-1$, 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

A permutation is stored 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*) Function

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*) Function

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*) Function

This function initializes the permutation p to the identity, i.e. $(0, 1, 2, \ldots, n-1)$.

`void` **gsl_permutation_free** (`gsl_permutation *` *p*) Function

This function frees all the memory used by the permutation p.

int **gsl_permutation_memcpy** (gsl_permutation * *dest*, const gsl_permutation * *src*) Function

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*) Function

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.

int **gsl_permutation_swap** (gsl_permutation * *p*, const size_t *i*, const size_t *j*) Function

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*) Function

This function returns the size of the permutation *p*.

size_t * **gsl_permutation_data** (const gsl_permutation * *p*) Function

This function returns a pointer to the array of elements in the permutation *p*.

int **gsl_permutation_valid** (gsl_permutation * *p*) Function

This function checks that the permutation *p* is valid. The *n* elements should contain each of the numbers 0 .. *n*-1 once and only once.

9.5 Permutation functions

void **gsl_permutation_reverse** (gsl_permutation * *p*) Function

This function reverses the elements of the permutation *p*.

int **gsl_permutation_inverse** (gsl_permutation * *inv*, const gsl_permutation * *p*) Function

This function computes the inverse of the permutation *p*, storing the result in *inv*.

int **gsl_permutation_next** (gsl_permutation * *p*) Function

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*) Function

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

`int` **gsl_permute** (`const size_t *` *p*, `double *` *data*, `size_t` *stride*, `size_t` *n*) Function

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*) Function

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*) Function

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*) Function

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_permutation_mul** (`gsl_permutation *` *p*, `const gsl_permutation *` *pa*, `const gsl_permutation *` *pb*) Function

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*) Function

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*) Function

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*) Function

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*. On a GNU system the type modifier `Z` represents `size_t`, so `"%Zu\n"` is a suitable format. The function returns `GSL_EFAILED` if there was a problem writing to the file.

int **gsl_permutation_fscanf** (FILE * *stream*, gsl_permutation * *p*) Function

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.

9.8 Permutations in Cyclic Form

A permutation can be represented in both linear and cyclic notations. The functions described in this section can be used to convert between the two forms.

The linear notation is an index mapping, and has already been described above. The cyclic notation represents a permutation as a series of circular rearrangements of groups of elements, or *cycles*.

Any permutation can be decomposed into a combination of 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*.

The cyclic notation for a permutation is not unique, but can be rearranged into a unique *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 between linear permutations defined by the canonical form has many important uses in the theory of permutations.

`int` **gsl_permutation_linear_to_canonical** (`gsl_permutation *` *q*, `const gsl_permutation *` *p*) — Function

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*) — Function

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*) — Function

This function counts the number of inversions in the permutation *p*.

`size_t` **gsl_permutation_linear_cycles** (`const gsl_permutation *` *p*) — Function

This function counts the number of cycles in the permutation *p*.

`size_t` **gsl_permutation_canonical_cycles** (`const gsl_permutation *` *q*) — Function

This function counts the number of cycles in the permutation *q*, where *q* is given in canonical form.

9.9 Examples

The example program below creates a random permutation by shuffling and finds its inverse.

```
#include <stdio.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#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");

  return 0;
}
```

Here is the output from the program,

```
bash$ ./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 3-rd order permutations, starting from the identity,

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

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);

   return 0;
 }
```

Here is the output from the program,

```
bash$ ./a.out
 0 1 2
 0 2 1
 1 0 2
 1 2 0
 2 0 1
 2 1 0
```

All 6 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 Knuth's *Sorting and Searching*,

> 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.

10 Combinations

This chapter describes functions for creating and manipulating combinations. A combination c is represented by an array of k integers in the range $0 .. n-1$, where each value c_i is from the range $0 .. n-1$ and 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

A combination is stored 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*) Function

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*) Function

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*) Function

This function initializes the combination c to the lexicographically first combination, i.e. $(0, 1, 2, ..., k-1)$.

`void` **gsl_combination_init_last** (`gsl_combination *` *c*) Function

This function initializes the combination c to the lexicographically last combination, i.e. $(n-k, n-k+1, ..., n-1)$.

`void` **gsl_combination_free** (`gsl_combination *` *c*) Function

This function frees all the memory used by the combination c.

10.3 Accessing combination elements

The following function can be used to access combinations elements.

`size_t` **gsl_combination_get** (`const gsl_combination *` *c*, `const size_t` *i*) Function

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.

10.4 Combination properties

`size_t` **gsl_combination_n** (`const gsl_combination *` *c*) Function

This function returns the *n* parameter of the combination *c*.

`size_t` **gsl_combination_k** (`const gsl_combination *` *c*) Function

This function returns the *k* parameter of the combination *c*.

`size_t *` **gsl_combination_data** (`const gsl_combination *` *c*) Function

This function returns a pointer to the array of elements in the combination *c*.

`int` **gsl_combination_valid** (`gsl_combination *` *c*) Function

This function checks that the combination *c* is valid. The *k* elements should contain numbers from range 0 .. *n*-1, each number at most once. The numbers have to be in increasing order.

10.5 Combination functions

`int` **gsl_combination_next** (`gsl_combination *` *c*) Function

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 fisrst combination and repeatedly applying this function will iterate through all possible combinations of a given order.

`int` **gsl_combination_prev** (`gsl_combination *` *c*) Function

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*) Function

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*) Function

This function reads into the combination *c* from the open stream *stream* 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*) Function

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*. On a GNU system the type modifier Z represents size_t, so "%Zu\n" is a suitable format. The function returns GSL_EFAILED if there was a problem writing to the file.

int **gsl_combination_fscanf** (FILE * *stream*, gsl_combination * *c*) Function

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 $\{1, 2, 3, 4\}$ 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);
      gsl_combination_free(c);
    }

  return 0;
}
```

Here is the output from the program,

```
bash$ ./a.out
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.

11 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. It does not require any additional storage and provides consistent performance. The running time for its worst-case (ordered data) is 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.

11.1 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*) — Function

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,

```
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*) — Function

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.

11.2 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*, `size_t` *stride*, `size_t` *n*) — Function

This function sorts the *n* elements of the array *data* with stride *stride* into ascending numerical order.

`void` **gsl_sort_vector** (`gsl_vector *` *v*) — Function

This function sorts the elements of the vector *v* into ascending numerical order.

`int` **gsl_sort_index** (`size_t *` *p*, `const double *` *data*, `size_t` *stride*, `size_t` *n*) — Function

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 to 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`) Function

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.

11.3 Selecting the k-th smallest or largest elements

The functions described in this section select the k-th 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.

void **gsl_sort_smallest** (`double * dest, size_t k, const double * src, size_t stride, size_t n`) Function

This function copies the k-th smallest elements of the array *src*, of size *n* and stride *stride*, in ascending numerical order in *dest*. The size of the subset *k* must be less than or equal to *n*. The data *src* is not modified by this operation.

void **gsl_sort_largest** (`double * dest, size_t k, const double * src, size_t stride, size_t n`) Function

This function copies the k-th largest elements of the array *src*, of size *n* and stride *stride*, in descending numerical order in *dest*. The size of the subset *k* must be less than or equal to *n*. The data *src* is not modified by this operation.

void **gsl_sort_vector_smallest** (`double * dest, size_t k, const gsl_vector * v`) Function

void **gsl_sort_vector_largest** (`double * dest, size_t k, const gsl_vector * v`) Function

These functions copy the k-th smallest or largest elements of the vector *v* into the array *dest*. The size of the subset *k* must be less than or equal to the length of the vector *v*.

The following functions find the indices of the k-th smallest or largest elements of a dataset,

void **gsl_sort_smallest_index** (`size_t * p, size_t k, const double * src, size_t stride, size_t n`) Function

This function stores the indices of the k-th 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. The size of the subset *k* must be less than or equal to *n*. The data *src* is not modified by this operation.

void **gsl_sort_largest_index** (size_t * *p*, size_t *k*, const double * *src*, size_t *stride*, size_t *n*) Function

This function stores the indices of the *k*-th 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. The size of the subset *k* must be less than or equal to *n*. The data *src* is not modified by this operation.

void **gsl_sort_vector_smallest_index** (size_t * *p*, size_t *k*, const gsl_vector * *v*) Function

void **gsl_sort_vector_largest_index** (size_t * *p*, size_t *k*, const gsl_vector * *v*) Function

These functions store the indices of *k*-th smallest or largest elements of the vector *v* in the array *p*. The size of the subset *k* must be less than or equal to the length of the vector *v*.

11.4 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);
}
```

11.5 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;

  int i, k = 5, N = 100000;

  double * x = malloc (N * sizeof(double));
  double * small = malloc (k * sizeof(double));

  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("%d smallest values from %d\n", k, N);

  for (i = 0; i < k; i++)
    {
      printf ("%d: %.18f\n", i, small[i]);
    }
  return 0;
}
```

The output lists the 5 smallest values, in ascending order,

```
$ ./a.out
5 smallest values from 100000
0: 0.000005466630682349
1: 0.000012384494766593
2: 0.000017581274732947
3: 0.000025131041184068
4: 0.000031369971111417
```

11.6 References and Further Reading

The subject of sorting is covered extensively in Knuth's *Sorting and Searching*,

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.

12 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, which is declared in the file `gsl_blas.h`. This 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.

The interface for the `gsl_cblas` layer is specified in the file `gsl_cblas.h`. This interface corresponds the BLAS Technical Forum's draft 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 draft CBLAS standard and can be obtained from Netlib. The complete set of CBLAS functions is listed in an appendix (see Appendix D [GSL CBLAS Library], page 404).

There are three levels of BLAS operations,

Level 1 Vector operations, e.g. $y = \alpha x + y$

Level 2 Matrix-vector operations, e.g. $y = \alpha A x + \beta y$

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 type of matrices are,

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".

12.1 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`.

12.1.1 Level 1

`int` **gsl_blas_sdsdot** (`float` *alpha*, `const gsl_vector_float *` *x*, `const gsl_vector_float *` *y*, `float *` *result*) — Function

`int` **gsl_blas_dsdot** (`const gsl_vector_float *` *x*, `const gsl_vector_float *` *y*, `double *` *result*) — Function

These functions compute 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*) — Function

`int` **gsl_blas_ddot** (`const gsl_vector *` *x*, `const gsl_vector *` *y*, `double *` *result*) — Function

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*) — Function

`int` **gsl_blas_zdotu** (`const gsl_vector_complex *` *x*, `const gsl_vector_complex *` *y*, `gsl_complex *` *dotu*) — Function

These functions compute the complex scalar product $x^T y$ for the vectors *x* and *y*, returning the result in *result* `int` **gsl_blas_cdotc** (`const gsl_vector_complex_float *` *x*, `const gsl_vector_complex_float *` *y*, `gsl_complex_float *` *dotc*) Function

`int` **gsl_blas_zdotc** (`const gsl_vector_complex *` *x*, `const gsl_vector_complex *` *y*, `gsl_complex *` *dotc*) Function

These functions compute the complex conjugate scalar product $x^H y$ for the vectors *x* and *y*, returning the result in *result*

`float` **gsl_blas_snrm2** (`const gsl_vector_float *` *x*) Function

`double` **gsl_blas_dnrm2** (`const gsl_vector *` *x*) Function

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*) Function

`double` **gsl_blas_dznrm2** (`const gsl_vector_complex *` *x*) Function

These functions compute the Euclidean norm of the complex vector *x*,

$$||x||_2 = \sqrt{\sum (\mathrm{Re}(x_i)^2 + \mathrm{Im}(x_i)^2)}.$$

`float` **gsl_blas_sasum** (`const gsl_vector_float *` *x*) Function

`double` **gsl_blas_dasum** (`const gsl_vector *` *x*) Function

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*) Function

`double` **gsl_blas_dzasum** (`const gsl_vector_complex *` *x*) Function

These functions compute the absolute sum $\sum |\mathrm{Re}(x_i)| + |\mathrm{Im}(x_i)|$ of the elements of the vector *x*.

`CBLAS_INDEX_t` **gsl_blas_isamax** (`const gsl_vector_float *` *x*) Function

`CBLAS_INDEX_t` **gsl_blas_idamax** (`const gsl_vector *` *x*) Function

`CBLAS_INDEX_t` **gsl_blas_icamax** (`const gsl_vector_complex_float *` *x*) Function

`CBLAS_INDEX_t` **gsl_blas_izamax** (`const gsl_vector_complex *` *x*) Function

These functions return the index of the largest element of the vector *x*. The largest element is determined by its absolute magnitude for real vector and by the sum of the magnitudes of the real and imaginary parts $|\mathrm{Re}(x_i)| + |\mathrm{Im}(x_i)|$ 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*) Function

`int` **gsl_blas_dswap** (`gsl_vector *` *x*, `gsl_vector *` *y*) Function

`int` **gsl_blas_cswap** (`gsl_vector_complex_float *` *x*, `gsl_vector_complex_float *` *y*) Function

`int` **gsl_blas_zswap** (`gsl_vector_complex *` *x*, `gsl_vector_complex *` *y*) Function

These functions exchange the elements of the vectors *x* and *y*.

int **gsl_blas_scopy** (const gsl_vector_float * *x*, gsl_vector_float * *y*) Function
int **gsl_blas_dcopy** (const gsl_vector * *x*, gsl_vector * *y*) Function
int **gsl_blas_ccopy** (const gsl_vector_complex_float * *x*, gsl_vector_complex_float * *y*) Function
int **gsl_blas_zcopy** (const gsl_vector_complex * *x*, gsl_vector_complex * *y*) Function

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*) Function
int **gsl_blas_daxpy** (double *alpha*, const gsl_vector * *x*, gsl_vector * *y*) Function
int **gsl_blas_caxpy** (const gsl_complex_float *alpha*, const gsl_vector_complex_float * *x*, gsl_vector_complex_float * *y*) Function
int **gsl_blas_zaxpy** (const gsl_complex *alpha*, const gsl_vector_complex * *x*, gsl_vector_complex * *y*) Function

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*) Function
void **gsl_blas_dscal** (double *alpha*, gsl_vector * *x*) Function
void **gsl_blas_cscal** (const gsl_complex_float *alpha*, gsl_vector_complex_float * *x*) Function
void **gsl_blas_zscal** (const gsl_complex *alpha*, gsl_vector_complex * *x*) Function
void **gsl_blas_csscal** (float *alpha*, gsl_vector_complex_float * *x*) Function
void **gsl_blas_zdscal** (double *alpha*, gsl_vector_complex * *x*) Function

These functions rescale the vector *x* by the multiplicative factor *alpha*.

int **gsl_blas_srotg** (float a[], float b[], float c[], float s[]) Function
int **gsl_blas_drotg** (double a[], double b[], double c[], double s[]) Function

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*) Function
int **gsl_blas_drot** (gsl_vector * *x*, gsl_vector * *y*, const double *c*, const double *s*) Function

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[]) Function
int **gsl_blas_drotmg** (double d1[], double d2[], double b1[], double *b2*, double P[]) Function

These functions compute a modified Given's transformation.

int **gsl_blas_srotm** (gsl_vector_float * *x*, gsl_vector_float * *y*, const float P[]) Function

int **gsl_blas_drotm** (gsl_vector * *x*, gsl_vector * *y*, const double P[]) Function

These functions apply a modified Given's transformation.

12.1.2 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*) Function

int **gsl_blas_dgemv** (CBLAS_TRANSPOSE_t *TransA*, double *alpha*, const gsl_matrix * *A*, const gsl_vector * *x*, double *beta*, gsl_vector * *y*) Function

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*) Function

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*) Function

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*) Function

int **gsl_blas_dtrmv** (CBLAS_UPLO_t *Uplo*, CBLAS_TRANSPOSE_t *TransA*, CBLAS_DIAG_t *Diag*, const gsl_matrix * *A*, gsl_vector * *x*) Function

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*) Function

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*) Function

These functions compute the matrix-vector product $x = \alpha op(A)x$ 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*) Function

int **gsl_blas_dtrsv** (CBLAS_UPLO_t *Uplo*, CBLAS_TRANSPOSE_t *TransA*, CBLAS_DIAG_t *Diag*, const gsl_matrix * *A*, gsl_vector * *x*) Function

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*) Function

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*) Function

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*) Function

int **gsl_blas_dsymv** (CBLAS_UPLO_t *Uplo*, double *alpha*, const gsl_matrix * *A*, const gsl_vector * *x*, double *beta*, gsl_vector * *y*) Function

These functions compute the matrix-vector product and sum $y = \alpha Ax + \beta y$ 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*) Function

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*) Function

These functions compute the matrix-vector product and sum $y = \alpha Ax + \beta y$ 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*) Function

int **gsl_blas_dger** (double *alpha*, const gsl_vector * *x*, const gsl_vector * *y*, gsl_matrix * *A*) Function

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*) Function

int **gsl_blas_zgeru** (const gsl_complex *alpha*, const gsl_vector_complex * *x*, const gsl_vector_complex * *y*, gsl_matrix_complex * *A*) Function

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*) Function

int **gsl_blas_zgerc** (const gsl_complex *alpha*, const gsl_vector_complex * *x*, const gsl_vector_complex * *y*, gsl_matrix_complex * *A*) Function

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*) Function

int **gsl_blas_dsyr** (CBLAS_UPLO_t *Uplo*, double *alpha*, const gsl_vector * *x*, gsl_matrix * *A*) Function

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*) Function

int **gsl_blas_zher** (CBLAS_UPLO_t *Uplo*, double *alpha*, const gsl_vector_complex * *x*, gsl_matrix_complex * *A*) Function

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*) Function

int **gsl_blas_dsyr2** (CBLAS_UPLO_t *Uplo*, double *alpha*, const gsl_vector * *x*, const gsl_vector * *y*, gsl_matrix * *A*) Function

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*) Function

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*) Function

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.

12.1.3 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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

These functions compute the matrix-matrix product $B = \alpha op(A) B$ for *Side* is CblasLeft and $B = \alpha B op(A)$ 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*) Function

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*) Function

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*) Function

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*) Function

These functions compute the matrix-matrix product $B = \alpha op(inv(A)) B$ for *Side* is CblasLeft and $B = \alpha B op(inv(A))$ 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*) Function

int **gsl_blas_dsyrk** (`CBLAS_UPLO_t` *Uplo*, `CBLAS_TRANSPOSE_t` *Trans*, `double` *alpha*, `const gsl_matrix *` *A*, `double` *beta*, `gsl_matrix *` *C*) Function

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*) Function

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*) Function

These functions compute a rank-k update of the symmetric matrix C, $C = \alpha A A^T + \beta C$ 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*) Function

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*) Function

These functions compute a rank-k update of the hermitian matrix C, $C = \alpha A A^H + \beta C$ when *Trans* is `CblasNoTrans` and $C = \alpha A^H A + \beta C$ when *Trans* is `CblasTrans`. 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*) Function

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*) Function

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*) Function

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*) Function

These functions compute a rank-2k update of the symmetric matrix C, $C = \alpha A B^T + \alpha B A^T + \beta C$ 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) — Function

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) — Function

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 `CblasTrans`. 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.

12.2 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,

```
$ ./a.out
[ 367.76, 368.12
  674.06, 674.72 ]
```

12.3 References and Further Reading

Information on the BLAS standards, including both the legacy and draft 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/cgi-bin/checkout/blast/blast.pl`

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.

13 Linear Algebra

This chapter describes functions for solving linear systems. The library provides simple linear algebra operations which operate directly on the `gsl_vector` and `gsl_matrix` objects. These are intended for use with "small" systems where simple algorithms are acceptable.

Anyone interested in large systems will want to use the sophisticated routines found in LAPACK. The Fortran version of LAPACK is recommended as the standard package for linear algebra. It supports blocked algorithms, specialized data representations and other optimizations.

The functions described in this chapter are declared in the header file '`gsl_linalg.h`'.

13.1 LU Decomposition

A general square matrix A has an LU decomposition into upper and lower triangular matrices,

$$PA = LU$$

where P is a permutation matrix, L is unit lower triangular matrix and U is upper triangular matrix. 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.

`int` **gsl_linalg_LU_decomp** (`gsl_matrix *` *A*, `gsl_permutation *` *p*, `int *`*signum*) — Function

`int` **gsl_linalg_complex_LU_decomp** (`gsl_matrix_complex *` *A*, `gsl_permutation *` *p*, `int *`*signum*) — Function

These functions factorize the square matrix A into the LU decomposition $PA = LU$. On output the diagonal and upper triangular part of the input matrix A contain the matrix U. The lower triangular 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. 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).

`int` **gsl_linalg_LU_solve** (`const gsl_matrix *` *LU*, `const gsl_permutation *` *p*, `const gsl_vector *` *b*, `gsl_vector *` *x*) — Function

`int` **gsl_linalg_complex_LU_solve** (`const gsl_matrix_complex *` *LU*, `const gsl_permutation *` *p*, `const gsl_vector_complex *` *b*, `gsl_vector_complex *` *x*) — Function

These functions solve the system $Ax = b$ using the LU decomposition of A into (LU, p) given by `gsl_linalg_LU_decomp` or `gsl_linalg_complex_LU_decomp`.

int **gsl_linalg_LU_svx** (const gsl_matrix * *LU*, const gsl_permutation * *p*, gsl_vector * *x*) Function

int **gsl_linalg_complex_LU_svx** (const gsl_matrix_complex * *LU*, const gsl_permutation * *p*, gsl_vector_complex * *x*) Function

These functions solve the system $Ax = b$ in-place using the 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 * *residual*) Function

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 * *residual*) Function

These functions apply an iterative improvement to *x*, the solution of $Ax = b$, using the LU decomposition of A into (*LU*,*p*). The initial residual $r = Ax - b$ is also computed and stored in *residual*.

int **gsl_linalg_LU_invert** (const gsl_matrix * *LU*, const gsl_permutation * *p*, gsl_matrix * *inverse*) Function

int **gsl_complex_linalg_LU_invert** (const gsl_matrix_complex * *LU*, const gsl_permutation * *p*, gsl_matrix_complex * *inverse*) Function

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 solving the system $Ax = b$ for each column of the identity matrix. It is preferable to avoid direct computation of the inverse whenever possible.

double **gsl_linalg_LU_det** (gsl_matrix * *LU*, int *signum*) Function

gsl_complex **gsl_linalg_complex_LU_det** (gsl_matrix_complex * *LU*, int *signum*) Function

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*) Function

double **gsl_linalg_complex_LU_lndet** (gsl_matrix_complex * *LU*) Function

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*) Function

`gsl_complex` **gsl_linalg_complex_LU_sgndet** (`gsl_matrix_complex *` *LU*, `int` *signum*) Function

These functions compute the sign or phase factor of the determinant of a matrix A, $det(A)/|det(A)|$, from its LU decomposition, LU.

13.2 QR Decomposition

A general rectangular M-by-N matrix A has a QR decomposition into the product of an orthogonal M-by-M square matrix Q (where $Q^T Q = I$) and an M-by-N right-triangular matrix R,

$$A = QR$$

This decomposition can be used to convert the linear system $Ax = b$ into the triangular system $Rx = Q^T b$, 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.

`int` **gsl_linalg_QR_decomp** (`gsl_matrix *` *A*, `gsl_vector *` *tau*) Function

This function factorizes 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 $k = \min(M, N)$. 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 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*) Function

This function solves the system $Ax = b$ using the QR decomposition of A into (QR, *tau*) given by `gsl_linalg_QR_decomp`.

`int` **gsl_linalg_QR_svx** (`const gsl_matrix *` *QR*, `const gsl_vector *` *tau*, `gsl_vector *` *x*) Function

This function solves the system $Ax = b$ in-place using the QR decomposition of A into (QR,*tau*) given by `gsl_linalg_QR_decomp`. 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*) Function

This function finds 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 uses the QR decomposition of A into (QR, *tau*) given by `gsl_linalg_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*) Function

This function applies the matrix Q^T encoded in the decomposition (QR,*tau*) to the vector *v*, storing the result $Q^T v$ 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.

int **gsl_linalg_QR_Qvec** (const gsl_matrix * *QR*, const gsl_vector * *tau*, gsl_vector * *v*) Function

This function applies 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_Rsolve** (const gsl_matrix * *QR*, const gsl_vector * *b*, gsl_vector * *x*) Function

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*) Function

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*) Function

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*) Function

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*) Function

This function performs a rank-1 update wv^T of the QR decomposition (Q, R). The update is given by $Q'R' = QR + wv^T$ 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*) Function

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*) Function

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.

13.3 QR Decomposition with Column Pivoting

The QR decomposition can be extended to the rank deficient case by introducing a column permutation P,

$$AP = QR$$

The first r columns of this 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 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 $A = QRP^T$.

`int` **gsl_linalg_QRPT_decomp** (`gsl_matrix *` *A*, `gsl_vector *` *tau*, `gsl_permutation *` *p*, `int *`*signum*, `gsl_vector *` *norm*) Function

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. On output the norms of each column of R are stored in the vector *norm*.

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*) Function

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*) Function

This function solves the system $Ax = b$ using the QRP^T decomposition of A into (QR, *tau*, p) given 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*) Function

This function solves the system $Ax = b$ in-place using the QRP^T decomposition of A into (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_QRsolve** (const gsl_matrix * *Q*, const gsl_matrix * *R*, const gsl_permutation * *p*, const gsl_vector * *b*, gsl_vector * *x*) Function

This function solves the system $RP^T x = Q^T b$ for x. It can be used when the QR decomposition of a matrix is available in unpacked form as (Q,R).

int **gsl_linalg_QRPT_update** (gsl_matrix * *Q*, gsl_matrix * *R*, const gsl_permutation * *p*, gsl_vector * *u*, const gsl_vector * *v*) Function

This function performs a rank-1 update wv^T of the QRP^T decomposition (Q, R,p). The update is given by $Q'R' = QR + wv^T$ 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*) Function

This function solves the triangular system $RP^T x = b$ 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*) Function

This function solves the triangular system $RP^T x = b$ 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.

13.4 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.

int **gsl_linalg_SV_decomp** (gsl_matrix * A, gsl_matrix * V, gsl_vector * S, gsl_vector * *work*) Function

This function factorizes the M-by-N matrix A into the singular value decomposition $A = USV^T$. 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*) Function

This function computes the SVD using the modified Golub-Reinsch algorithm, which is faster for $M >> N$. It requires the vector *work* 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) Function

This function computes the SVD using one-sided Jacobi orthogonalization (see references for details). The Jacobi method can compute singular values to higher relative accuracy than Golub-Reinsch algorithms.

int **gsl_linalg_SV_solve** (gsl_matrix * U, gsl_matrix * V, gsl_vector * S, const gsl_vector * b, gsl_vector * x) Function

This function solves the system $Ax = b$ using the singular value decomposition (U, S, V) of A given by `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 $||Ax - b||_2$.

13.5 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 ($Ly = b$, $L^T x = y$), which can be solved by forward and back-substitution.

int **gsl_linalg_cholesky_decomp** (gsl_matrix * A) Function

This function factorizes the positive-definite square matrix A into the Cholesky decomposition $A = LL^T$. On output the diagonal and lower triangular part of the input matrix A contain the matrix L. The upper triangular part of the input matrix contains 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`.

int gsl_linalg_cholesky_solve (const gsl_matrix * *cholesky*, const gsl_vector * *b*, gsl_vector * *x*) Function

This function solves the system $Ax = b$ using the Cholesky decomposition of A into the matrix *cholesky* given by `gsl_linalg_cholesky_decomp`.

int gsl_linalg_cholesky_svx (const gsl_matrix * *cholesky*, gsl_vector * *x*) Function

This function solves the system $Ax = b$ in-place using the Cholesky decomposition of A into the matrix *cholesky* given by `gsl_linalg_cholesky_decomp`. On input *x* should contain the right-hand side *b*, which is replaced by the solution on output.

13.6 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*) Function

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*) Function

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*) Function

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*.

13.7 Tridiagonal Decomposition of Hermitian Matrices

A hermitian matrix A can be factorized by similarity transformations into the form,

$$A = UTU^T$$

where U is an unitary matrix and T is a real symmetric tridiagonal matrix.

int **gsl_linalg_hermtd_decomp** (gsl_matrix_complex * *A*, gsl_vector_complex * *tau*) Function

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 orthogonal matrix Q. 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 * *Q*, gsl_vector * *diag*, gsl_vector * *subdiag*) Function

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*) Function

This function unpacks the diagonal and subdiagonal of the encoded tridiagonal decomposition (A, *tau*) obtained from `gsl_linalg_hermtd_decomp` into the real vectors *diag* and *subdiag*.

13.8 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*) Function

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*) Function

This function unpacks the bidiagonal decomposition of *A* given 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*.

int **gsl_linalg_bidiag_unpack2** (gsl_matrix * *A*, gsl_vector * *tau_U*, gsl_vector * *tau_V*, gsl_matrix * *V*) Function

This function unpacks the bidiagonal decomposition of *A* given 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*) Function

This function unpacks the diagonal and superdiagonal of the bidiagonal decomposition of *A* given by `gsl_linalg_bidiag_decomp`, into the diagonal vector *diag* and superdiagonal vector *superdiag*.

13.9 Householder solver for linear systems

int **gsl_linalg_HH_solve** (gsl_matrix * *A*, const gsl_vector * *b*, gsl_vector * *x*) Function

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*) Function

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.

13.10 Tridiagonal Systems

int **gsl_linalg_solve_symm_tridiag** (const gsl_vector * *diag*, const gsl_vector * *e*, const gsl_vector * *b*, gsl_vector * *x*) Function

This function solves the general N-by-N system $Ax = b$ where A is symmetric tridiagonal. The form of A for the 4-by-4 case is shown below,

$$A = \begin{pmatrix} d_0 & e_0 & & \\ e_0 & d_1 & e_1 & \\ & e_1 & d_2 & e_2 \\ & & e_2 & d_3 \end{pmatrix}$$

int gsl_linalg_solve_symm_cyc_tridiag (const gsl_vector * *diag*, const gsl_vector * *e*, const gsl_vector * *b*, gsl_vector * *x*) Function

This function solves the general N-by-N system $Ax = b$ where A is symmetric cyclic tridiagonal. The form of A for the 4-by-4 case is shown below,

$$A = \begin{pmatrix} d_0 & e_0 & & e_3 \\ e_0 & d_1 & e_1 & \\ & e_1 & d_2 & e_2 \\ e_3 & & e_2 & d_3 \end{pmatrix}$$

13.11 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);

  gsl_linalg_LU_solve (&m.matrix, p, &b.vector, x);

  printf ("x = \n");
```

```
    gsl_vector_fprintf(stdout, x, "%g");

    gsl_permutation_free (p);
    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 $Ax = b$.

13.12 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,

LAPACK Users' Guide (Third Edition, 1999), Published by SIAM, ISBN 0-89871-447-8.

`http://www.netlib.org/lapack`

The LAPACK source code can be found at the website above, along with an online copy of the users guide.

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 (1973), p 74—76

James Demmel, Kresimir 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.

14 Eigensystems

This chapter describes functions for computing eigenvalues and eigenvectors of matrices. There are routines for real symmetric and complex hermitian matrices, and eigenvalues can be computed with or without eigenvectors. The algorithms used are symmetric bidiagonalization followed by QR reduction.

These routines are intended for "small" systems where simple algorithms are acceptable. Anyone interested finding eigenvalues and eigenvectors of large matrices will want to use the sophisticated routines found in LAPACK. The Fortran version of LAPACK is recommended as the standard package for linear algebra.

The functions described in this chapter are declared in the header file '`gsl_eigen.h`'.

14.1 Real Symmetric Matrices

`gsl_eigen_symm_workspace *` **gsl_eigen_symm_alloc** (`const size_t` *n*) — Function

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*) — Function

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*) — Function

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.

`gsl_eigen_symmv_workspace *` **gsl_eigen_symmv_alloc** (`const size_t` *n*) — Function

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*) — Function

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*) — Function

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.

14.2 Complex Hermitian Matrices

gsl_eigen_herm_workspace * **gsl_eigen_herm_alloc** (const size_t *n*) Function

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*) Function

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*) Function

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.

gsl_eigen_hermv_workspace * **gsl_eigen_hermv_alloc** (const size_t *n*) Function

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*) Function

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*) Function

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.

14.3 Sorting Eigenvalues and Eigenvectors

int **gsl_eigen_symmv_sort** (gsl_vector * *eval*, gsl_matrix * *evec*, gsl_eigen_sort_t *sort_type*) Function

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*,

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*) Function

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.

14.4 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);

    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");
        }
    }

    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
```

```
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.

14.5 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,

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`http://www.netlib.org/lapack`

The LAPACK source code can be found at the website above along with an online copy of the users guide.

15 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 by 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 Section 15.8 [FFT References and Further Reading], page 160)

15.1 Mathematical Definitions

Fast Fourier Transforms are efficient algorithms for calculating the discrete fourier transform (DFT),

$$x_j = \sum_{k=0}^{N-1} z_k \exp(-2\pi i j k/N)$$

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 $f_1 f_2 \ldots f_n$ 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,

$$x_j = \sum_{k=0}^{N-1} z_k \exp(-2\pi i j k/N)$$

and the definition of the *inverse fourier transform*, $x = \mathrm{IFFT}(z)$, is,

$$z_j = \frac{1}{N} \sum_{k=0}^{N-1} x_k \exp(2\pi i j k/N).$$

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.

15.2 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,

```
gsl_complex_packed_array data[6];
```

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])
```

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.

The array indices have the same ordering as those in the definition of the DFT — i.e. there are no index transformations or permutations of the data.

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))
.        ........        ..................
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.

15.3 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 these functions 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*) Function

`int` **gsl_fft_complex_radix2_transform** (`gsl_complex_packed_array` *data*[], `size_t` *stride*, `size_t` *n*) Function

`int` **gsl_fft_complex_radix2_backward** (`gsl_complex_packed_array` *data*[], `size_t` *stride*, `size_t` *n*) Function

`int` **gsl_fft_complex_radix2_inverse** (`gsl_complex_packed_array` *data*[], `size_t` *stride*, `size_t` *n*) Function

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.

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*) Function

`int` **gsl_fft_complex_radix2_dif_transform** (`gsl_complex_packed_array` *data*[], `size_t` *stride*, `size_t` *n*) Function

`int` **gsl_fft_complex_radix2_dif_backward** (`gsl_complex_packed_array` *data*[], `size_t` *stride*, `size_t` *n*) Function

`int` **gsl_fft_complex_radix2_dif_inverse** (`gsl_complex_packed_array` *data*[], `size_t` *stride*, `size_t` *n*) Function

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>
```

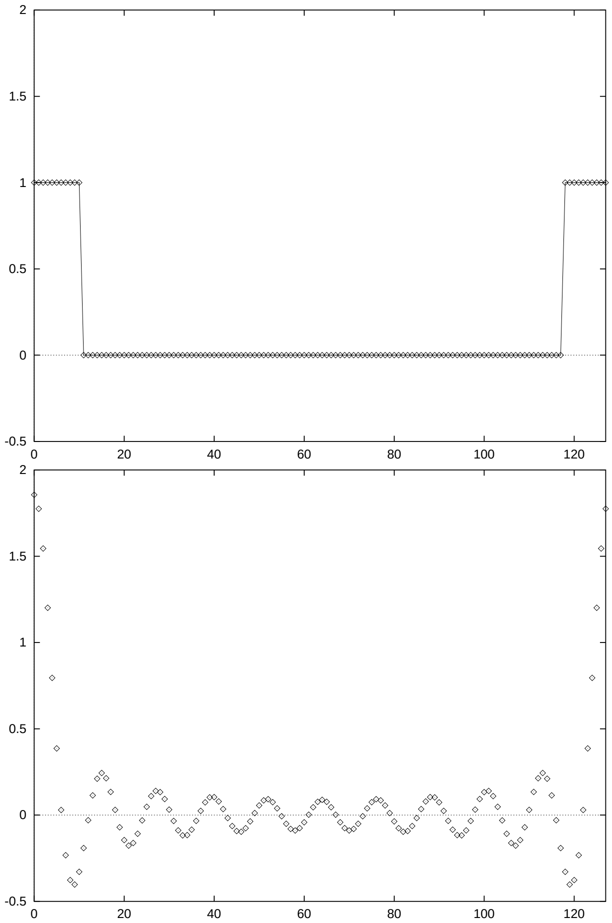
```
#include <gsl/gsl_fft_complex.h>

#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");

  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 sin function.

$$\int_{-a}^{+a} e^{-2\pi ikx} dx = \frac{\sin(2\pi ka)}{\pi k}$$



A pulse and its discrete fourier transform, output from the example program.

15.4 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 the Fortran FFTPACK library by Paul Swarztrauber. 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 these functions are declared in the header file '`gsl_fft_complex.h`'.

`gsl_fft_complex_wavetable *` **gsl_fft_complex_wavetable_alloc** (`size_t` *n*) Function

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*) Function

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`'.

gsl_fft_complex_wavetable Data Type

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.

The mixed radix algorithms require an additional working space to hold the intermediate steps of the transform.

`gsl_fft_complex_workspace *` **gsl_fft_complex_workspace_alloc** (`size_t` *n*) Function

This function allocates a workspace for a complex transform of length *n*.

`void` **gsl_fft_complex_workspace_free** (`gsl_fft_complex_workspace *` *workspace*) Function

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*) Function

`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*) Function

`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*) Function

`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*) Function

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*.

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>

#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].real = 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 < wavetable->nf; i++)
      {
         printf("# factor %d: %d\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);
    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.

15.5 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,

$$c_k = \sum_{j=0}^{N-1} x_k \exp(-2\pi i jk/N)$$

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 constrain 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. This is desirable for better locality of memory accesses.

15.6 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*) Function

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,

```
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].real  =    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]
```

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*) Function

int **gsl_fft_halfcomplex_radix2_backward** (double *data*[], size_t *stride*, size_t *n*) Function

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.

15.7 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, $n = 5$ 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`'.

`gsl_fft_real_wavetable *` **gsl_fft_real_wavetable_alloc** (`size_t` *n*) — Function

`gsl_fft_halfcomplex_wavetable *` **gsl_fft_halfcomplex_wavetable_alloc** (`size_t` *n*) — Function

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*) — Function

`void` **gsl_fft_halfcomplex_wavetable_free** (`gsl_fft_halfcomplex_wavetable *` *wavetable*) — Function

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 an additional working space to hold the intermediate steps of the transform,

gsl_fft_real_workspace * **gsl_fft_real_workspace_alloc** (size_t *n*) — Function

This function allocates a workspace for a real transform of length *n*. The same workspace is used for both forward real and inverse halfcomplex transforms.

void **gsl_fft_real_workspace_free** (gsl_fft_real_workspace * *workspace*) — Function

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*) — Function

int **gsl_fft_halfcomplex_transform** (double *data*[], size_t *stride*, size_t *n*, const gsl_fft_halfcomplex_wavetable * *wavetable*, gsl_fft_real_workspace * *work*) — Function

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*) — Function

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].real
      = real_coefficient[i];
    complex_coefficient[i].imag
      = 0.0;
  }
```

int **gsl_fft_halfcomplex_unpack** (const double *halfcomplex_coefficient*[], gsl_complex_packed_array *complex_coefficient*[], size_t *stride*, size_t *n*) — Function

This function converts *halfcomplex_coefficient*, an array of half-complex coefficients as returned by `gsl_fft_real_transform`, into an ordinary complex array, *com-*

plex_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,

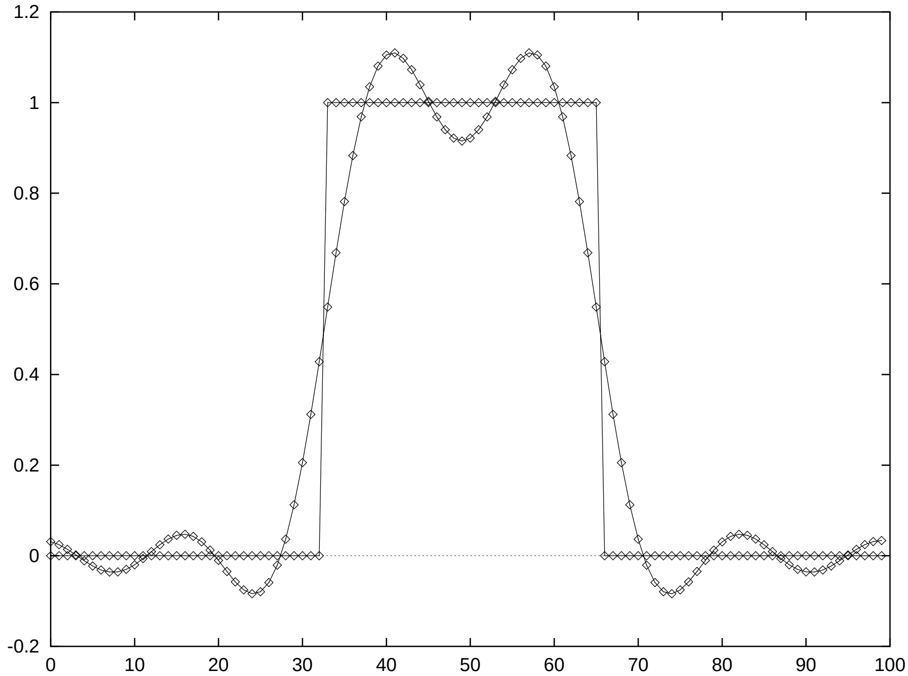
```
complex_coefficient[0].real
  = halfcomplex_coefficient[0];
complex_coefficient[0].imag
  = 0.0;

for (i = 1; i < n - i; i++)
  {
    double hc_real
      = halfcomplex_coefficient[2 * i - 1];
    double hc_imag
      = halfcomplex_coefficient[2 * i];
    complex_coefficient[i].real = hc_real;
    complex_coefficient[i].imag = hc_imag;
    complex_coefficient[n - i].real = hc_real;
    complex_coefficient[n - i].imag = -hc_imag;
  }

if (i == n - i)
  {
    complex_coefficient[i].real
      = halfcomplex_coefficient[n - 1];
    complex_coefficient[i].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);
    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;
  }
```



Low-pass filtered version of a real pulse,
output from the example program.

15.8 References and Further Reading

A good starting point for learning more about the FFT is the review article *Fast Fourier Transforms: A Tutorial Review and A State of the Art* by Duhamel and Vetterli,

> 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 latex 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 serious 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/`

16 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, Doncker-Kapenga, Uberhuber and Kahaner. Fortran code for QUADPACK is available on Netlib.

The functions described in this chapter are declared in the header file '`gsl_integration.h`'.

16.1 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,

$$|RESULT - I| \leq ABSERR \leq \max(epsabs, epsrel|I|)$$

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

`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.

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.

For integrands with weight functions the algorithms use Clenshaw-Curtis quadrature rules. A Clenshaw-Curtis rule begins with an n-th order Chebyschev polynomial approximation to the integrand. This polynomial can be integrated exactly to give an approximation to the integral of the original function. The Chebyschev expansion can be extended to higher orders to improve the approximation. The presence of singularities (or other behavior) in the integrand can cause slow convergence in the Chebyschev 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 Chebyschev polynomials to precompute *modified Chebyschev moments*. Combining the moments with the Chebyschev 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.

16.2 QNG non-adaptive Gauss-Kronrod integration

The QNG algorithm is non-adaptive procedure which uses fixed Gauss-Kronrod 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*) Function

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.

16.3 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 a `gsl_integration_workspace` struct, which handles the memory for the subinterval ranges, results and error estimates.

`gsl_integration_workspace * ` **gsl_integration_workspace_alloc** `(size_t` *n*`)` Function

This function allocates a workspace sufficient to hold *n* double precision intervals, their integration results and error estimates.

`void` **gsl_integration_workspace_free** `(gsl_integration_workspace *` *w*`)` Function

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*`)` Function

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,

```
GSL_INTEG_GAUSS15  (key = 1)
GSL_INTEG_GAUSS21  (key = 2)
GSL_INTEG_GAUSS31  (key = 3)
GSL_INTEG_GAUSS41  (key = 4)
GSL_INTEG_GAUSS51  (key = 5)
GSL_INTEG_GAUSS61  (key = 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.

16.4 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*`)` Function

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.

16.5 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*) Function

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 `QAGS`.

16.6 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*) Function

This function computes the integral of the function *f* over the infinite interval $(-\infty, +\infty)$. The integral is mapped onto the 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*) Function

This function computes the integral of the function f over the semi-infinite interval $(a,+\infty)$. The integral is mapped onto the 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*) Function

This function computes the integral of the function f over the semi-infinite interval $(-\infty,b)$. The integral is mapped onto the region $(0,1]$ 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.

16.7 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*) Function

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.

16.8 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 Chebyschev moments.

gsl_integration_qaws_table * **gsl_integration_qaws_table_alloc** (double *alpha*, double *beta*, int *mu*, int *nu*) — Function

This function allocates space for a gsl_integration_qaws_table struct and associated workspace 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,

$$\begin{array}{ll} W(x) = (x-a)^\alpha (b-x)^\beta & (\mu = 0, \nu = 0) \\ W(x) = (x-a)^\alpha (b-x)^\beta \log(x-a) & (\mu = 1, \nu = 0) \\ W(x) = (x-a)^\alpha (b-x)^\beta \log(b-x) & (\mu = 0, \nu = 1) \\ W(x) = (x-a)^\alpha (b-x)^\beta \log(x-a) \log(b-x) & (\mu = 1, \nu = 1) \end{array}$$

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 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*) — Function

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*) — Function

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*) — Function

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.

16.9 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 Chebyschev 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*) — Function

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*) — Function

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*) — Function

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*) — Function

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*) — Function

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, $d\omega > 4$ are computed using a 25-point Clenshaw-Curtis integration rule, which handles the oscillatory behavior. Subintervals with a "small" width $d\omega < 4$ are computed using a 15-point Gauss-Kronrod integration.

16.10 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*) — Function

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 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 $c = (2\,\mathrm{floor}(|\omega|) + 1)\pi/|\omega|$. 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,

$$TOL_k = u_k \max(abserr, \max_{i<k}\{E_i\})$$

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.

16.11 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.

16.12 Examples

The integrator `QAGS` will handle a large class of definite integrals. For example, consider the following integral, which has a 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);
  printf("exact result    = % .18f\n", expected);
  printf("estimated error = % .18f\n", error);
  printf("actual error    = % .18f\n", result - expected);
  printf("intervals =  %d\n", w->size);

  return 0;
}
```

The results below show that the desired accuracy is achieved after 8 subdivisions.

```
bash$ ./a.out
result          = -3.999999999999973799
exact result    = -4.000000000000000000
estimated error =  0.000000000000246025
actual error    =  0.000000000000026201
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.

16.13 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. Uberhuber, D.K. Kahaner. QUADPACK *A subroutine package for automatic integration* Springer Verlag, 1983.

17 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`'.

17.1 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".

17.2 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.

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'.

17.3 Random number generator initialization

`gsl_rng *` **gsl_rng_alloc** (`const gsl_rng_type *` *T*) Random

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` (see Section 17.6 [Random number environment variables], page 175).

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*) Random

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* 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`.

`void` **gsl_rng_free** (`gsl_rng *` *r*) Random

This function frees all the memory associated with the generator *r*.

17.4 Sampling from a random number generator

The following functions return uniformly distributed random numbers, either as integers or double precision floating point numbers. To obtain non-uniform distributions see Chapter 19 [Random Number Distributions], page 192.

`unsigned long int` **gsl_rng_get** (`const gsl_rng *` *r*) Random

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 determined using the auxiliary functions `gsl_rng_max (r)` and `gsl_rng_min (r)`.

double **gsl_rng_uniform** (const gsl_rng * *r*) Random

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*) Random

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*) Random

This function returns a random integer from 0 to *n-1* inclusive. All integers in the range [0,*n-1*] are equally likely, regardless of the generator used. An offset correction is applied so that zero is always returned with the correct probability, for any minimum value of the underlying generator.

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.

17.5 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*) Random

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*) Random

`gsl_rng_max` returns the largest value that `gsl_rng_get` can return.

unsigned long int **gsl_rng_min** (const gsl_rng * *r*) Random

`gsl_rng_min` 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*) Random
size_t **gsl_rng_size** (const gsl_rng * *r*) Random

These function 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) Random

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);
  }
```

17.6 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.

const gsl_rng_type * **gsl_rng_env_setup** (void) Function

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`. These global variables are defined as follows,

```
extern const gsl_rng_type *gsl_rng_default
extern unsigned long int gsl_rng_default_seed
```

The environment variable `GSL_RNG_TYPE` should be the name of a generator, such as `taus` or `mt19937`. The environment variable `GSL_RNG_SEED` should contain the desired seed value. It 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>

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 = %u\n", gsl_rng_default_seed);
  printf("first value = %u\n", gsl_rng_get (r));
  return 0;
}
```

Running the program without any environment variables uses the initial defaults, an `mt19937` generator with a seed of 0,

```
bash$ ./a.out
generator type: mt19937
seed = 0
first value = 2867219139
```

By setting the two variables on the command line we can change the default generator and the seed,

```
bash$ 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
```

17.7 Saving and restoring random number generator state

The above methods ignore 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*) Random

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*) Random

This function returns a pointer to a newly created generator which is an exact copy of the generator *r*.

`void` **gsl_rng_print_state** (`const gsl_rng *` *r*) Random

This function prints a hex-dump of the state of the generator *r* to `stdout`. At the moment its only use is for debugging.

17.8 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.

gsl_rng_mt19937 Generator

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.

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_19937` 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 alternate generators `gsl_rng_mt19937_1999` and `gsl_rng_mt19937_1998`.

gsl_rng_ranlxs0 Generator
gsl_rng_ranlxs1 Generator
gsl_rng_ranlxs2 Generator

The generator `ranlxs0` is a second-generation version of the RANLUX algorithm of Lüscher, which produces "luxury random numbers". This generator provides single precision output (24 bits) at three luxury levels `ranlxs0`, `ranlxs1` and `ranlxs2`. 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 additional decorrelation between samples as an additional safety margin.

gsl_rng_ranlxd1 Generator
gsl_rng_ranlxd2 Generator

These generators produce double precision output (48 bits) from the RANLXS generator. The library provides two luxury levels `ranlxd1` and `ranlxd2`.

gsl_rng_ranlux Generator
gsl_rng_ranlux389 Generator

The `ranlux` generator is an implementation of the original algorithm developed by Lüscher. 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 Lüscher 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. Lüscher, "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 Lüscher", *Computer Physics Communications*, 79 (1994) 111-114

gsl_rng_cmrg Generator

This is a combined multiple recursive generator by L'Ecuyer. Its sequence is,

$$z_n = (x_n - y_n) \bmod m_1$$

where the two underlying generators x_n and y_n are,

$$x_n = (a_1 x_{n-1} + a_2 x_{n-2} + a_3 x_{n-3}) \bmod m_1$$
$$y_n = (b_1 y_{n-1} + b_2 y_{n-2} + b_3 y_{n-3}) \bmod m_2$$

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 2^{205} (about 10^{61}). 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_mrg Generator

This is a fifth-order multiple recursive generator by L'Ecuyer, Blouin and Coutre. Its sequence is,

$$x_n = (a_1 x_{n-1} + a_5 x_{n-5}) \bmod m$$

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_taus Generator

gsl_rng_taus2 Generator

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,

$$s^1_{n+1} = (((s^1_n \& 4294967294) \ll 12) \oplus (((s^1_n \ll 13) \oplus s^1_n) \gg 19))$$
$$s^2_{n+1} = (((s^2_n \& 4294967288) \ll 4) \oplus (((s^2_n \ll 2) \oplus s^2_n) \gg 25))$$
$$s^3_{n+1} = (((s^3_n \& 4294967280) \ll 17) \oplus (((s^3_n \ll 3) \oplus s^3_n) \gg 11))$$

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_gfsr4 Generator

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 the one ones in this implementation), then the sequence is said to be maximal. I'm not sure what that means, but I would guess that means all states are part of the same cycle, which would mean that the period for this generator is astronomical; it is $(2^K)^D \approx 10^{93334}$ where $K = 32$ is the number of bits in the word, and D is the longest lag. This would also mean that any one random number could easily be zero; ie $0 \leq r < 2^{32}$.

Ziff doesn't say so, but it seems to me that the bits are completely independent here, so one could use this as an efficient bit generator; each number supplying 32 random bits. The quality of the generated bits depends on the underlying seeding procedure, which may need to be improved in some circumstances.

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.

17.9 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_rand Generator

This is the BSD `rand()` generator. Its sequence is

$$x_{n+1} = (a x_n + c) \bmod m$$

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_random_bsd Generator
gsl_rng_random_libc5 Generator
gsl_rng_random_glibc2 Generator

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_rand48 Generator

This is the Unix rand48 generator. Its sequence is

$$x_{n+1} = (a x_n + c) \bmod m$$

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).

17.10 Numerical Recipes generators

The following generators are provided for compatibility with *Numerical Recipes*. Note that the original Numerical Recipes functions used single precision while we use double precision. This will lead to minor discrepancies, but only at the level of single-precision rounding error. If necessary you can force the returned values to single precision by storing them in a volatile float, which prevents the value being held in a register with double or extended precision. Apart from this difference the underlying algorithms for the integer part of the generators are the same.

gsl_rng_ran0 Generator

Numerical recipes ran0 implements Park and Miller's MINSTD algorithm with a modified seeding procedure.

gsl_rng_ran1 Generator

Numerical recipes ran1 implements Park and Miller's MINSTD algorithm with a 32-element Bayes-Durham shuffle box.

gsl_rng_ran2 Generator

Numerical recipes ran2 implements a L'Ecuyer combined recursive generator with a 32-element Bayes-Durham shuffle-box.

gsl_rng_ran3 Generator

Numerical recipes ran3 implements Knuth's portable subtractive generator.

17.11 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_ranf Generator

This is the CRAY random number generator `RANF`. Its sequence is

$$x_{n+1} = (a x_n) \bmod m$$

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 compatibile 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_ranmar Generator

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_r250 Generator

This is the shift-register generator of Kirkpatrick and Stoll. The sequence is

$$x_n = x_{n-103} \oplus x_{n-250}$$

where $\oplus$ denote "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_tt800 Generator

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_vax Generator

This is the VAX generator `MTH$RANDOM`. Its sequence is,

$$x_{n+1} = (a x_n + c) \bmod m$$

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_transputer Generator

This is the random number generator from the INMOS Transputer Development system. Its sequence is,

$$x_{n+1} = (a x_n) \bmod m$$

with $a = 1664525$ and $m = 2^{32}$. The seed specifies the initial value, x_1.

gsl_rng_randu Generator

This is the IBM `RANDU` generator. Its sequence is

$$x_{n+1} = (a x_n) \bmod m$$

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_minstd Generator

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,

$$x_{n+1} = (a x_n) \bmod m$$

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 is used in the IMSL Library (subroutine RNUN) and in MATLAB (the RAND function). 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_uni Generator
gsl_rng_uni32 Generator

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_slatec Generator

This is the SLATEC random number generator RAND. It is ancient. The original source code is available from NETLIB.

gsl_rng_zuf Generator

This is the ZUFALL lagged Fibonacci series generator of Peterson. Its sequence is,

$$t = u_{n-273} + u_{n-607}$$
$$u_n = t - \mathrm{floor}(t)$$

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_borosh13 Generator

This is the Borosh, Niederreiter random number generator. It is taken from Knuth's *Seminumerical Algorithms*, 3rd Ed., pages 106-108. Its sequence is,

$$x_{n+1} = (a x_n) \bmod m$$

with $a = 1812433253$ and $m = 2^{32}$. The seed specifies the initial value, x_1.

gsl_rng_coveyou Generator

This is the Coveyou random number generator. It is taken from Knuth's *Seminumerical Algorithms*, 3rd Ed., Section 3.2.2. Its sequence is,

$$x_{n+1} = (x_n (x_n + 1)) \bmod m$$

with $m = 2^{32}$. The seed specifies the initial value, x_1.

gsl_rng_fishman18 Generator

This is the Fishman, Moore III random number generator. It is taken from Knuth's *Seminumerical Algorithms*, 3rd Ed., pages 106-108. Its sequence is,

$$x_{n+1} = (a x_n) \bmod m$$

with $a = 62089911$ and $m = 2^{31} - 1$. The seed specifies the initial value, x_1.

gsl_rng_fishman20 Generator

This is the Fishman random number generator. It is taken from Knuth's *Seminumerical Algorithms*, 3rd Ed., page 108. Its sequence is,

$$x_{n+1} = (a x_n) \bmod m$$

with $a = 48271$ and $m = 2^{31} - 1$. The seed specifies the initial value, x_1.

gsl_rng_fishman2x Generator

This is the L'Ecuyer - Fishman random number generator. It is taken from Knuth's *Seminumerical Algorithms*, 3rd Ed., page 108. Its sequence is,

$$z_{n+1} = (x_n - y_n) \bmod m$$

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_knuthran2 Generator

This is a second-order multiple recursive generator described by Knuth in *Seminumerical Algorithms*, 3rd Ed., page 108. Its sequence is,

$$x_n = (a_1 x_{n-1} + a_2 x_{n-2}) \bmod m$$

with $a_1 = 271828183$, $a_2 = 314159269$, and $m = 2^{31} - 1$.

gsl_rng_knuthran Generator

This is a second-order multiple recursive generator described by Knuth in *Seminumerical Algorithms*, 3rd Ed., Section 3.6. Knuth provides its C code.

gsl_rng_lecuyer21 Generator

This is the L'Ecuyer random number generator. It is taken from Knuth's *Seminumerical Algorithms*, 3rd Ed., page 106-108. Its sequence is,

$$x_{n+1} = (a x_n) \bmod m$$

with $a = 40692$ and $m = 2^{31} - 249$. The seed specifies the initial value, x_1.

gsl_rng_waterman14 Generator

This is the Waterman random number generator. It is taken from Knuth's *Seminumerical Algorithms*, 3rd Ed., page 106-108. Its sequence is,

$$x_{n+1} = (a x_n) \bmod m$$

with $a = 1566083941$ and $m = 2^{32}$. The seed specifies the initial value, x_1.

17.12 Random Number Generator Performance

The following table shows the relative performance of a selection the available random number generators. The simulation quality generators which offer the best performance are `taus`, `gfsr4` and `mt19937`.

```
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

1852 k ints/sec,    935 k doubles/sec, ran3
 813 k ints/sec,    575 k doubles/sec, ran0
 787 k ints/sec,    476 k doubles/sec, ran1
 379 k ints/sec,    292 k doubles/sec, ran2
```

17.13 Examples

The following program demonstrates the use of a random number generator to produce uniform random numbers in 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,

```
$ ./a.out
0.66758
0.36908
0.72483
0.68776
0.57365
0.81078
0.27108
0.83777
0.13736
0.95745
```

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 mutiple-recursive generator `mrg`,

```
$ GSL_RNG_SEED=123 GSL_RNG_TYPE=mrg ./a.out
GSL_RNG_TYPE=mrg
GSL_RNG_SEED=123
0.33050
0.86631
0.32982
0.67620
0.53391
0.06457
0.16847
0.70229
0.04371
0.86374
```

17.14 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`'.

On the World Wide Web, see the pLab home page (`http://random.mat.sbg.ac.at/`) for a lot of information on the state-of-the-art in random number generation, and for numerous links to various "random" WWW sites.

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/`

17.15 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 Lüscher for providing notes and source code for the RANLXS and RANLXD generators.

18 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.

The functions described in this section are declared in the header file 'gsl_qrng.h'.

18.1 Quasi-random number generator initialization

gsl_qrng * **gsl_qrng_alloc** (const gsl_qrng_type * *T*, unsigned int *d*) Function

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*) Function

This function frees all the memory associated with the generator *q*.

void **gsl_qrng_init** (gsl_qrng * *q*) Function

This function reinitializes the generator *q* to its starting point.

18.2 Sampling from a quasi-random number generator

int **gsl_qrng_get** (const gsl_qrng * *q*, double *x*[]) Function

This function returns the next point *x* from the sequence generator *q*. 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.

18.3 Auxiliary quasi-random number generator functions

const char * **gsl_qrng_name** (const gsl_qrng * *q*) Function

This function returns a pointer to the name of the generator.

size_t **gsl_qrng_size** (const gsl_qrng * *q*) Function
void * **gsl_qrng_state** (const gsl_qrng * *q*) Function

These function 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);
```

18.4 Saving and resorting quasi-random number generator state

int **gsl_qrng_memcpy** (gsl_qrng * *dest*, const gsl_qrng * *src*) Function

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*) Function

This function returns a pointer to a newly created generator which is an exact copy of the generator *r*.

18.5 Quasi-random number generator algorithms

The following quasi-random sequence algorithms are available,

gsl_qrng_niederreiter_2 Generator

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_sobol Generator

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.

18.6 Examples

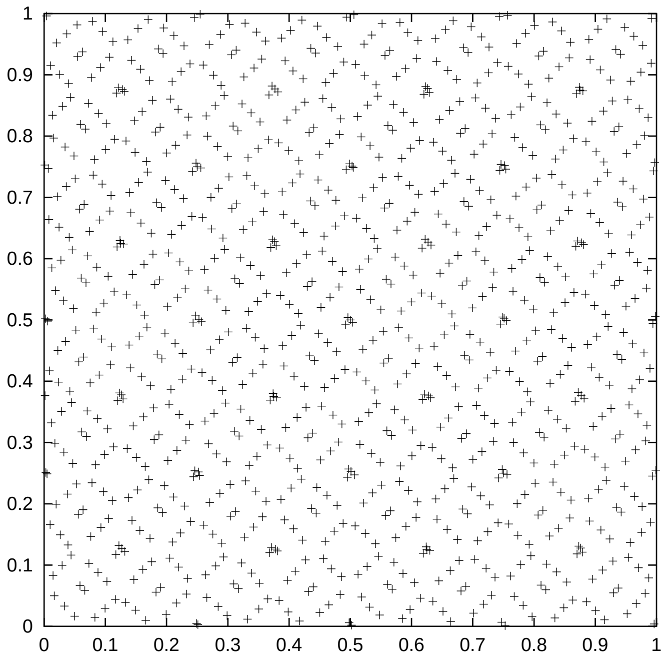
The following program prints the first 1024 points of the 2-dimensional Sobol sequence.

```
#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. The following plot shows the distribution in the x-y plane of the first 1024 points from the Sobol sequence,



Distribution of the first 1024 points
from the quasi-random Sobol sequence

18.7 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", Transactions on Mathematical Software, Vol. 20, No. 4, December, 1994, p. 494-495.

19 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 functions described in this section are declared in '`gsl_randist.h`'.

19.1 The Gaussian Distribution

`double` **gsl_ran_gaussian** (`const gsl_rng *` *r*, `double` *sigma*) Random

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-Mueller algorithm which requires two calls the random number generator *r*.

`double` **gsl_ran_gaussian_pdf** (`double` *x*, `double` *sigma*) Function

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_ratio_method** (`const gsl_rng *` *r*, `const double` *sigma*) Function

This function computes a gaussian random variate using the Kinderman-Monahan ratio method.

`double` **gsl_ran_ugaussian** (`const gsl_rng *` *r*) Random
`double` **gsl_ran_ugaussian_pdf** (`double` *x*) Function
`double` **gsl_ran_ugaussian_ratio_method** (`const gsl_rng *` *r*) Random

These functions compute results for the unit Gaussian distribution. They are equivalent to the functions above with a standard deviation of one, *sigma* = 1.

19.2 The Gaussian Tail Distribution

`double` **gsl_ran_gaussian_tail** (`const gsl_rng *` *r*, `double` *a*, `double` *sigma*) Random

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,

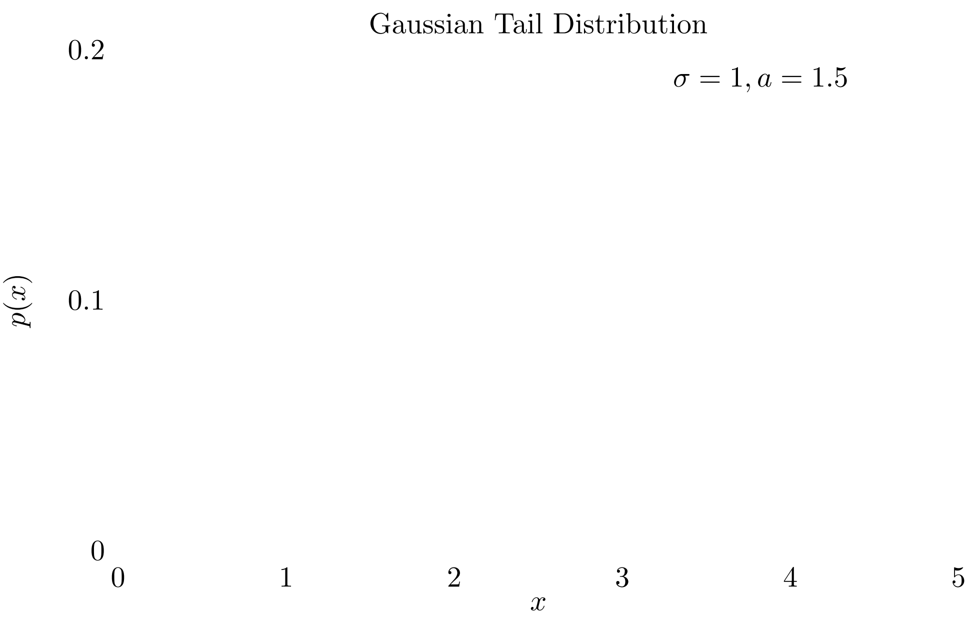
$$p(x)dx = \frac{1}{N(a;\sigma)} \exp(-x^2/2\sigma^2)dx$$

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*) Function

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*) Random

`double` **gsl_ran_ugaussian_tail_pdf** (`double` *x*, `double` *a*) Function

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.

19.3 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*) — Random

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,

$$p(x, y)dxdy = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}} \exp\left(\frac{-(x^2 + y^2 - 2\rho xy)}{2\sigma_x^2\sigma_y^2(1-\rho^2)}\right) dxdy$$

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*) — Function

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.

Bivariate Gaussian Distribution

$\sigma_x = 1, \sigma_y = 1, \rho = 0.9$

2

1

0 y

-1

-2

-2 -1 0 1 2

x

19.4 The Exponential Distribution

`double` **gsl_ran_exponential** (`const gsl_rng *` *r*, `double` *mu*) Random

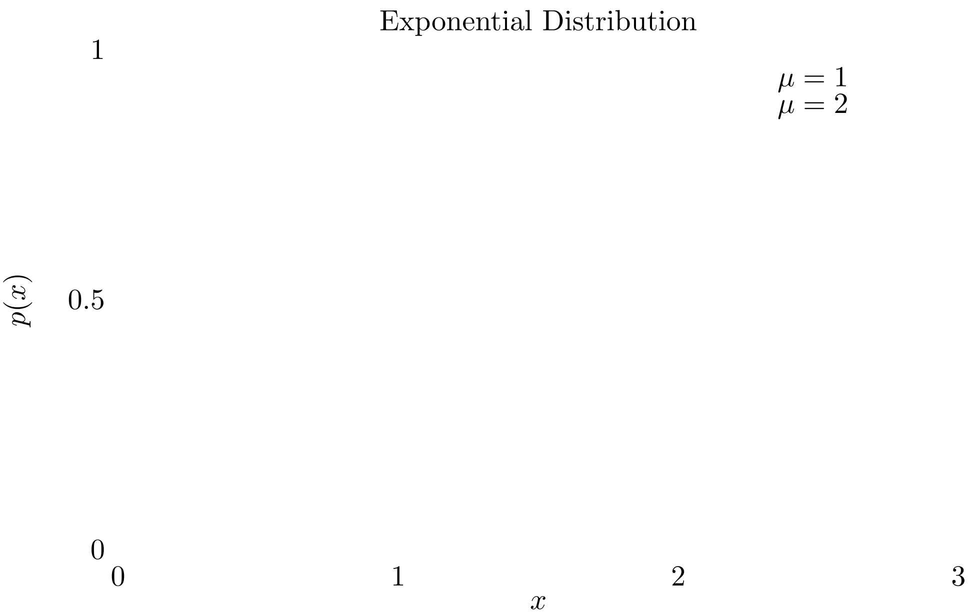
This function returns a random variate from the exponential distribution with mean *mu*. The distribution is,

$$p(x)dx = \frac{1}{\mu}\exp(-x/\mu)dx$$

for $x \geq 0$.

`double` **gsl_ran_exponential_pdf** (`double` *x*, `double` *mu*) Function

This function computes the probability density $p(x)$ at x for an exponential distribution with mean *mu*, using the formula given above.



19.5 The Laplace Distribution

double **gsl_ran_laplace** (const gsl_rng * *r*, double *a*) Random

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*) Function

This function computes the probability density $p(x)$ at x for a Laplace distribution with mean a, using the formula given above.

19.6 The Exponential Power Distribution

double **gsl_ran_exppow** (const gsl_rng * *r*, double *a*, double *b*) Random

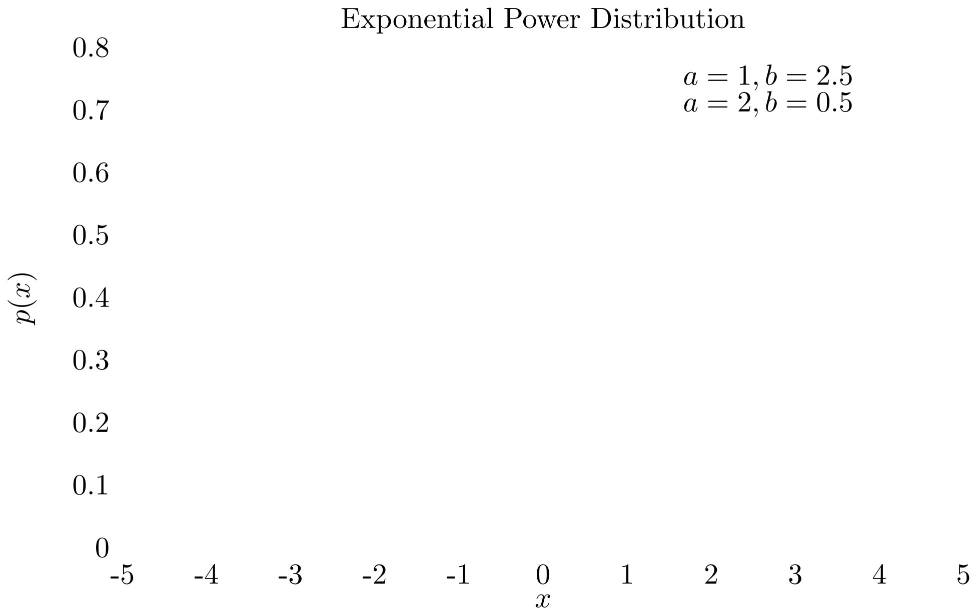
This function returns a random variate from the exponential power distribution with scale parameter *a* and exponent *b*. The distribution is,

$$p(x)dx = \frac{1}{2a\Gamma(1+1/b)} \exp(-|x/a|^b)dx$$

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*) Function

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.



19.7 The Cauchy Distribution

`double` **gsl_ran_cauchy** (`const gsl_rng *` *r*, `double` *a*) Random

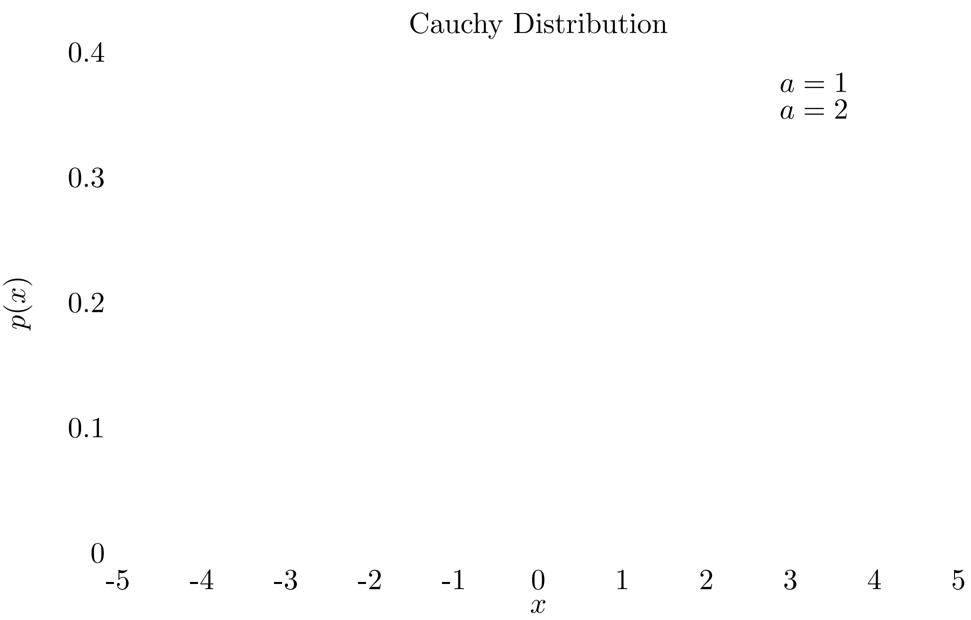
This function returns a random variate from the Cauchy distribution with scale parameter *a*. The probability distribution for Cauchy random variates is,

$$p(x)dx = \frac{1}{a\pi(1+(x/a)^2)}dx$$

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*) Function

This function computes the probability density $p(x)$ at x for a Cauchy distribution with scale parameter a, using the formula given above.



19.8 The Rayleigh Distribution

`double` **gsl_ran_rayleigh** (`const gsl_rng *` *r*, `double` *sigma*) Random

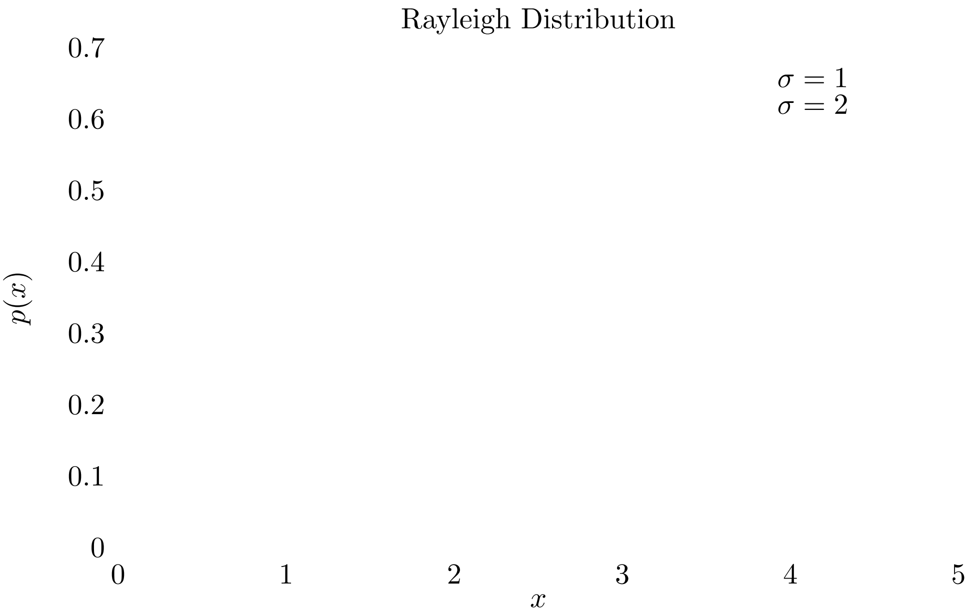
This function returns a random variate from the Rayleigh distribution with scale parameter *sigma*. The distribution is,

$$p(x)dx = \frac{x}{\sigma^2} \exp(-x^2/(2\sigma^2))dx$$

for $x > 0$.

`double` **gsl_ran_rayleigh_pdf** (`double` *x*, `double` *sigma*) Function

This function computes the probability density $p(x)$ at x for a Rayleigh distribution with scale parameter *sigma*, using the formula given above.



19.9 The Rayleigh Tail Distribution

`double` **gsl_ran_rayleigh_tail** (`const gsl_rng *` *r*, `double` *a* `double` *sigma*) — Random

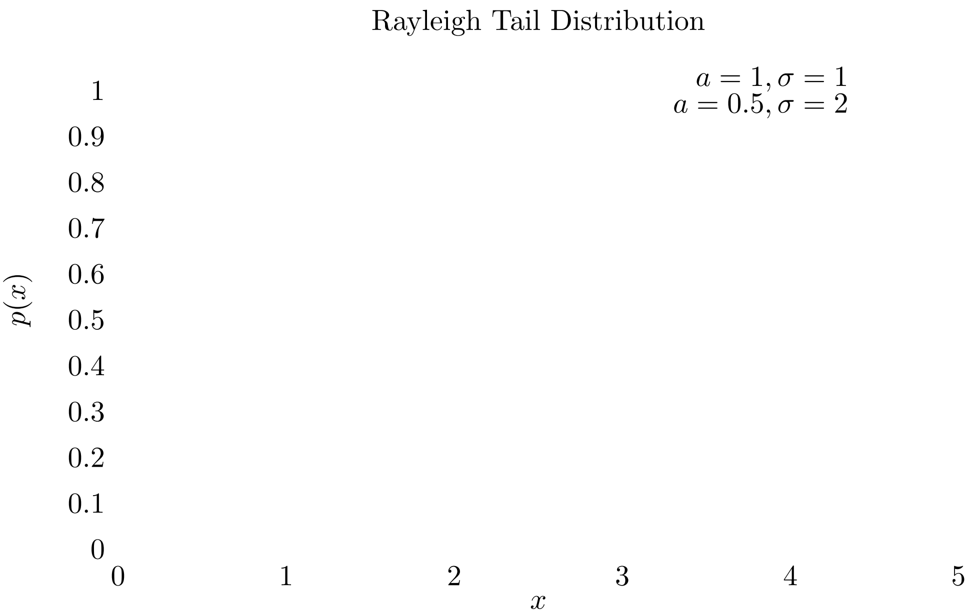
This function returns a random variate from the tail of the Rayleigh distribution with scale parameter *sigma* and a lower limit of *a*. The distribution is,

$$p(x)dx = \frac{x}{\sigma^2} \exp((a^2 - x^2)/(2\sigma^2)) dx$$

for $x > a$.

`double` **gsl_ran_rayleigh_tail_pdf** (`double` *x*, `double` *a*, `double` *sigma*) — Function

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.



19.10 The Landau Distribution

`double` **gsl_ran_landau** (`const gsl_rng *` *r*) [Random]

This function returns a random variate from the Landau distribution. The probability distribution for Landau random variates is defined analytically by the complex integral,

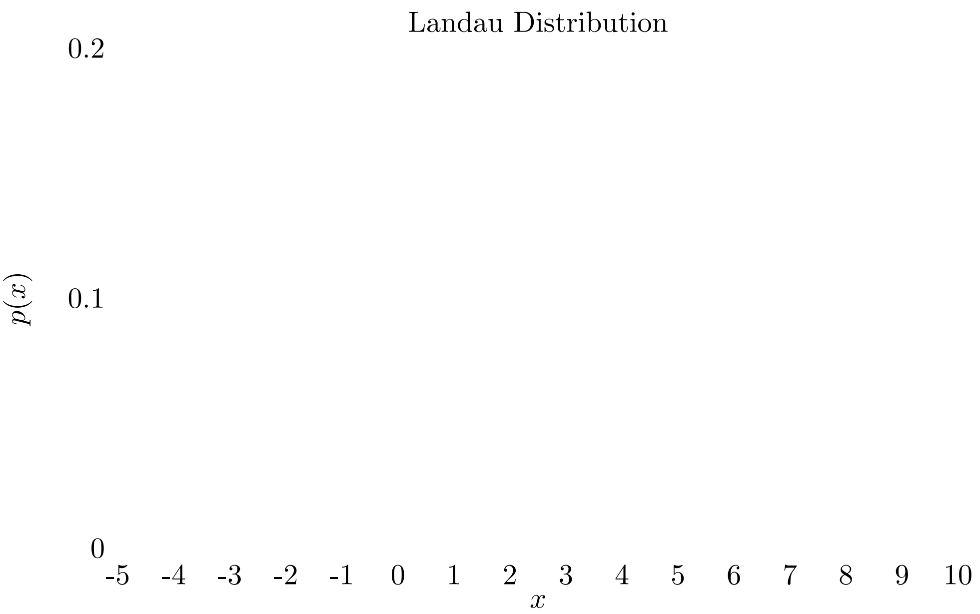
$$p(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \, \exp(s \log(s) + xs)$$

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*) [Function]

This function computes the probability density $p(x)$ at x for the Landau distribution using an approximation to the formula given above.



19.11 The Levy alpha-Stable Distributions

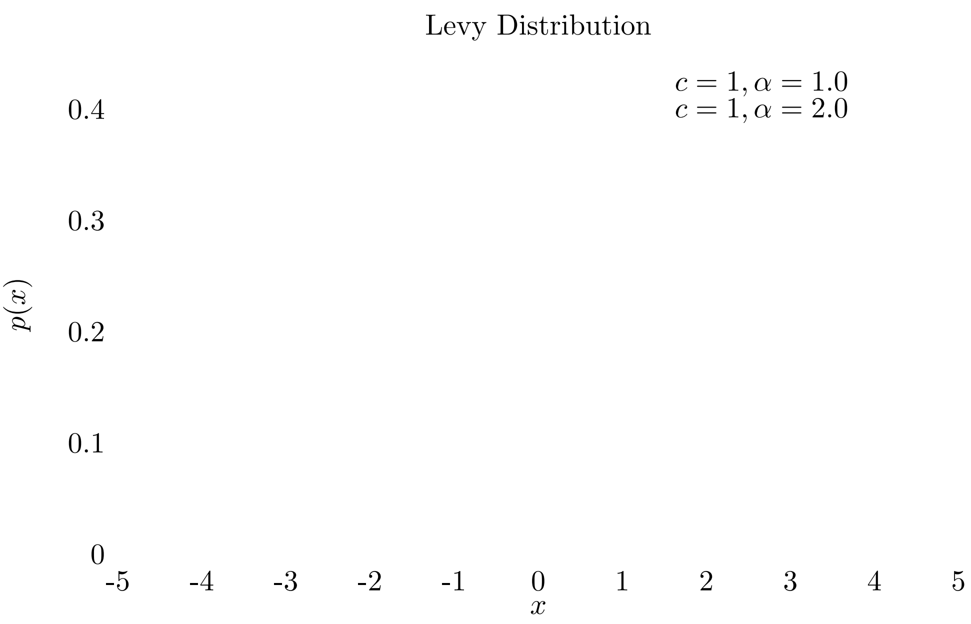
`double` **gsl_ran_levy** (`const gsl_rng *` *r*, `double` *c*, `double` *alpha*) Random

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 $0 < \alpha \leq 2$.



19.12 The Levy skew alpha-Stable Distribution

`double` **gsl_ran_levy_skew** (`const gsl_rng *` *r*, `double` *c*, `double` *alpha*, `double` *beta*) — Random

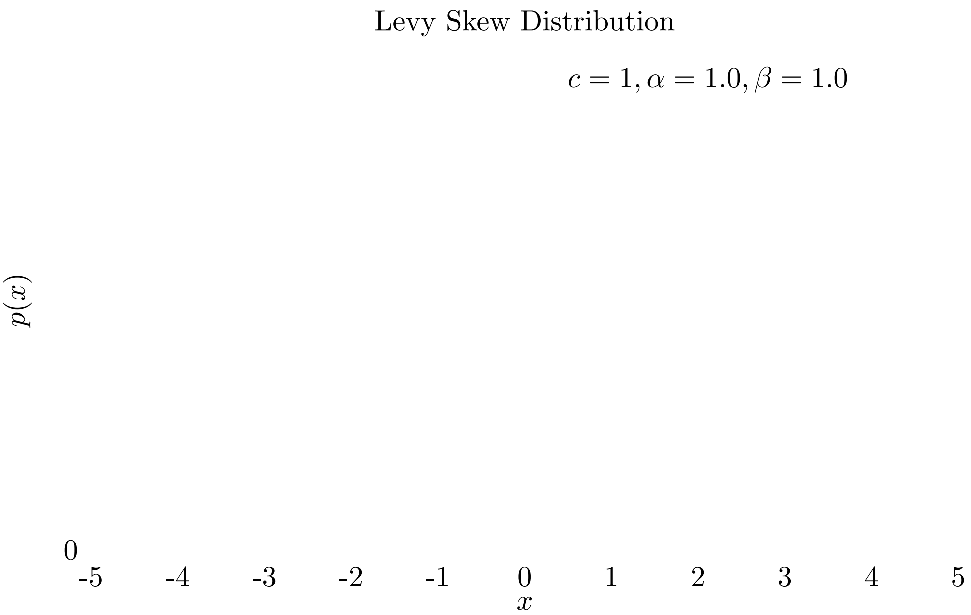
This function returns a random variate from the Levy skew stable distribution with scale *c*, exponent *alpha* and skewness parameter *beta*. The skewness parameter must lie in the range $[-1, 1]$. The Levy skew stable probability distribution is defined by a fourier transform,

$$p(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \exp(-itx - |ct|^{\alpha}(1 - i\beta sign(t) \tan(\pi\alpha/2)))$$

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 $0 < \alpha \leq 2$.

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 $Y = X_1 + X_2 + \ldots + X_N$ will also be distributed as an alpha-stable variate, $p(N^{1/\alpha}c, \alpha, \beta)$.



19.13 The Gamma Distribution

double **gsl_ran_gamma** (const gsl_rng * *r*, double *a*, double *b*) Random

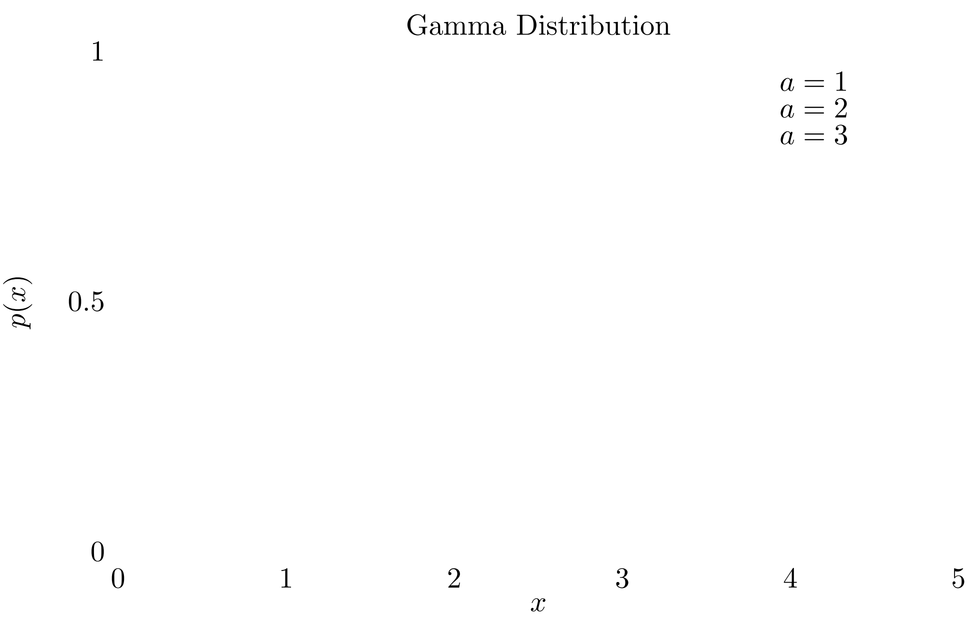
This function returns a random variate from the gamma distribution. The distribution function is,

$$p(x)dx = \frac{1}{\Gamma(a)b^a} x^{a-1} e^{-x/b} dx$$

for $x > 0$.

double **gsl_ran_gamma_pdf** (double *x*, double *a*, double *b*) Function

This function computes the probability density $p(x)$ at x for a gamma distribution with parameters a and b, using the formula given above.



19.14 The Flat (Uniform) Distribution

`double` **gsl_ran_flat** (`const gsl_rng *` r, `double` a, `double` b) Random

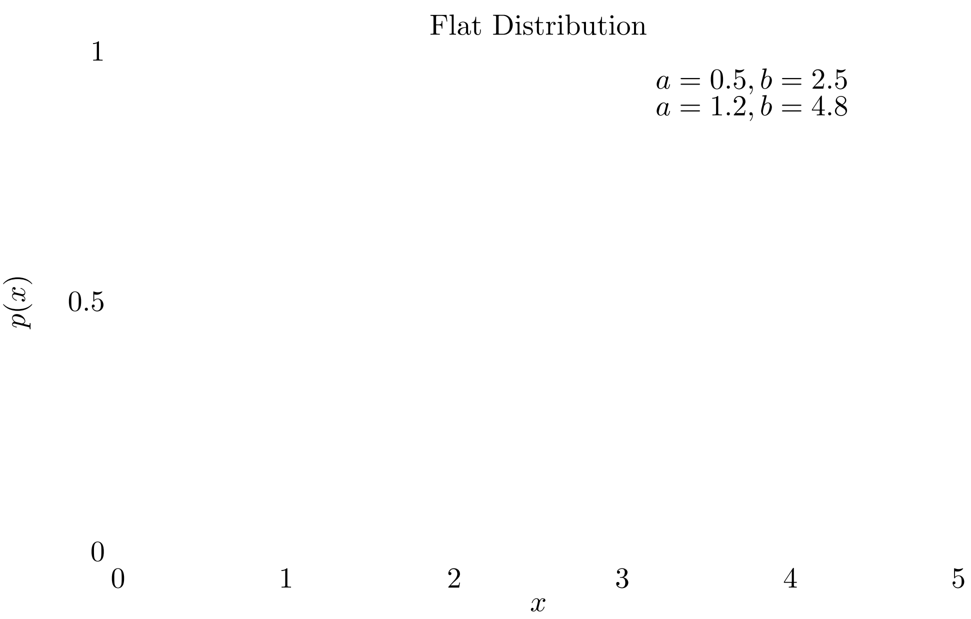
This function returns a random variate from the flat (uniform) distribution from a to b. The distribution is,

$$p(x)dx = \frac{1}{(b-a)}dx$$

if $a \leq x < b$ and 0 otherwise.

`double` **gsl_ran_flat_pdf** (`double` x, `double` a, `double` b) Function

This function computes the probability density $p(x)$ at x for a uniform distribution from a to b, using the formula given above.



19.15 The Lognormal Distribution

`double` **gsl_ran_lognormal** (`const gsl_rng *` *r*, `double` *zeta*, `double` *sigma*) [Random]

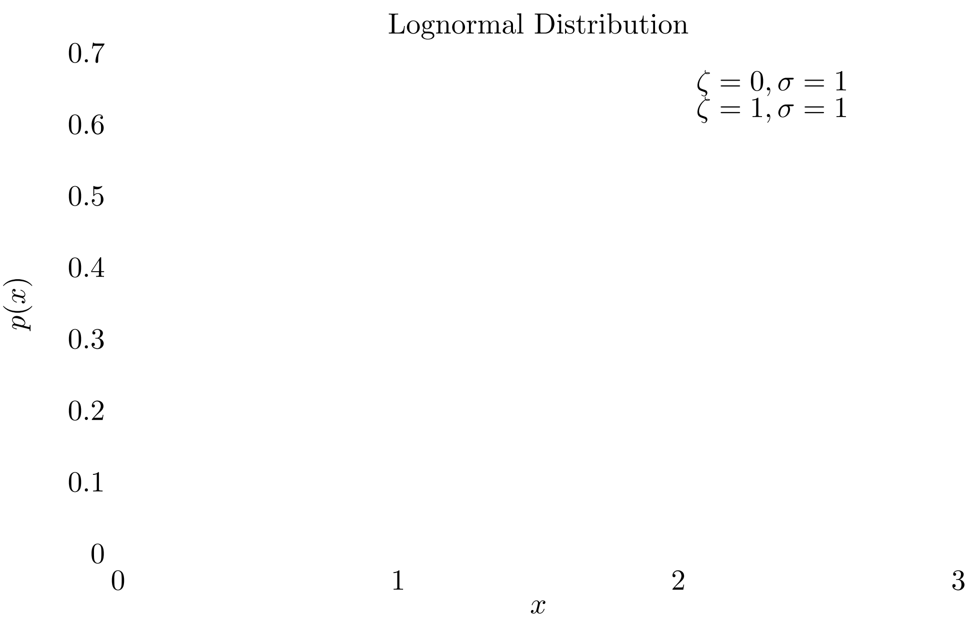
This function returns a random variate from the lognormal distribution. The distribution function is,

$$p(x)dx = \frac{1}{x\sqrt{2\pi\sigma^2}} \exp(-(\ln(x) - \zeta)^2/2\sigma^2)dx$$

for $x > 0$.

`double` **gsl_ran_lognormal_pdf** (`double` *x*, `double` *zeta*, `double` *sigma*) [Function]

This function computes the probability density $p(x)$ at x for a lognormal distribution with parameters *zeta* and *sigma*, using the formula given above.



19.16 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*) Random

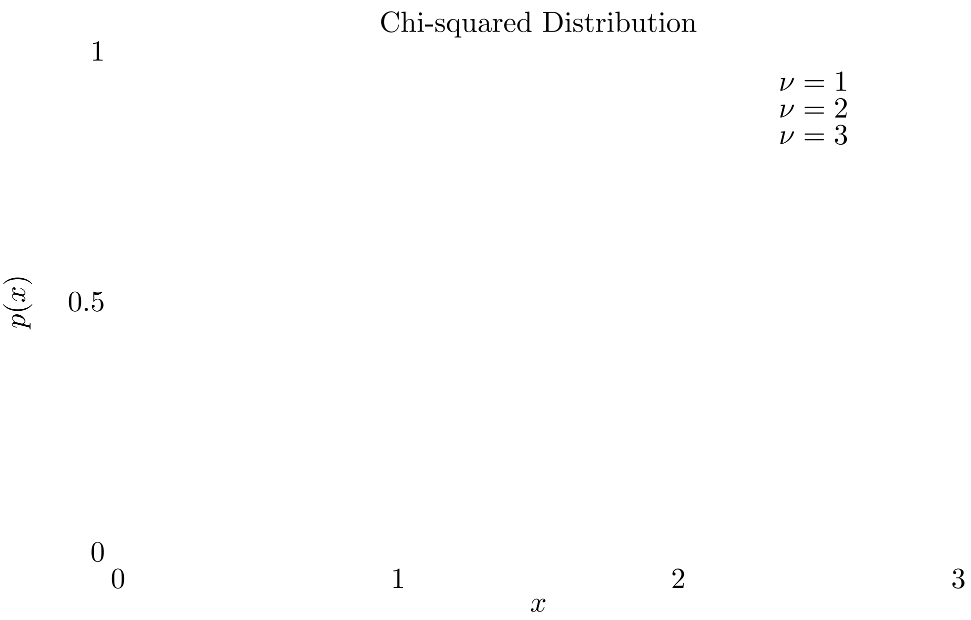
This function returns a random variate from the chi-squared distribution with *nu* degrees of freedom. The distribution function is,

$$p(x)dx = \frac{1}{\Gamma(\nu/2)} (x/2)^{\nu/2-1} \exp(-x/2) dx$$

for $x \geq 0$.

`double` **gsl_ran_chisq_pdf** (`double` *x*, `double` *nu*) Function

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.



19.17 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*) Random

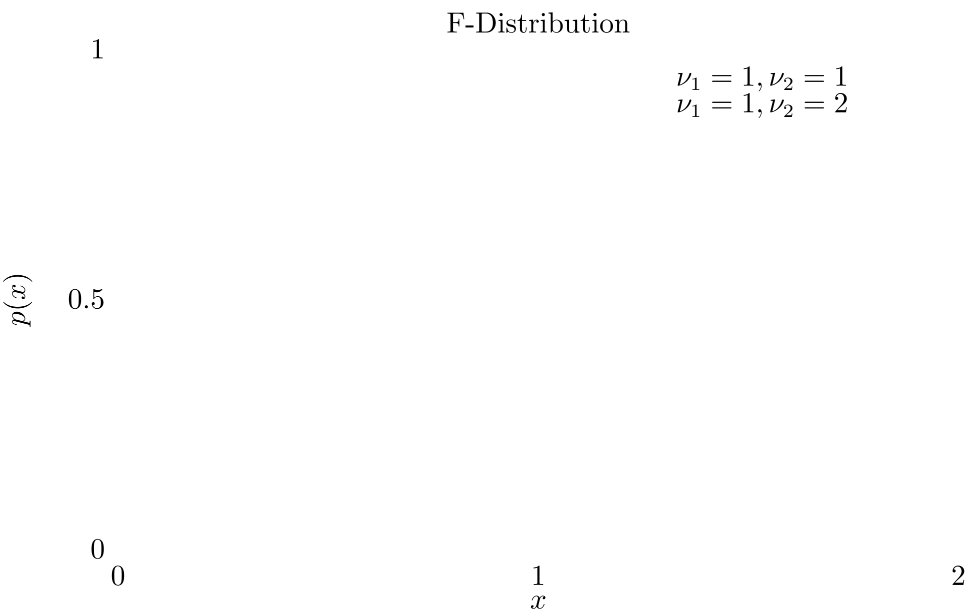
This function returns a random variate from the F-distribution with degrees of freedom *nu1* and *nu2*. The distribution function is,

$$p(x)dx = \frac{\Gamma((\nu_1 + \nu_2)/2)}{\Gamma(\nu_1/2)\Gamma(\nu_2/2)} \nu_1^{\nu_1/2} \nu_2^{\nu_2/2} x^{\nu_1/2-1} (\nu_2 + \nu_1 x)^{-\nu_1/2-\nu_2/2}$$

for $x \geq 0$.

`double` **gsl_ran_fdist_pdf** (`double` *x*, `double` *nu1*, `double` *nu2*) Function

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.



19.18 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*) Random

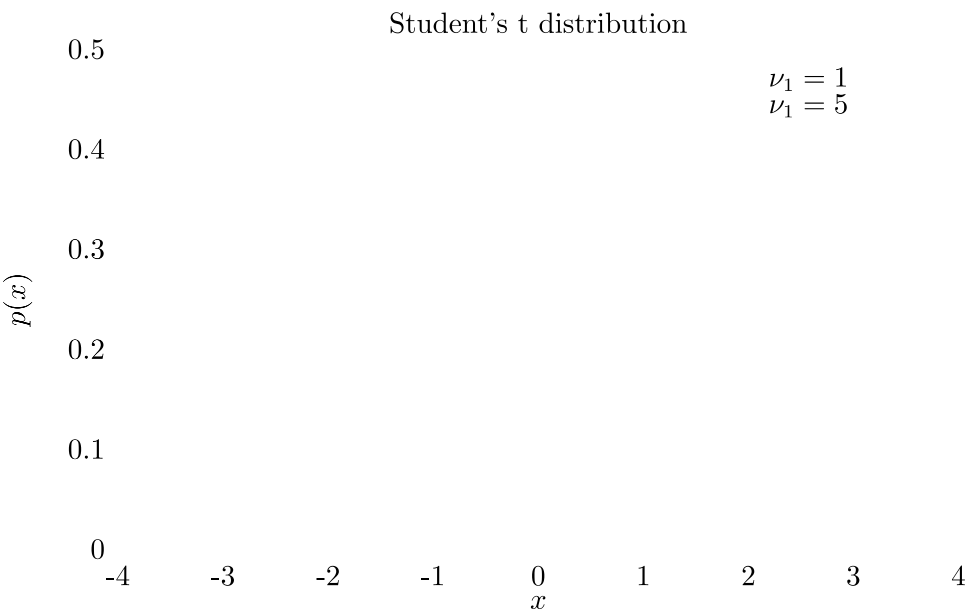
This function returns a random variate from the t-distribution. The distribution function is,

$$p(x)dx = \frac{\Gamma((\nu+1)/2)}{\sqrt{\pi\nu}\Gamma(\nu/2)}(1 + x^2/\nu)^{-(\nu+1)/2}dx$$

for $-\infty < x < +\infty$.

`double` **gsl_ran_tdist_pdf** (`double` *x*, `double` *nu*) Function

This function computes the probability density $p(x)$ at x for a t-distribution with *nu* degrees of freedom, using the formula given above.



19.19 The Beta Distribution

`double` **gsl_ran_beta** (`const gsl_rng *` *r*, `double` *a*, `double` *b*) Random

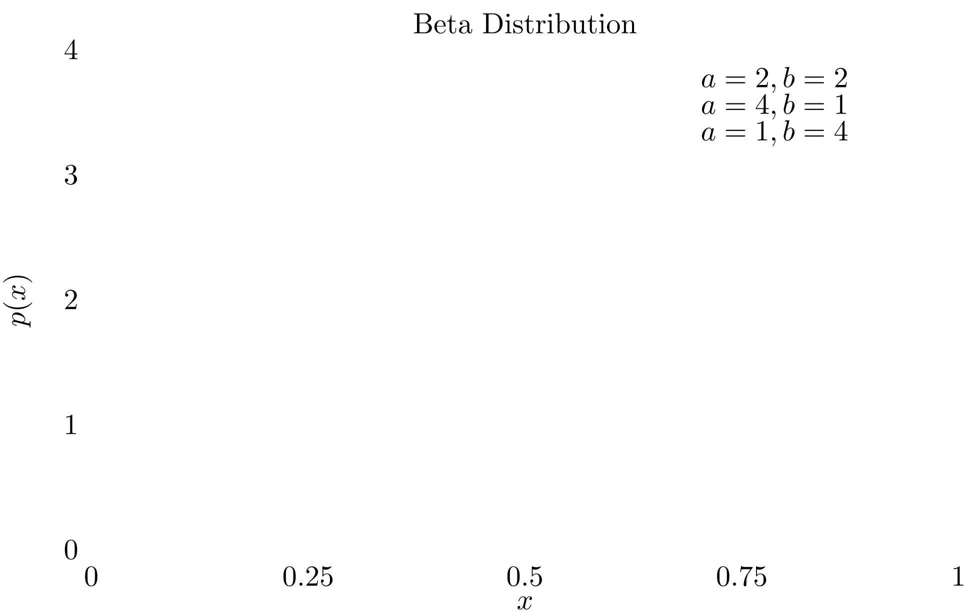
This function returns a random variate from the beta distribution. The distribution function is,

$$p(x)dx = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} x^{a-1}(1-x)^{b-1}dx$$

for $0 \le x \le 1$.

`double` **gsl_ran_beta_pdf** (`double` *x*, `double` *a*, `double` *b*) Function

This function computes the probability density $p(x)$ at x for a beta distribution with parameters a and b, using the formula given above.



19.20 The Logistic Distribution

double **gsl_ran_logistic** (const gsl_rng * *r*, double *a*) Random

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*) Function

This function computes the probability density $p(x)$ at x for a logistic distribution with scale parameter a, using the formula given above.

19.21 The Pareto Distribution

`double` **gsl_ran_pareto** (`const gsl_rng *` *r*, `double` *a*, `double` *b*) Random

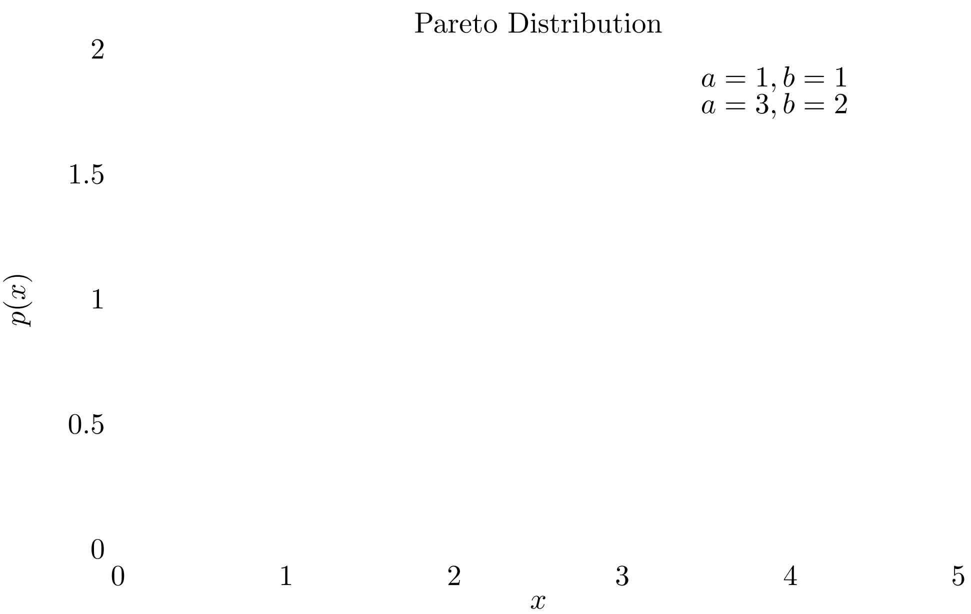
This function returns a random variate from the Pareto distribution of order a. The distribution function is,

$$p(x)dx = (a/b)/(x/b)^{a+1}dx$$

for $x \geq b$.

`double` **gsl_ran_pareto_pdf** (`double` *x*, `double` *a*, `double` *b*) Function

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.



19.22 The Spherical Distribution (2D & 3D)

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*) Random
`void` **gsl_ran_dir_2d_trig_method** (`const gsl_rng *` *r*, `double *`*x*, `double *`*y*) Random

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 my home Pentium (but not the case for my Sun Sparcstation 20 at work). Once 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 $y = uv/(u^2 + v^2)$.

`void` **gsl_ran_dir_3d** (`const gsl_rng *` *r*, `double *`*x*, `double *`*y*, `double *` *z*) Random

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 3d).

`void` **gsl_ran_dir_nd** (`const gsl_rng *` *r*, `size_t` *n*, `double *`*x*) Random

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).

19.23 The Weibull Distribution

double **gsl_ran_weibull** (const gsl_rng * *r*, double *a*, double *b*) Random

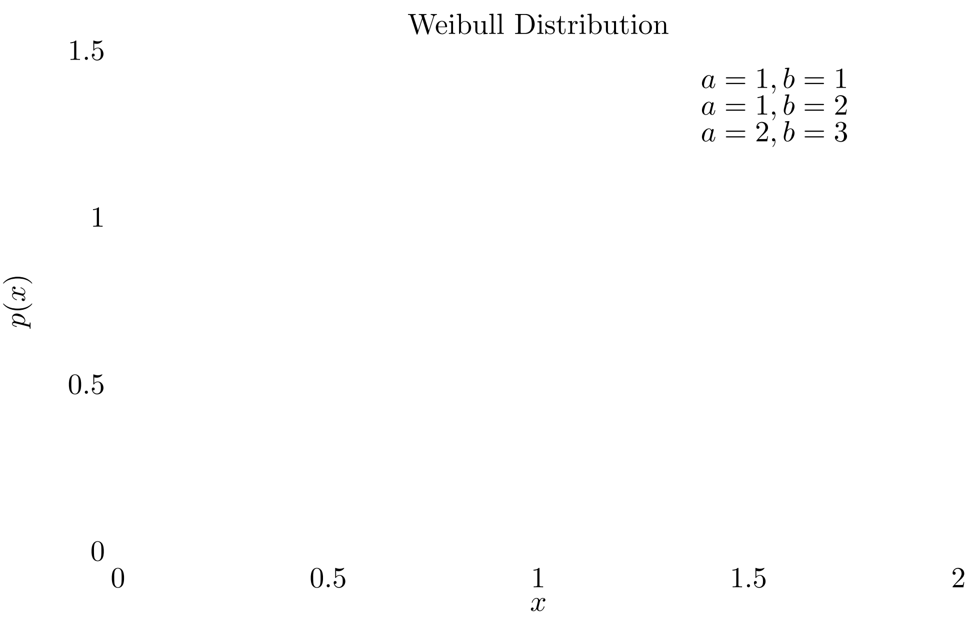
This function returns a random variate from the Weibull distribution. The distribution function is,

$$p(x)dx = \frac{b}{a^b} x^{b-1} \exp(-(x/a)^b) dx$$

for $x \geq 0$.

double **gsl_ran_weibull_pdf** (double *x*, double *a*, double *b*) Function

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.



19.24 The Type-1 Gumbel Distribution

`double` **gsl_ran_gumbel1** (`const gsl_rng *` *r*, `double` *a*, `double` *b*) Random

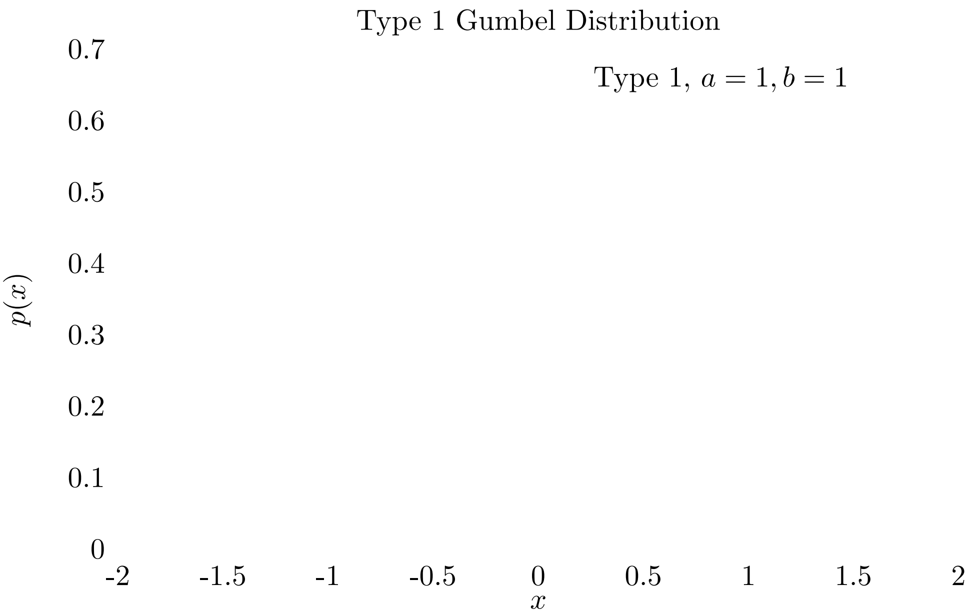
This function returns a random variate from the Type-1 Gumbel distribution. The Type-1 Gumbel distribution function is,

$$p(x)dx = ab\exp(-(b\exp(-ax) + ax))dx$$

for $-\infty < x < \infty$.

`double` **gsl_ran_gumbel1_pdf** (`double` *x*, `double` *a*, `double` *b*) Function

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.



19.25 The Type-2 Gumbel Distribution

`double` **gsl_ran_gumbel2** (`const gsl_rng *` *r*, `double` *a*, `double` *b*) Random

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*) Function

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.

19.26 The Dirichlet Distribution

`void` **gsl_ran_dirichlet** (`const gsl_rng *` *r*, `const size_t` *K*, `const double` *alpha*[], `double` *theta*[]) Random

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 $\alpha_i \geq 0$. 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** (`const size_t` *K*, `const double` *alpha*[], `const double` *theta*[]) Function

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** (`const size_t` *K*, `const double` *alpha*[], `const double` *theta*[]) Function

This function computes the logarithm of the probability density $p(\theta_1, \ldots, \theta_K)$ for a Dirichlet distribution with parameters *alpha*[*K*].

19.27 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 $C[k] \le u < C[k+1]$. 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 numbers 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 if for something like the Poisson Distribution, a modification would have to be made, since it only takes a finite set of K outcomes.

`gsl_ran_discrete_t *` **gsl_ran_discrete_preproc** (`size_t` *K*, `const double *` *P*) — Function

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*) — Random

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*) Function

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*) Function

De-allocates the lookup table pointed to by g.

19.28 The Poisson Distribution

`unsigned int` **gsl_ran_poisson** (`const gsl_rng *` *r*, `double` *mu*) Random

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*) Function

This function computes the probability $p(k)$ of obtaining k from a Poisson distribution with mean *mu*, using the formula given above.

19.29 The Bernoulli Distribution

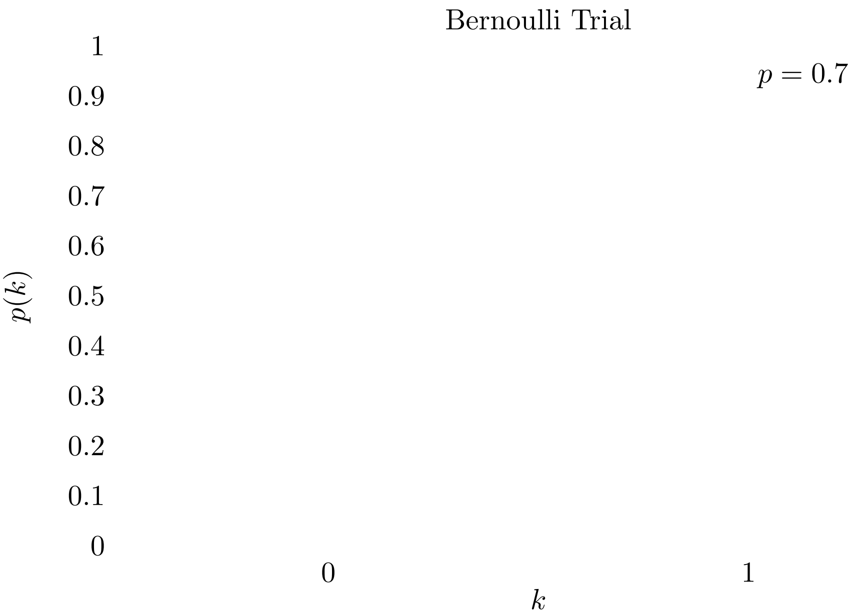
`unsigned int` **gsl_ran_bernoulli** (`const gsl_rng *` *r*, `double` *p*) Random

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*) Function

This function computes the probability $p(k)$ of obtaining k from a Bernoulli distribution with probability parameter p, using the formula given above.



19.30 The Binomial Distribution

`unsigned int` **gsl_ran_binomial** (`const gsl_rng *` r, `double` p, `unsigned int` n) Random

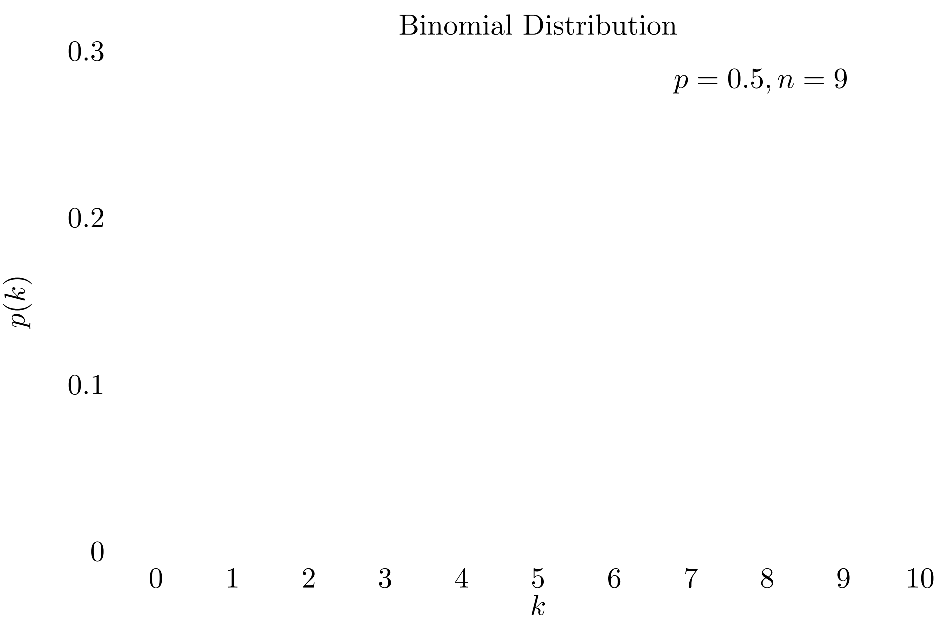
This function returns a random integer from the binomial distribution, the number of successes in n independent trials with probability p. The probability distribution for binomial variates is,

$$p(k) = \frac{n!}{k!(n-k)!} p^k (1-p)^{n-k}$$

for $0 \le k \le n$.

`double` **gsl_ran_binomial_pdf** (`unsigned int` k, `double` p, `unsigned int` n) Function

This function computes the probability $p(k)$ of obtaining k from a binomial distribution with parameters p and n, using the formula given above.



19.31 The Multinomial Distribution

void **gsl_ran_multinomial** (const gsl_rng * r, const size_t K, const unsigned int N, const double $p[]$, unsigned int $n[]$) — Random

This function returns an array of K random variates from a multinomial distribution. The distribution function 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.

Random variates are generated using the conditional binomial method (see C.S. David, *The computer generation of multinomial random variates*, Comp. Stat. Data Anal. 16 (1993) 205-217 for details).

double **gsl_ran_multinomial_pdf** (const size_t K, const double $p[]$, const unsigned int $n[]$) — Function

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** (const size_t K, const double $p[]$, const unsigned int $n[]$) — Function

This function returns the logarithm of the probability for the multinomial distribution $P(n_1, n_2, \ldots, n_K)$ with parameters $p[K]$.

19.32 The Negative Binomial Distribution

`unsigned int` **gsl_ran_negative_binomial** (`const gsl_rng *` *r*, `double` *p*, `double` *n*) — Random

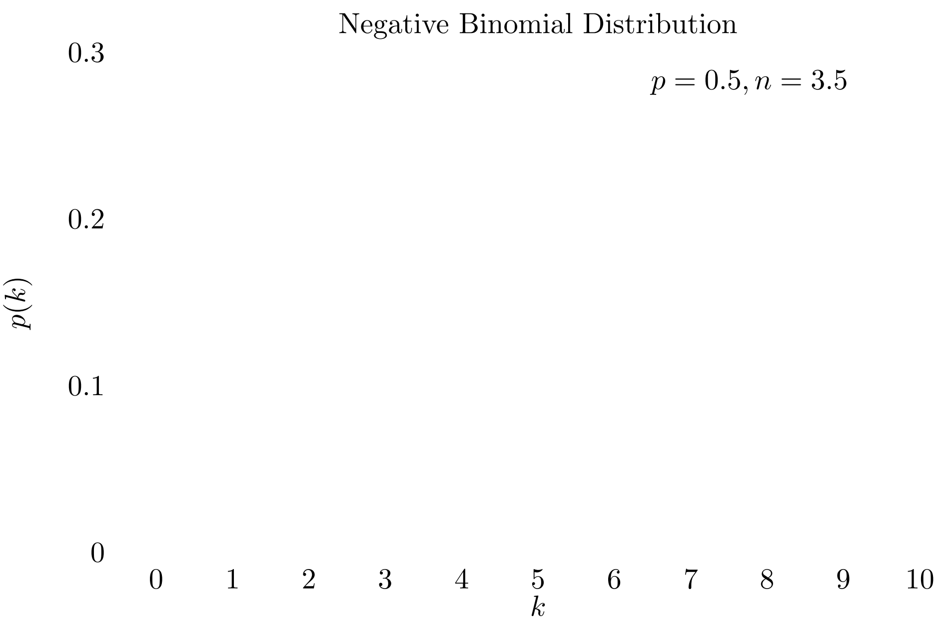
This function returns a random integer from the negative binomial distribution, the number of failures occurring before n successes in independent trials with probability p of success. The probability distribution for negative binomial variates is,

$$p(k) = \frac{\Gamma(n+k)}{\Gamma(k+1)\Gamma(n)} p^n (1-p)^k$$

Note that n is not required to be an integer.

`double` **gsl_ran_negative_binomial_pdf** (`unsigned int` *k*, `double` *p*, `double` *n*) — Function

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.



19.33 The Pascal Distribution

`unsigned int` **gsl_ran_pascal** (`const gsl_rng *` *r*, `double` *p*, `unsigned int` *k*) [Random]

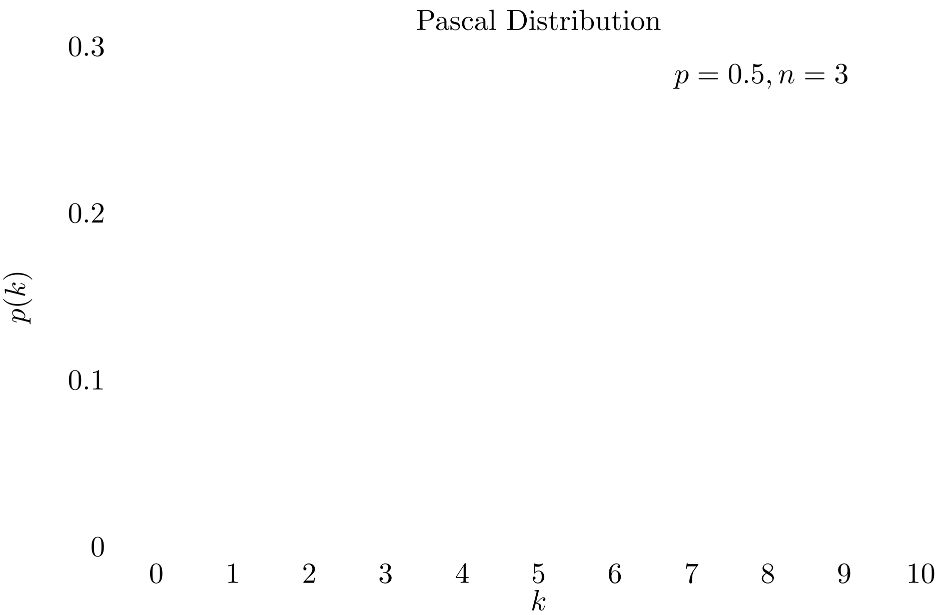
This function returns a random integer from the Pascal distribution. The Pascal distribution is simply a negative binomial distribution with an integer value of n.

$$p(k) = \frac{(n + k - 1)!}{k!(n - 1)!} p^n (1 - p)^k$$

for $k \geq 0$

`double` **gsl_ran_pascal_pdf** (`unsigned int` *k*, `double` *p*, `unsigned int` *n*) [Function]

This function computes the probability $p(k)$ of obtaining k from a Pascal distribution with parameters p and n, using the formula given above.



19.34 The Geometric Distribution

`unsigned int` **gsl_ran_geometric** (`const gsl_rng *` r, `double` p) Random

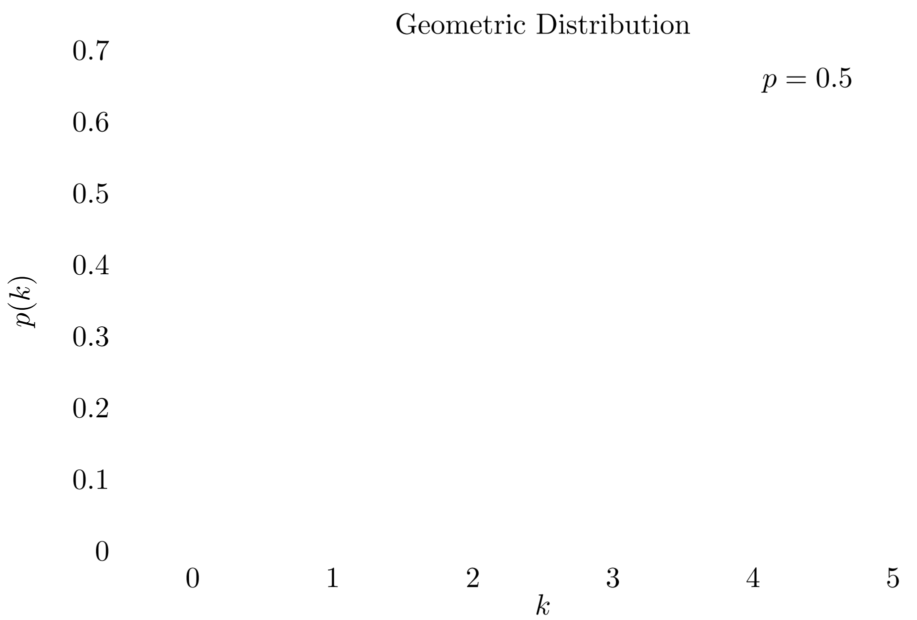
This function returns a random integer from the geometric distribution, the number of independent trials with probability p until the first success. The probability distribution for geometric variates is,

$$p(k) = p(1-p)^{k-1}$$

for $k \geq 1$.

`double` **gsl_ran_geometric_pdf** (`unsigned int` k, `double` p) Function

This function computes the probability $p(k)$ of obtaining k from a geometric distribution with probability parameter p, using the formula given above.



19.35 The Hypergeometric Distribution

`unsigned int` **gsl_ran_hypergeometric** (`const gsl_rng *` *r*, `unsigned int` *n1*, `unsigned int` *n2*, `unsigned int` *t*) Random

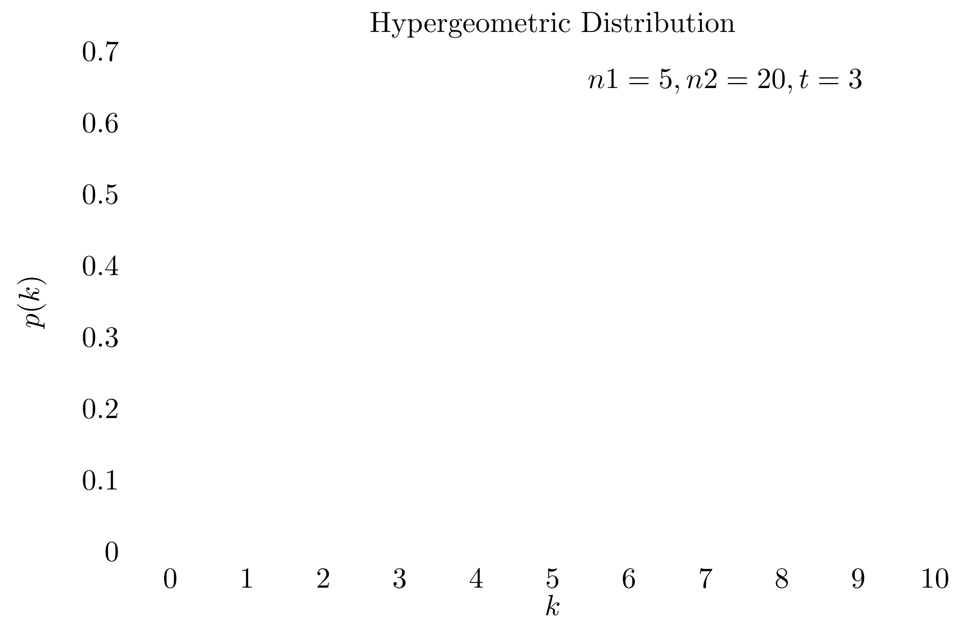
This function returns a random integer from the hypergeometric distribution. The probability distribution for hypergeometric random variates is,

$$p(k) = C(n_1, k)C(n_2, t - k)/C(n_1 + n_2, k)$$

where $C(a, b) = a!/(b!(a - b)!)$. The domain of k is $\max(0\, t - n_2), \ldots, \max(t, n_1)$.

`double` **gsl_ran_hypergeometric_pdf** (`unsigned int` *k*, `unsigned int` *n1*, `unsigned int` *n2*, `unsigned int` *t*) Function

This function computes the probability $p(k)$ of obtaining k from a hypergeometric distribution with parameters *n1*, *n2*, *n3*, using the formula given above.



19.36 The Logarithmic Distribution

`unsigned int` **gsl_ran_logarithmic** (`const gsl_rng *` *r*, `double` *p*) Random

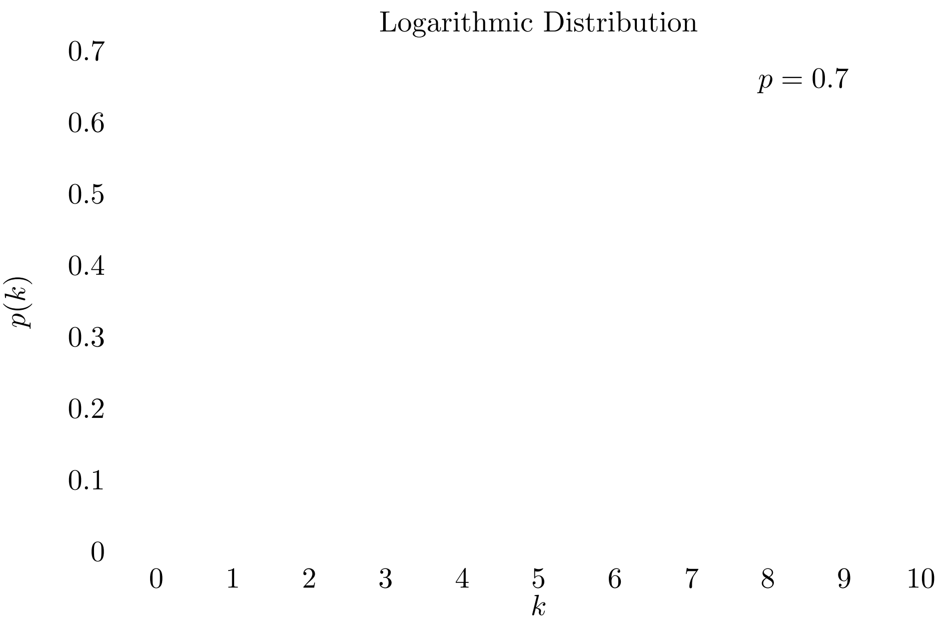
This function returns a random integer from the logarithmic distribution. The probability distribution for logarithmic random variates is,

$$p(k) = \frac{-1}{\log(1-p)} \left(\frac{p^k}{k} \right)$$

for $k \geq 1$.

`double` **gsl_ran_logarithmic_pdf** (`unsigned int` *k*, `double` *p*) Function

This function computes the probability $p(k)$ of obtaining k from a logarithmic distribution with probability parameter p, using the formula given above.



19.37 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 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*) Random

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*) Random

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*[k]. 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*) Random

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.

19.38 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");
  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 demo.c -lgsl -lgslcblas -lm
```

Here is the output of the program,

```
$ ./a.out
 4 2 3 3 1 3 4 1 3 5
```

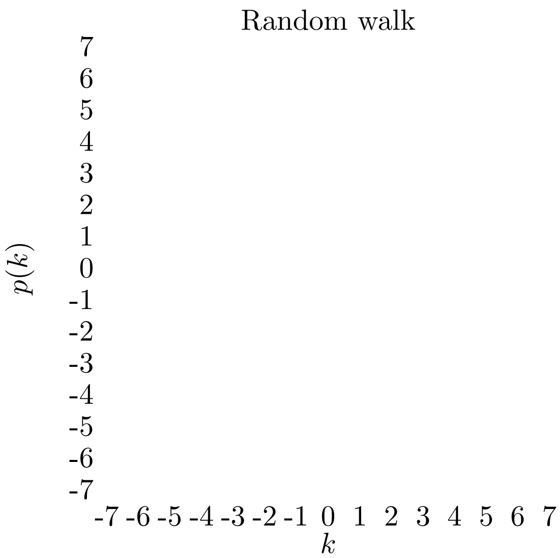
The variates depend on the seed used by the generator. The seed for the default generator type `gsl_rng_default` can be changed with the `GSL_RNG_SEED` environment variable to produce a different stream of variates,

```
$ GSL_RNG_SEED=123 ./a.out
GSL_RNG_SEED=123
 1 1 2 1 2 6 2 1 8 7
```

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);
    }
  return 0;
}
```

Example output from the program, three 10-step random walks from the origin.



19.39 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.

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.

20 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 files '`gsl_statistics_int.h`'.

20.1 Mean, Standard Deviation and Variance

`double` **gsl_stats_mean** (`const double` *data*[], `size_t` *stride*, `size_t` *n*) — Statistics

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*) — Statistics

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*) — Statistics

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*) Statistics

`double` **gsl_stats_sd_m** (`const double` *data*[], `size_t` *stride*, `size_t` *n*, `double` *mean*) Statistics

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_variance_with_fixed_mean** (`const double` *data*[], `size_t` *stride*, `size_t` *n*, `double` *mean*) Statistics

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*) Statistics

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.

20.2 Absolute deviation

`double` **gsl_stats_absdev** (`const double` *data*[], `size_t` *stride*, `size_t` *n*) Statistics

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*) Statistics

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).

20.3 Higher moments (skewness and kurtosis)

`double` **gsl_stats_skew** (`const double` *data*[], `size_t` *stride*, `size_t` *n*) Statistics

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*) Statistics

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*) Statistics

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*) Statistics

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.

20.4 Autocorrelation

double **gsl_stats_lag1_autocorrelation** (const double data[], const size_t *stride*, const size_t *n*) — Function

This function computes the lag-1 autocorrelation of the dataset *data*.

$$a_1 = \frac{\sum_{i=1}^{n}(x_i - \hat{\mu})(x_{i-1} - \hat{\mu})}{\sum_{i=1}^{n}(x_i - \hat{\mu})(x_i - \hat{\mu})}$$

double **gsl_stats_lag1_autocorrelation_m** (const double data[], const size_t *stride*, const size_t *n*, const double *mean*) — Function

This function computes the lag-1 autocorrelation of the dataset *data* using the given value of the mean *mean*.

20.5 Covariance

double **gsl_stats_covariance** (const double *data1*[], const size_t *stride1*, const double data2[], const size_t *stride2*, const size_t *n*) — Function

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 *n*, const double *mean1*, const double *mean2*) — Function

This function computes the covariance of the datasets *data1* and *data2* using the given values of the means, *mean1* and *mean2*.

20.6 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*) — Statistics

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*) — Statistics

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 defined 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*) — Statistics

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*) — Statistics

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*) — Statistics

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*) — Statistics

This function computes an unbiased estimate of the variance of 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*) — Statistics

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_wabsdev** (`const double` *w*[], `size_t` *wstride*, `const double` *data*[], `size_t` *stride*, `size_t` *n*) — Statistics

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*) Statistics

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*) Statistics

This function computes the weighted skewness of the dataset *data*.

$$skew = \frac{\sum w_i ((x_i - xbar)/\sigma)^3}{\sum w_i}$$

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*) Statistics

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*) Statistics

This function computes the weighted kurtosis of the dataset *data*.

$$kurtosis = \frac{\sum w_i ((x_i - xbar)/sigma)^4}{\sum w_i} - 3$$

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*) Statistics

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*.

20.7 Maximum and Minimum values

double **gsl_stats_max** (const double *data*[], size_t *stride*, size_t *n*) Statistics

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*) Statistics

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*) Statistics

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*) Statistics

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*) Statistics

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*) Statistics

This function returns the indexes *min_index*, *max_index* of the minimum and maximum values in *data* in a single pass.

20.8 Median and Percentiles

The median and percentile functions described in this section operate on sorted data. 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*[], size_t *stride*, size_t *n*) Statistics

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_quantile_from_sorted_data** (`const double` *sorted_data*[], `size_t` *stride*, `size_t` *n*, `double` *f*) Statistics

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.

20.9 Example statistical programs

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 4.2984
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);

  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
```

20.10 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 `http://pdg.lbl.gov/`.

21 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 real data.

The functions are declared in the header files '`gsl_histogram.h`' and '`gsl_histogram2d.h`'.

21.1 The histogram struct

A histogram is defined by the following struct,

gsl_histogram Data Type

`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,

$$\text{bin[i] corresponds to range[i]} \le x < \text{range[i+1]}$$

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[5] )
  ---|---------|---------|---------|---------|---------|---   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 ($r \le x$), 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`'.

21.2 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*) Function

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*) Function

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*) Function

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) Function

This function frees the histogram *h* and all of the memory associated with it.

21.3 Copying Histograms

int **gsl_histogram_memcpy** (gsl_histogram * *dest*, const gsl_histogram * *src*) Function

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*) Function

This function returns a pointer to a newly created histogram which is an exact copy of the histogram *src*.

21.4 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) Function

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 histogram 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*) Function

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*) Function

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*) Function

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*) Function
`double` **gsl_histogram_min** (`const gsl_histogram *` *h*) Function
`size_t` **gsl_histogram_bins** (`const gsl_histogram *` *h*) Function

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*) Function

This function resets all the bins in the histogram *h* to zero.

21.5 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*) Function

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.

21.6 Histogram Statistics

`double` **gsl_histogram_max_val** (`const gsl_histogram *` *h*) Function

This function returns the maximum value contained in the histogram bins.

`size_t` **gsl_histogram_max_bin** (`const gsl_histogram *` *h*) Function

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*) Function

This function returns the minimum value contained in the histogram bins.

`size_t` **gsl_histogram_min_bin** (`const gsl_histogram *` *h*) Function

This function returns the index of the bin containing the minimum value. In the case where several bins contain the same maximum value the smallest index is returned.

double **gsl_histogram_mean** (const gsl_histogram * *h*) Function

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*) Function

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*) Function

This function returns the sum of all bin values. Negative bin values are included in the sum.

21.7 Histogram Operations

int **gsl_histogram_equal_bins_p** (const gsl_histogram **h1*, const gsl_histogram **h2*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

This function shifts the contents of the bins of histogram *h* by the constant *offset*, i.e. $h'_1(i) = h_1(i) + offset$.

21.8 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*) Function

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*) Function

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*) Function

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*) Function

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.

21.9 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.

21.10 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.

gsl_histogram_pdf Data Type

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) Function

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*) — Function

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*) — Function

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*) — Function

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,

$$s = \mathrm{range}[i] + \delta * (\mathrm{range}[i+1] - \mathrm{range}[i])$$

where i is the index which satisfies $sum[i] \leq r < sum[i+1]$ and *delta* is $(r - sum[i])/(sum[i+1] - sum[i])$.

21.11 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");
```

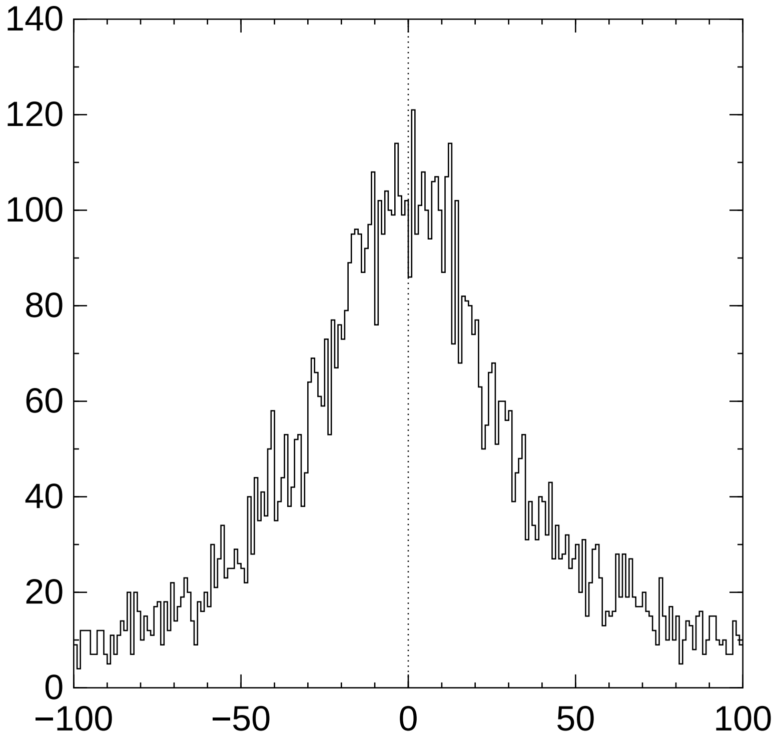
```
        exit (0);
      }

    a = atof (argv[1]);
    b = atof (argv[2]);
    n = atoi (argv[3]);

    {
      int status;
      double x;

      gsl_histogram * h = gsl_histogram_alloc (n);

      gsl_histogram_set_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
```

A plot of the resulting histogram shows the familiar shape of the Cauchy distribution and the fluctuations caused by the finite sample size.

```
$ awk '{print $1, $3 ; print $2, $3}' histogram.dat
   | graph -T X
```



21.12 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 $n(x, E)$.

21.13 The 2D histogram struct

Two dimensional histograms are defined by the following struct,

gsl_histogram2d Data Type

`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* 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,

$$\begin{array}{cc} \text{bin(i,j) corresponds to} & xrange[i] \le x < xrange[i+1] \\ \text{and} & yrange[j] \le y < yrange[j+1] \end{array}$$

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`'.

21.14 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*) Function

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*) Function

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*) Function

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*) Function

This function frees the 2D histogram *h* and all of the memory associated with it.

21.15 Copying 2D Histograms

int **gsl_histogram2d_memcpy** (gsl_histogram2d * *dest*, const gsl_histogram2d * *src*) Function

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*) Function

This function returns a pointer to a newly created histogram which is an exact copy of the histogram *src*.

21.16 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*) Function

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 bins are modified. The error handler is not called, since it is often necessary to compute histogram 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*) Function

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*) Function

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*) Function

int **gsl_histogram2d_get_yrange** (const gsl_histogram2d * *h*, size_t *j*, double * *ylower*, double * *yupper*) Function

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*) Function
`double` **gsl_histogram2d_xmin** (`const gsl_histogram2d *` *h*) Function
`size_t` **gsl_histogram2d_nx** (`const gsl_histogram2d *` *h*) Function
`double` **gsl_histogram2d_ymax** (`const gsl_histogram2d *` *h*) Function
`double` **gsl_histogram2d_ymin** (`const gsl_histogram2d *` *h*) Function
`size_t` **gsl_histogram2d_ny** (`const gsl_histogram2d *` *h*) Function

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*) Function

This function resets all the bins of the histogram *h* to zero.

21.17 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*) Function

This function finds and sets the indices *i* and *j* to the to the bin which covers the coordinates (*x*,*y*). The bin is located using a binary search. The search includes an optimization for histogram 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.

21.18 2D Histogram Statistics

`double` **gsl_histogram2d_max_val** (`const gsl_histogram2d *` *h*) Function

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*) Function

This function returns the indices (*i*,*j*) of the bin containing the maximum value in the histogram *h*. 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*) Function

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*) Function

This function returns the indices (*i*,*j*) of the bin containing the minimum value in the histogram *h*. 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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

This function returns the sum of all bin values. Negative bin values are included in the sum.

21.19 2D Histogram Operations

`int` **gsl_histogram2d_equal_bins_p** (`const gsl_histogram2d *`*h1*, `const gsl_histogram2d *`*h2*) Function

This function returns 1 if the all of the individual bin ranges of the two histograms are identical, and 0 otherwise.

`int` **gsl_histogram2d_add** (`gsl_histogram2d` **h1*, `const gsl_histogram2d` **h2*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

This function shifts the contents of the bins of histogram *h* by the constant *offset*, i.e. $h'_1(i,j) = h_1(i,j) + offset$.

21.20 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*) Function

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*) Function

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*) Function

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*) Function

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_histogram_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.

21.21 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.

gsl_histogram2d_pdf Data Type

`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`) Function

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*) Function

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*) Function

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*) Function

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*.

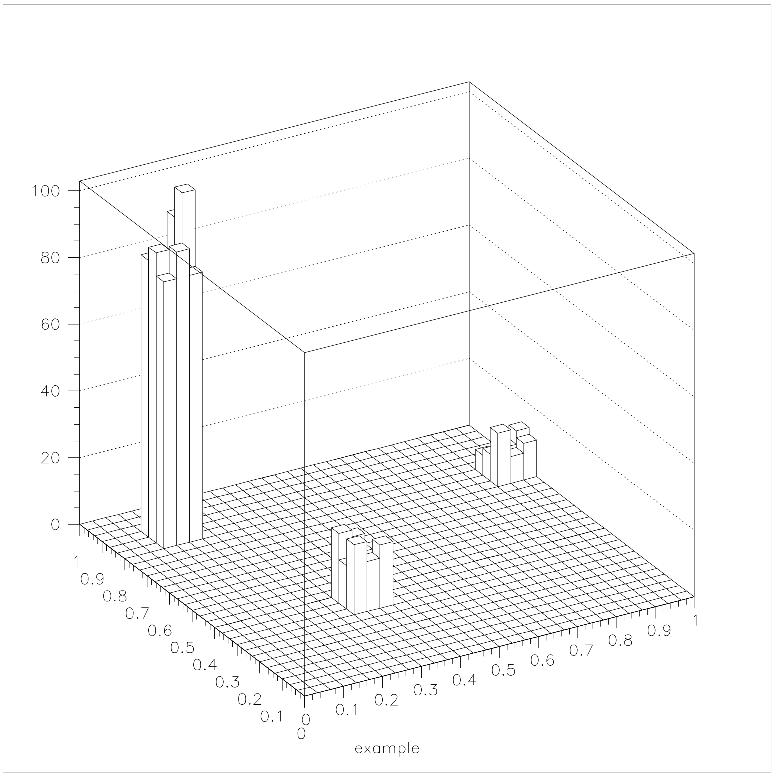
21.22 Example programs for 2D histograms

This program demonstrates two features of two-dimensional histograms. First a 10 by 10 2d-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);

  {
    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);

        int status
         = gsl_histogram2d_pdf_sample (p, u, v, &x, &y);

        printf("%g %g\n", x, y);
      }
    }

   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.



22 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 an 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 entry for each event.

All the ntuple functions are defined in the header file '`gsl_ntuple.h`'

22.1 The ntuple struct

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;
```

22.2 Creating ntuples

`gsl_ntuple *` **gsl_ntuple_create** (`char *` *filename*, `void *` *ntuple_data*, `size_t` *size*) Function

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.

22.3 Opening an existing ntuple file

`gsl_ntuple *` **gsl_ntuple_open** (`char *` *filename*, `void *` *ntuple_data*, `size_t` *size*) Function

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.

22.4 Writing ntuples

int **gsl_ntuple_write** (gsl_ntuple * *ntuple*) Function

This function writes the current ntuple *ntuple->ntuple_data* of size *ntuple->size* to the corresponding file.

int **gsl_ntuple_bookdata** (gsl_ntuple * *ntuple*) Function

This function is a synonym for `gsl_ntuple_write`

22.5 Reading ntuples

int **gsl_ntuple_read** (gsl_ntuple * *ntuple*) Function

This function reads the current row of the ntuple file for *ntuple* and stores the values in *ntuple->data*

22.6 Closing an ntuple file

int **gsl_ntuple_close** (gsl_ntuple * *ntuple*) Function

This function closes the ntuple file *ntuple* and frees its associated allocated memory.

22.7 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.

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.

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*) Function

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.

22.8 Example programs

The following example programs demonstrate the use of ntuples in managing a large dataset. The first program creates a set of 100,000 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 <config.h>
#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);

  for (i = 0; i < 10000; i++)
    {
      ntuple_row.x = gsl_ran_ugaussian (r);
```

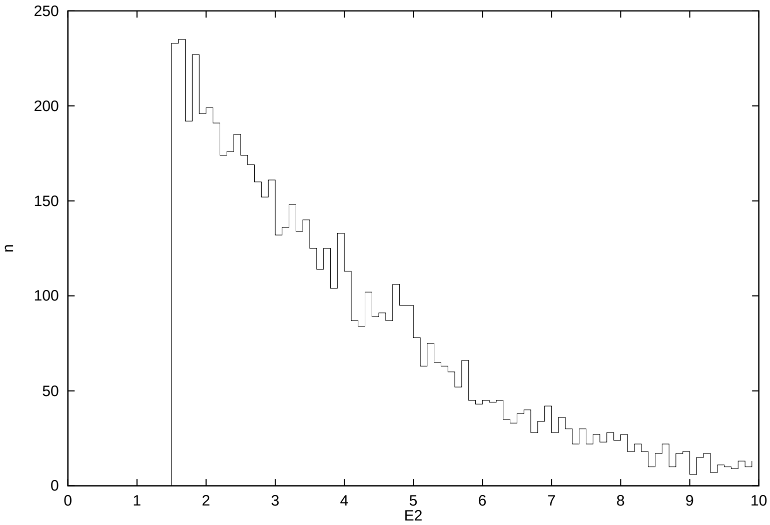
```
      ntuple_row.y = gsl_ran_ugaussian (r);
      ntuple_row.z = gsl_ran_ugaussian (r);

      gsl_ntuple_write (ntuple);
    }

  gsl_ntuple_close(ntuple);
  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 <config.h>
#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;
  int i;

  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;

  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)
{
  double x, y, z, E, scale;
  scale = *(double *) params;

  x = ((struct data *) ntuple_data)->x;
  y = ((struct data *) ntuple_data)->y;
  z = ((struct data *) ntuple_data)->z;

  E2 = x * x + y * y + z * z;

  return E2 > scale;
}

double
val_func (void *ntuple_data, void *params)
{
  double x, y, z;

  x = ((struct data *) ntuple_data)->x;
  y = ((struct data *) ntuple_data)->y;
  z = ((struct data *) ntuple_data)->z;

  return x * x + y * y + z * z;
}
```

The following plot shows the distribution of the selected events. Note the cut-off at the lower bound.



22.9 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).

23 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,

$$I = \int_{x_l}^{x_u} dx \int_{y_l}^{y_u} dy \ldots f(x, y, \ldots)$$

over a hypercubic region $((x_l, x_u), (y_l, y_u), \ldots)$ 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`’.

23.1 Interface

All of the Monte Carlo integration routines use the same 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`’.

gsl_monte_function Data Type

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 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.function = &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)->function))(x,(F)->dim,(F)->params)
```

23.2 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,

$$\sigma^2(E; N) = \frac{V}{N}\sum_i^N (f(x_i) - \langle f\rangle)^2$$

For large N this variance decreases asymptotically as $var(f)/N$, where $var(f)$ 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'.

gsl_monte_plain_state * **gsl_monte_plain_alloc** (size_t *dim*) Function

This function allocates and initializes a workspace for Monte Carlo integration in *dim* dimensions.

int **gsl_monte_plain_init** (gsl_monte_plain_state* *s*) Function

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*, double * *xl*, double * *xu*, size_t *dim*, size_t *calls*, gsl_rng * *r*, gsl_monte_plain_state * *s*, double * *result*, double * *abserr*) Function

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*), Function

This function frees the memory associated with the integrator state *s*.

23.3 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 $Var(f)$ of the combined estimate $E(f) = \frac{1}{2}(E_a(f) + E_b(f))$ is given by,

$$Var(f) = \frac{\sigma_a^2(f)}{4N_a} + \frac{\sigma_b^2(f)}{4N_b}$$

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`'.

`gsl_monte_miser_state *` **gsl_monte_miser_alloc** (`size_t` *dim*) Function

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*) Function

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*, `double *` *xl*, `double *` *xu*, `size_t` *dim*, `size_t` *calls*, `gsl_rng *` *r*, `gsl_monte_miser_state *` *s*, `double *` *result*, `double *` *abserr*) Function

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*), Function

This function frees the memory associated with the integrator state *s*.

The MISER algorithm has several configurable parameters. The following variables can be accessed through the `gsl_monte_miser_state` struct,

`double` **estimate_frac** Variable

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** Variable

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** Variable

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** Variable

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,

$$Var(f) = \frac{\sigma_a}{N_a^\alpha} + \frac{\sigma_b}{N_b^\alpha}$$

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** Variable

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 integration region. The default value of dither is zero, so no variation is introduced. If needed, a typical value of *dither* is around 0.1.

23.4 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,

$$Var_g(f; N) = Var(f/g; N)$$

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 in fixed number of points (the goal is 2). Each box can then have a fractional number of bins, but if bins/box is less than two, Vegas switches to a kind variance reduction (rather than importance sampling).

`gsl_monte_vegas_state *` **gsl_monte_vegas_alloc** (`size_t` *dim*) Function

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*) Function

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*) Function

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*), Function

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 VEGAS algorithm is highly configurable. The following variables can be accessed through the `gsl_monte_vegas_state` struct,

`double` **result** — Variable
`double` **sigma** — Variable

These parameters contain the raw value of the integral *result* and its error *sigma* from the last iteration of the algorithm.

`double` **chisq** — Variable

This parameter gives the chi-squared per degree of freedom for the weighted estimate of the integral. The value of *chisq* should be close to 1. A value of *chisq* 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.

`double` **alpha** — Variable

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** — Variable

The number of iterations to perform for each call to the routine. The default value is 5 iterations.

`int` **stage** — Variable

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** — Variable

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** Variable

`FILE *` **ostream** Variable

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.

23.5 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) */

/* 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)
{
  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 = %.1g 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);

    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, s->chisq);
        }
      while (fabs (s->chisq - 1.0) > 0.5);

      display_results ("vegas final", res, err);

      gsl_monte_vegas_free (s);
    }
    return 0;
  }
```

With 500,000 function calls the plain Monte Carlo algorithm achieves a fractional error of 0.6%. The estimated error `sigma` is consistent with the actual error, and the computed result differs from the true result by about one standard deviation,

```
plain ==================
result =  1.385867
sigma  =  0.007938
exact  =  1.393204
error  = -0.007337 = 0.9 sigma
```

The MISER algorithm reduces the error by a factor of two, and also correctly estimates the error,

```
miser ==================
result =  1.390656
sigma  =  0.003743
exact  =  1.393204
error  = -0.002548 = 0.7 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 =  1.386925
sigma  =  0.002651
exact  =  1.393204
error  = -0.006278 = 2 sigma
converging...
result =  1.392957 sigma =  0.000452 chisq/dof = 1.1
vegas final ==================
result =  1.392957
sigma  =  0.000452
exact  =  1.393204
error  = -0.000247 = 0.5 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.

23.6 References and Further Reading

The MISER algorithm is described in the following article,

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

24 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`'.

24.1 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 $E_{i+1} \le E_i$.

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.

24.2 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*) Function

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:

```
number_of_iterations temperature x x-(*x0_p) Ef(x)
```

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.

gsl_siman_Efunc_t Data Type

This function type should return the energy of a configuration *xp*.

```
double (*gsl_siman_Efunc_t) (void *xp)
```

gsl_siman_step_t Data Type

This function type should modify the configuration *xp* using a random step taken from the generator *r*, up to a maximium distance of *step_size*.

```
void (*gsl_siman_step_t) (const gsl_rng *r, void *xp,
                          double step_size)
```

gsl_siman_metric_t Data Type

This function type should return the distance between two configurations *xp* and *yp*.

```
double (*gsl_siman_metric_t) (void *xp, void *yp)
```

gsl_siman_print_t Data Type

This function type should print the contents of the configuration *xp*.

```
void (*gsl_siman_print_t) (void *xp)
```

gsl_siman_copy_t Data Type

This function type should copy the configuration *dest* into *source*.

```
void (*gsl_siman_copy_t) (void *source, void *dest)
```

gsl_siman_copy_construct_t Data Type

This function type should create a new copy of the configuration *xp*.

```
void * (*gsl_siman_copy_construct_t) (void *xp)
```

gsl_siman_destroy_t Data Type

This function type should destroy the configuration *xp*, freeing its memory.

```
void (*gsl_siman_destroy_t) (void *xp)
```

gsl_siman_params_t Data Type

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

24.3 Examples with Simulated Annealing

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.

24.3.1 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.

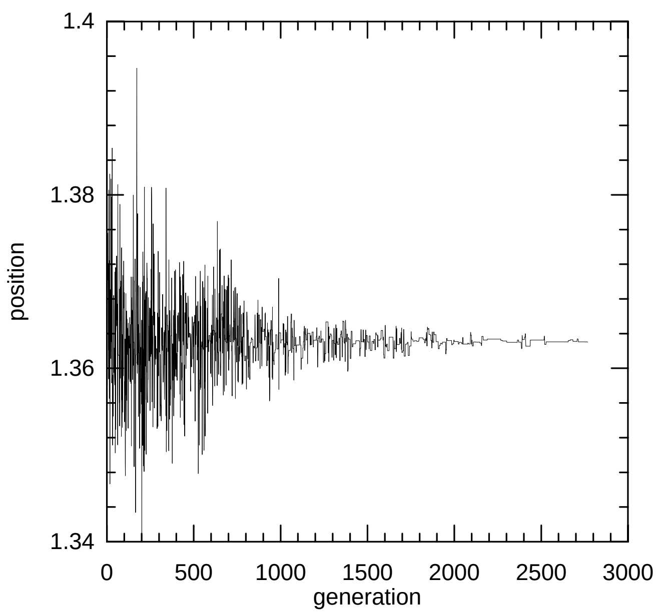
```
#include <math.h>
#include <stdlib.h>
#include <gsl/gsl_siman.h>

/* 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 10

/* max step size in random walk */
#define STEP_SIZE 10

/* Boltzmann constant */
```

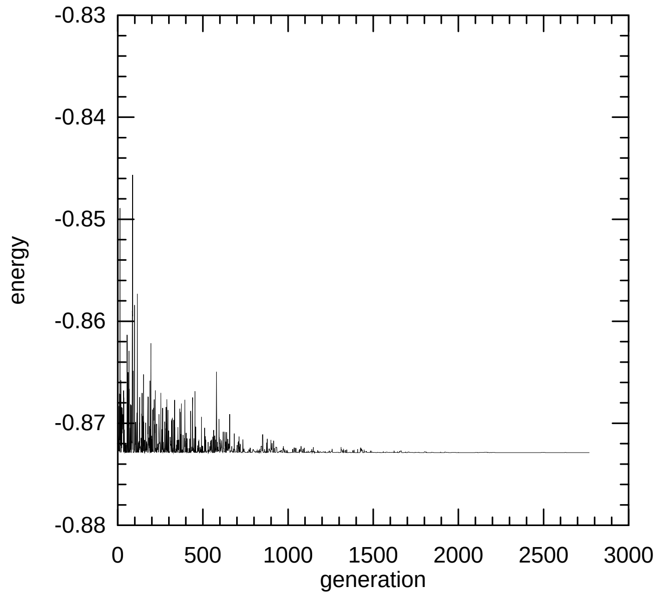
```
#define K 1.0

/* initial temperature */
#define T_INITIAL 0.002

/* damping factor for temperature */
#define MU_T 1.005
#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(int argc, char *argv[])
{
  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);

  gsl_siman_solve(r, &x_initial, E1, S1, M1, P1,
                  NULL, NULL, NULL,
                  sizeof(double), params);
  return 0;
}
```

Here are a couple of plots that are generated by running `siman_test` in the following way:

```
./siman_test | grep -v "^#"
  | xyplot -xyil -y -0.88 -0.83 -d "x...y"
  | xyps -d > siman-test.eps
./siman_test | grep -v "^#"
  | xyplot -xyil -xl "generation" -yl "energy" -d "x..y"
  | xyps -d > siman-energy.eps
```





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.

24.3.2 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 can be found in '`siman/siman_tsp.c`', but I include here some plots generated with in the following way:

```
./siman_tsp > tsp.output
grep -v "^#" tsp.output
  | xyplot -xyil -d "x...............y"
          -lx "generation" -ly "distance"
          -lt "TSP -- 12 southwest cities"
  | xyps -d > 12-cities.eps
grep initial_city_coord tsp.output
  | awk '{print $2, $3, $4, $5}'
  | xyplot -xyil -lb0 -cs 0.8
          -lx "longitude (- means west)"
          -ly "latitude"
          -lt "TSP -- initial-order"
  | xyps -d > initial-route.eps
grep final_city_coord tsp.output
  | awk '{print $2, $3, $4, $5}'
  | xyplot -xyil -lb0 -cs 0.8
          -lx "longitude (- means west)"
```

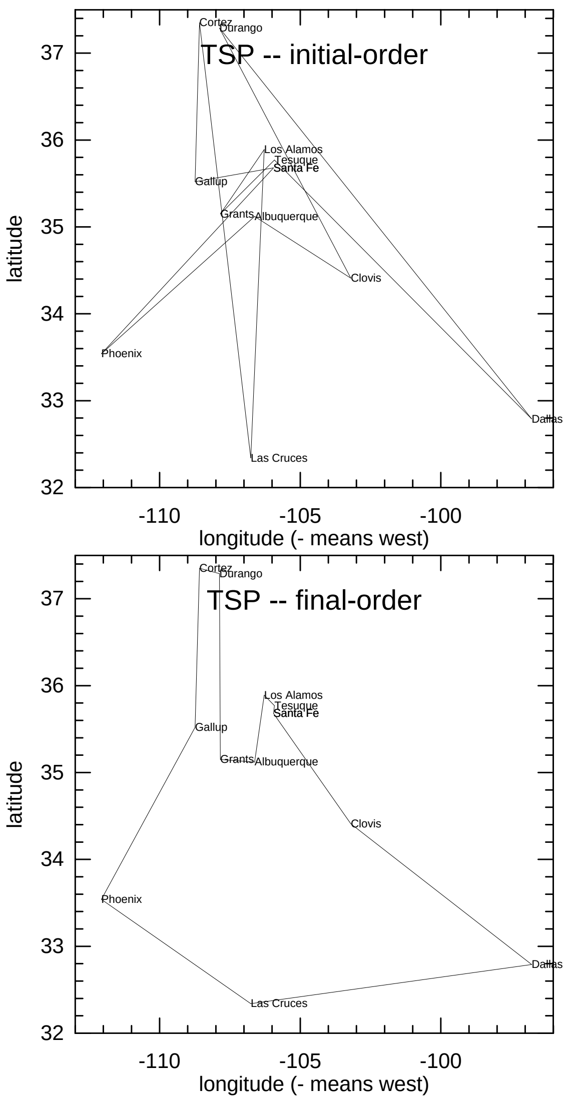
```
           -ly "latitude"
           -lt "TSP -- final-order"
   | xyps -d > final-route.eps
```

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
```

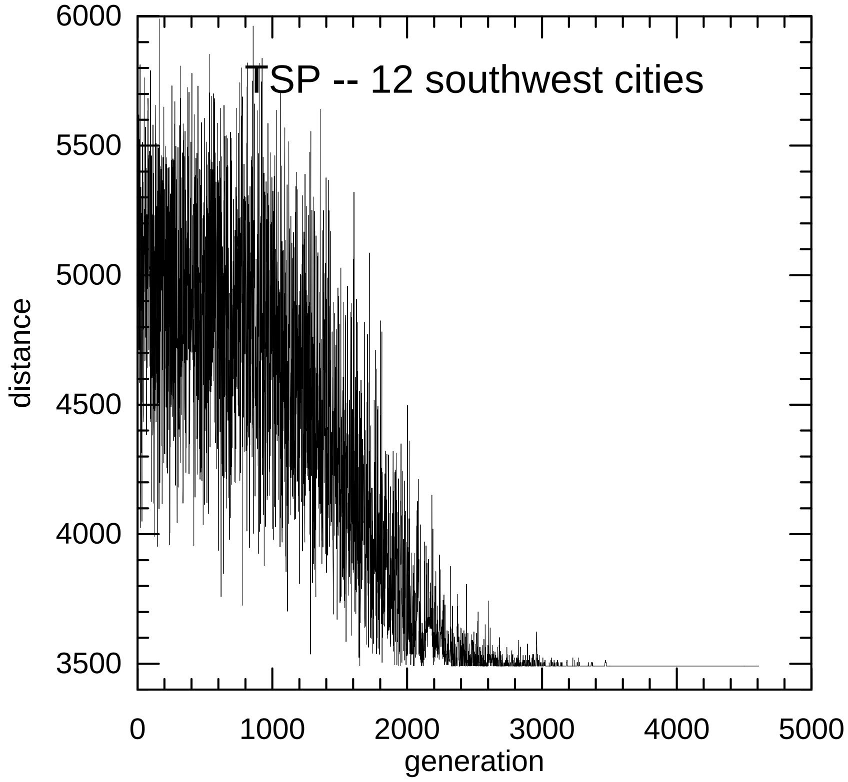
The optimal route turns out to be:

```
# final coordinates of cities (longitude and latitude)
###final_city_coord: -105.95 35.68 Santa Fe
###final_city_coord: -106.28 35.89 Los Alamos
###final_city_coord: -106.62 35.12 Albuquerque
###final_city_coord: -107.84 35.15 Grants
###final_city_coord: -107.87 37.29 Durango
###final_city_coord: -108.58 37.35 Cortez
###final_city_coord: -108.74 35.52 Gallup
###final_city_coord: -112.07 33.54 Phoenix
###final_city_coord: -106.76 32.34 Las Cruces
###final_city_coord: -96.77 32.79 Dallas
###final_city_coord: -103.2 34.41 Clovis
###final_city_coord: -105.92 35.77 Tesuque
###final_city_coord: -105.95 35.68 Santa Fe
```



Initial and final (optimal) route for the 12 southwestern cities Flying Salesman Problem.

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:



Example of a simulated annealing run for the 12 southwestern cities Flying Salesman Problem.

25 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.

These functions are declared in the header file '`gsl_odeiv.h`'.

25.1 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_odeiv_system` datatype.

gsl_odeiv_system Data Type

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*

`int (*` *jacobian*`) (double t, const double y[], double * dfdy, double dfdt[], void * params);`

This function should store the vector 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 * dim + j]` where `dim` is the dimension of the system.

Some of the simpler solver algorithms do not make use of the Jacobian matrix, so it is not always strictly necessary to provide it (this element of the struct can be replace by a null pointer). However, it is useful to provide the Jacobian to allow the solver algorithms to be interchanged – the best algorithms make use of the Jacobian.

`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.

25.2 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.

`gsl_odeiv_step *` **gsl_odeiv_step_alloc** (`const gsl_odeiv_step_type *` *T*, `size_t` *dim*) Function

This function returns a pointer to a newly allocated instance of a stepping function of type T for a system of *dim* dimensions.

`int` **gsl_odeiv_step_reset** (`gsl_odeiv_step *` *s*) Function

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_odeiv_step_free** (`gsl_odeiv_step *` *s*) Function

This function frees all the memory associated with the stepping function *s*.

`const char *` **gsl_odeiv_step_name** (`const gsl_odeiv_step *` *s*) Function

This function returns a pointer to the name of the stepping function. For example,

```
printf("step method is '%s'\n",
        gsl_odeiv_step_name (s));
```

would print something like `step method is 'rk4'`.

`unsigned int` **gsl_odeiv_step_order** (`const gsl_odeiv_step *` *s*) Function

This function returns the order of the stepping function on the previous step. This order can vary if the stepping function itself is adaptive.

`int` **gsl_odeiv_step_apply** (`gsl_odeiv_step *` *s*, `double` *t*, `double` *h*, `double y[]`, `double yerr[]`, `const double dydt_in[]`, `double dydt_out[]`, `const gsl_odeiv_system *` *dydt*) Function

This function applies the stepping function *s* to the system of equations defined by *dydt*, 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 following algorithms are available,

gsl_odeiv_step_rk2 Step Type

Embedded 2nd order Runge-Kutta with 3rd order error estimate.

gsl_odeiv_step_rk4 Step Type

4th order (classical) Runge-Kutta.

gsl_odeiv_step_rkf45 Step Type

Embedded 4th order Runge-Kutta-Fehlberg method with 5th order error estimate. This method is a good general-purpose integrator.

gsl_odeiv_step_rkck Step Type

Embedded 4th order Runge-Kutta Cash-Karp method with 5th order error estimate.

gsl_odeiv_step_rk8pd Step Type

Embedded 8th order Runge-Kutta Prince-Dormand method with 9th order error estimate.

gsl_odeiv_step_rk2imp Step Type

Implicit 2nd order Runge-Kutta at Gaussian points

gsl_odeiv_step_rk4imp Step Type

Implicit 4th order Runge-Kutta at Gaussian points

gsl_odeiv_step_bsimp Step Type

Implicit Bulirsch-Stoer method of Bader and Deuflhard. This algorithm requires the Jacobian.

gsl_odeiv_step_gear1 Step Type

M=1 implicit Gear method

gsl_odeiv_step_gear2 Step Type

M=2 implicit Gear method

25.3 Adaptive Step-size Control

The control function examines the proposed change to the solution and its error estimate produced by a stepping function and attempts to determine the optimal step-size for a user-specified level of error.

`gsl_odeiv_control *` **gsl_odeiv_control_standard_new** (`double` *eps_abs*, `double` *eps_rel*, `double` *a_y*, `double` *a_dydt*) Function

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,

$$D_i = \epsilon_{abs} + \epsilon_{rel} * (a_y |y_i| + a_{dydt} h |y'_i|)$$

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,

$$h_{new} = h_{old} * S * (D/E)^{1/q}$$

where q is the consistency order of method (e.g. $q = 4$ for 4(5) embedded RK), and S is a safety factor of 0.9. The ratio D/E is taken to be the maximum of the ratios D_i/E_i.

If the observed error E is less than 50% of the desired error level D for the maximum ratio D_i/E_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.

`gsl_odeiv_control *` **gsl_odeiv_control_y_new** (`double` *eps_abs*, `double` *eps_rel*) Function

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_odeiv_control *` **gsl_odeiv_control_yp_new** (`double` *eps_abs*, `double` *eps_rel*) Function

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_odeiv_control *` **gsl_odeiv_control_scaled_new** (`double` *eps_abs*, `double` *eps_rel*, `double` *a_y*, `double` *a_dydt*, `const double` *scale_abs*[], `size_t` *dim*) Function

This function creates a new control object which uses the same algorithm as `gsl_odeiv_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,

$$D_i = \epsilon_{abs} s_i + \epsilon_{rel} * (a_y |y_i| + a_{dydt} h |y'_i|)$$

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_odeiv_control *` **gsl_odeiv_control_alloc** (`const gsl_odeiv_control_type *` *T*) Function

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_odeiv_control_init** (`gsl_odeiv_control *` *c*, `double` *eps_abs*, `double` *eps_rel*, `double` *a_y*, `double` *a_dydt*) Function

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_odeiv_control_free** (gsl_odeiv_control * *c*) Function

This function frees all the memory associated with the control function *c*.

int **gsl_odeiv_control_hadjust** (gsl_odeiv_control * *c*, gsl_odeiv_step * *s*, const double y0[], const double yerr[], const double dydt[], double * *h*) Function

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_odeiv_control_name** (const gsl_odeiv_control * *c*) Function

This function returns a pointer to the name of the control function. For example,

```
printf("control method is '%s'\n",
       gsl_odeiv_control_name (c));
```

would print something like `control method is 'standard'`

25.4 Evolution

The highest level of the system is the evolution function which combines the results of a stepping function and control function to reliably advance the solution forward over an interval (t_0, t_1). If the control function signals that the step-size should be decreased the evolution function backs out of the current step and tries the proposed smaller step-size. This is process is continued until an acceptable step-size is found.

gsl_odeiv_evolve * **gsl_odeiv_evolve_alloc** (size_t *dim*) Function

This function returns a pointer to a newly allocated instance of an evolution function for a system of *dim* dimensions.

int **gsl_odeiv_evolve_apply** (gsl_odeiv_evolve * *e*, gsl_odeiv_control * *con*, gsl_odeiv_step * *step*, const gsl_odeiv_system * *dydt*, double * *t*, double *t1*, double * *h*, double y[]) Function

This function advances the system (*e*, *dydt*) 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*, but this will be modified using the control function *c* to achieve the appropriate error bound if necessary. The routine may make several calls to *step* in order to determine the optimum step-size. If the step-size has been changed the value of *h* will be modified on output. 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_odeiv_evolve_reset** (`gsl_odeiv_evolve *` *e*) Function

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_odeiv_evolve_free** (`gsl_odeiv_evolve *` *e*) Function

This function frees all the memory associated with the evolution function *e*.

25.5 Examples

The following program solves the second-order nonlinear Van der Pol oscillator equation,

$$x''(t) + \mu x'(t)(x(t)^2 - 1) + x(t) = 0$$

This can be converted into a first order system suitable for use with the library by introducing a separate variable for the velocity, $y = x'(t)$,

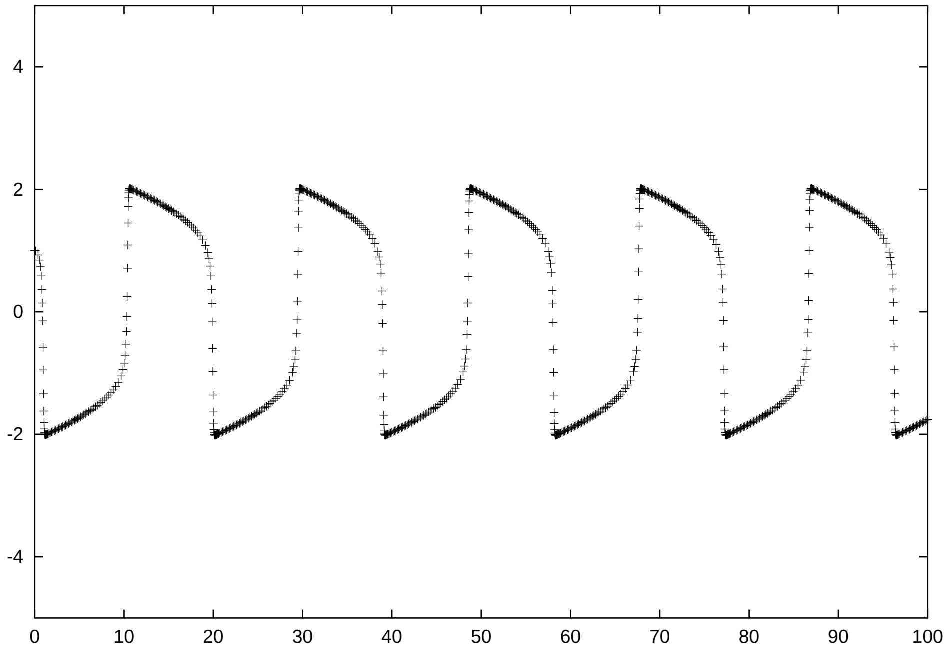
$$x' = y$$
$$y' = -x + \mu y(1 - x^2)$$

The program begins by defining functions for these derivatives and their Jacobian,

```
#include <stdio.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_odeiv.h>

int
func (double t, const double y[], double f[],
      void *params)
{
  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)
{
  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));
  dfdt[0] = 0.0;
  dfdt[1] = 0.0;
  return GSL_SUCCESS;
```

```
}

int
main (void)
{
  const gsl_odeiv_step_type * T
    = gsl_odeiv_step_rk8pd;

  gsl_odeiv_step * s
    = gsl_odeiv_step_alloc (T, 2);
  gsl_odeiv_control * c
    = gsl_odeiv_control_y_new (1e-6, 0.0);
  gsl_odeiv_evolve * e
    = gsl_odeiv_evolve_alloc (2);

  double mu = 10;
  gsl_odeiv_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_odeiv_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_odeiv_evolve_free(e);
  gsl_odeiv_control_free(c);
  gsl_odeiv_step_free(s);
  return 0;
}
```

The main loop of the program evolves the solution from $(y, y') = (1, 0)$ 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 y.



Numerical solution of the Van der Pol oscillator equation
using Prince-Dormand 8th order Runge-Kutta.

To obtain the values at regular intervals, rather than the variable spacings chosen by the control function, the main loop can be modified to advance the solution from one point to the next. For example, the following main loop prints the solution at the fixed points $t = 0, 1, 2, \ldots, 100$,

```
  for (i = 1; i <= 100; i++)
    {
      double ti = i * t1 / 100.0;

      while (t < ti)
        {
          gsl_odeiv_evolve_apply (e, c, s,
                                  &sys,
                                  &t, ti, &h,
                                  y);
        }

      printf("%.5e %.5e %.5e\n", t, y[0], y[1]);
    }
```

It is also possible to work with a non-adaptive integrator, using only the stepping function itself. The following program uses the rk4 fourth-order Runge-Kutta stepping function with a fixed stepsize of 0.01,

```
int
main (void)
{
  const gsl_odeiv_step_type * T
    = gsl_odeiv_step_rk4;

  gsl_odeiv_step * s
```

```
    = gsl_odeiv_step_alloc (T, 2);

  double mu = 10;
  gsl_odeiv_system sys = {func, jac, 2, &mu};

  double t = 0.0, t1 = 100.0;
  double h = 1e-2;
  double y[2] = { 1.0, 0.0 }, y_err[2];
  double dfdy[4], dydt_in[2], dydt_out[2];

  /* initialise dydt_in */
  GSL_ODEIV_JA_EVAL(&sys, t, y, dfdy, dydt_in);

  while (t < t1)
    {
      int status = gsl_odeiv_step_apply (s, t, h,
                                         y, y_err,
                                         dydt_in,
                                         dydt_out,
                                         &sys);

      if (status != GSL_SUCCESS)
          break;

      dydt_in[0] = dydt_out[0];
      dydt_in[1] = dydt_out[1];

      t += h;

      printf("%.5e %.5e %.5e\n", t, y[0], y[1]);
    }

  gsl_odeiv_step_free(s);
  return 0;
}
```

The derivatives and jacobian must be initialised for the starting point $t = 0$ before the first step is taken. Subsequent steps use the output derivatives *dydt_out* as inputs to the next step by copying their values into *dydt_in*.

25.6 References and Further Reading

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.

26 Interpolation

This chapter describes functions for performing interpolation. The library provides a variety of interpolation methods, including Cubic splines and Akima 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.

The functions described in this section are declared in the header files 'gsl_interp.h' and 'gsl_spline.h'.

26.1 Introduction

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 $y_i = y(x_i)$. The interpolation is piecewise smooth, and its behavior at the end-points is determined by the type of interpolation used.

26.2 Interpolation Functions

The interpolation function for a given dataset is stored in a `gsl_interp` object. These are created by the following functions.

`gsl_interp *` **gsl_interp_alloc** (`const gsl_interp_type *` *T*, `size_t` *size*) Function

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*) Function

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; the behavior for other arrangements is not defined.

`void` **gsl_interp_free** (`gsl_interp *` *interp*) Function

This function frees the interpolation object *interp*.

26.3 Interpolation Types

The interpolation library provides five interpolation types:

gsl_interp_linear Interpolation Type

Linear interpolation. This interpolation method does not require any additional memory.

gsl_interp_polynomial Interpolation Type

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_cspline Interpolation Type

Cubic spline with natural boundary conditions.

gsl_interp_cspline_periodic Interpolation Type

Cubic spline with periodic boundary conditions

gsl_interp_akima Interpolation Type

Akima spline with natural boundary conditions.

gsl_interp_akima_periodic Interpolation Type

Akima spline with periodic boundary conditions.

The following related functions are available:

`const char *` **gsl_interp_name** (`const gsl_interp *` *interp*) Function

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*) Function

This function returns the minimum number of points required by the interpolation type of *interp*. For example, Akima spline interpolation requires a minimum of 5 points.

26.4 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. 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*) Function

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*].

`gsl_interp_accel *` **gsl_interp_accel_alloc** (`void`) Function

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.

`size_t` **gsl_interp_accel_find** (`gsl_interp_accel *` *a*, `const double` `x_array[]`, `size_t` *size*, `double` *x*) Function

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 `xarray[i] <= x < xarray[i+1]`.

`void` **gsl_interp_accel_free** (`gsl_interp_accel*` *a*) Function

This function frees the accelerator object *a*.

26.5 Evaluation of Interpolating Functions

`double` **gsl_interp_eval** (`const gsl_interp *` *interp*, `const double` *xa*[], `const double` *ya*[], `double` *x*, `gsl_interp_accel *` *a*) Function

`int` **gsl_interp_eval_e** (`const gsl_interp *` *interp*, `const double` *xa*[], `const double` *ya*[], `double` *x*, `gsl_interp_accel *` *a*, `double *` *y*) Function

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 *a*.

`double` **gsl_interp_eval_deriv** (`const gsl_interp *` *interp*, `const double` *xa*[], `const double` *ya*[], `double` *x*, `gsl_interp_accel *` *a*) Function

`int` **gsl_interp_eval_deriv_e** (`const gsl_interp *` *interp*, `const double` *xa*[], `const double` *ya*[], `double` *x*, `gsl_interp_accel *` *a*, `double *` *d*) Function

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 *a*.

`double` **gsl_interp_eval_deriv2** (`const gsl_interp *` *interp*, `const double` *xa*[], `const double` *ya*[], `double` *x*, `gsl_interp_accel *` *a*) Function

`int` **gsl_interp_eval_deriv2_e** (`const gsl_interp *` *interp*, `const double` *xa*[], `const double` *ya*[], `double` *x*, `gsl_interp_accel *` *a*, `double *` *d2*) Function

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 *a*.

double **gsl_interp_eval_integ** (const gsl_interp * *interp*, const double *xa*[], const double *ya*[], double *a*, double *b*double *x*, gsl_interp_accel * *a*) Function

int **gsl_interp_eval_integ_e** (const gsl_interp * *interp*, const double *xa*[], const double *ya*[], , double *a*, double *b*, gsl_interp_accel * *a*, double * *result*) Function

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 *a*.

26.6 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`'.

gsl_spline * **gsl_spline_alloc** (const gsl_interp_type * *T*, size_t *n*) Function

int **gsl_spline_init** (gsl_spline * *spline*, const double xa[], const double *ya*[], size_t *size*) Function

void **gsl_spline_free** (gsl_spline * *spline*) Function

double **gsl_spline_eval** (const gsl_spline * *spline*, double *x*, gsl_interp_accel * *a*) Function

int **gsl_spline_eval_e** (const gsl_spline * *spline*, double *x*, gsl_interp_accel * *a*, double * *y*) Function

double **gsl_spline_eval_deriv** (const gsl_spline * *spline*, double *x*, gsl_interp_accel * *a*) Function

int **gsl_spline_eval_deriv_e** (const gsl_spline * *spline*, double *x*, gsl_interp_accel * *a*, double * *d*) Function

double **gsl_spline_eval_deriv2** (const gsl_spline * *spline*, double *x*, gsl_interp_accel * *a*) Function

int **gsl_spline_eval_deriv2_e** (const gsl_spline * *spline*, double *x*, gsl_interp_accel * *a*, double * *d2*) Function

double **gsl_spline_eval_integ** (const gsl_spline * *spline*, double *a*, double *b*, gsl_interp_accel * *acc*) Function

int **gsl_spline_eval_integ_e** (const gsl_spline * *spline*, double *a*, double *b*, gsl_interp_accel * *acc*, double * *result*) Function

26.7 Examples

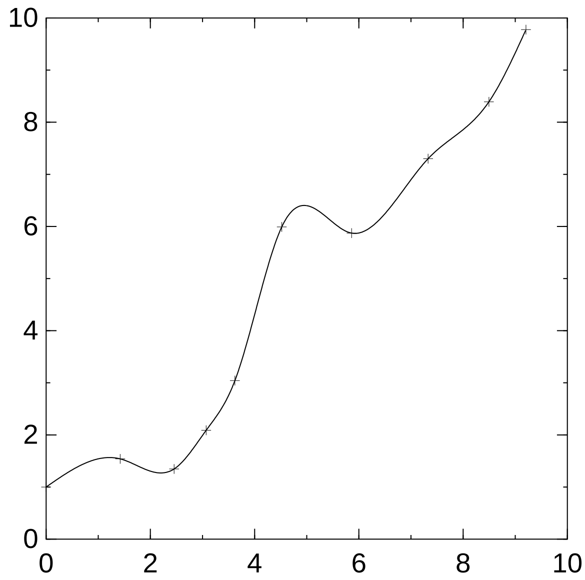
The following program demonstrates the use of the interpolation and spline functions. It computes a cubic spline interpolation of the 10-point dataset (x_i, y_i) where $x_i = i + \sin(i)/2$ and $y_i = i + \cos(i^2)$ for $i = 0 \ldots 9$.

```
#include <config.h>
#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=2\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
```



The result shows a smooth interpolation of the original points. The interpolation method can changed simply by varying the first argument of `gsl_spline_alloc`.

26.8 References and Further Reading

Descriptions of the interpolation algorithms and further references can be found in the following book,

C.W. Ueberhuber, *Numerical Computation (Volume 1), Chapter 9* "*Interpolation*", Springer (1997), ISBN 3-540-62058-3.

27 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_diff.h'

27.1 Functions

int **gsl_diff_central** (const gsl_function **f*, double *x*, double **result*, double **abserr*) — Function

This function computes the numerical derivative of the function *f* at the point *x* using an adaptive central difference algorithm. The derivative is returned in *result* and an estimate of its absolute error is returned in *abserr*.

int **gsl_diff_forward** (const gsl_function **f*, double *x*, double **result*, double **abserr*) — Function

This function computes the numerical derivative of the function *f* at the point *x* using an adaptive forward difference algorithm. The function is evaluated only at points greater than *x* and 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 singularity or is undefined for values less than *x*.

int **gsl_diff_backward** (const gsl_function **f*, double *x*, double **result*, double **abserr*) — Function

This function computes the numerical derivative of the function *f* at the point *x* using an adaptive backward difference algorithm. The function is evaluated only at points less than *x* and 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 singularity or is undefined for values greater than *x*.

27.2 Example

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_diff_forward`.

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

double f (double x, void * params)
{
  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_diff_central (&F, 2.0, &result, &abserr);
  printf("x = 2.0\n");
  printf("f'(x) = %.10f +/- %.5f\n", result, abserr);
  printf("exact = %.10f\n\n", 1.5 * sqrt(2.0));

  gsl_diff_forward (&F, 0.0, &result, &abserr);
  printf("x = 0.0\n");
  printf("f'(x) = %.10f +/- %.5f\n", result, abserr);
  printf("exact = %.10f\n", 0.0);

  return 0;
}
```

Here is the output of the program,

```
$ ./demo
f(x) = x^(3/2)

x = 2.0
f'(x) = 2.1213203435 +/- 0.01490
exact = 2.1213203436

x = 0.0
f'(x) = 0.0012172897 +/- 0.05028
exact = 0.0000000000
```

27.3 References and Further Reading

The algorithms used by these functions are described in the following book,

S.D. Conte and Carl de Boor, *Elementary Numerical Analysis: An Algorithmic Approach*, McGraw-Hill, 1972.

28 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, $T_0(x) = 1$, $T_1(x) = x$, $T_2(x) = 2x^2 - 1$.

The functions described in this chapter are declared in the header file 'gsl_chebyshev.h'.

28.1 The gsl_cheb_series struct

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_struct
```

The approximation is made over the range $[a, b]$ using *order*+1 terms, including the coefficient $c[0]$.

28.2 Creation and Calculation of Chebyshev Series

gsl_cheb_series * **gsl_cheb_alloc** (const size_t *n*) Function

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*) Function

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*) Function

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.

28.3 Chebyshev Series Evaluation

double **gsl_cheb_eval** (const gsl_cheb_series * *cs*, double *x*) Function

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*) Function

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*) Function

This function evaluates the Chebyshev series *cs* at a given point *n*, 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*) Function

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.

28.4 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*) Function

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*) Function

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*.

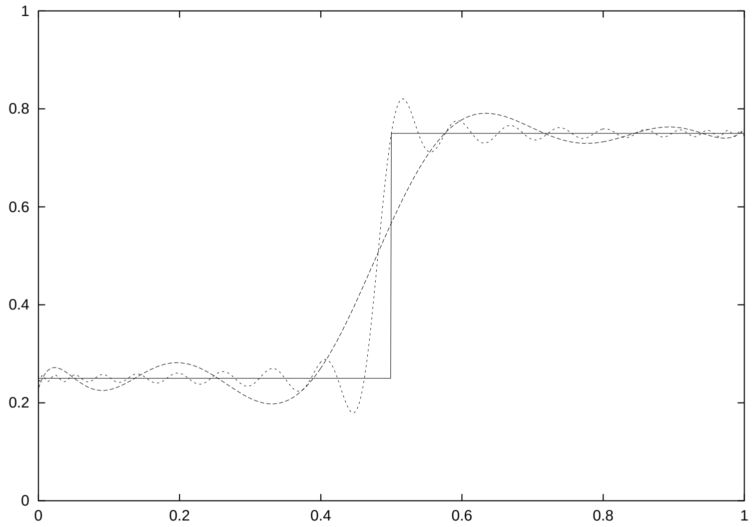
28.5 Examples

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)
{
  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;
}
```

The output from the program gives the original function, 10-th order approximation and 40-th order approximation, all sampled at intervals of 0.001 in x.



28.6 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)

29 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'.

29.1 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. .

gsl_sum_levin_u_workspace * **gsl_sum_levin_u_alloc** (size_t *n*) Function

This function allocates a workspace for a Levin u-transform of n terms. The size of the workspace is $O(2n^2 + 3n)$.

int **gsl_sum_levin_u_free** (gsl_sum_levin_u_workspace * *w*) Function

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*) Function

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.

29.2 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 converge 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.

`gsl_sum_levin_utrunc_workspace *` **gsl_sum_levin_utrunc_alloc** (`size_t` *n*) Function

This function allocates a workspace for a Levin u-transform of *n* terms, without error estimation. The size of the workspace is $O(3n)$.

`int` **gsl_sum_levin_utrunc_free** (`gsl_sum_levin_utrunc_workspace * `*w*) Function

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*) Function

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.

29.3 Example of accelerating a series

The following code calculates an estimate of $\zeta(2) = \pi^2/6$ using the series,

$$\zeta(2) = 1 + 1/2^2 + 1/3^2 + 1/4^2 + \ldots$$

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;

  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 %d terms\n",
         w->sum_plain, w->terms_used);

  printf("exact value      = % .16f\n", zeta_2);
  printf("accelerated sum  = % .16f using %d 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.

```
bash$ ./a.out
term-by-term sum =  1.5961632439130233 using 20 terms
term-by-term sum =  1.5759958390005426 using 13 terms
```

```
exact value      =  1.6449340668482264
accelerated sum  =  1.6449340668166479 using 13 terms
estimated error  =  0.0000000000508580
actual error     = -0.0000000000315785
```

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.

29.4 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://xxx.lanl.gov/abs/math/0005209`

30 Discrete Hankel Transforms

This chapter describes functions for performing Discrete Hankel Transforms (DHTs). The functions are declared in the header file 'gsl_dht.h'.

30.1 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 zeroes 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.

Specifically, let $f(t)$ be a function on the unit interval. Then the finite ν-Hankel transform of $f(t)$ is defined to be the set of numbers g_m given by

$$g_m = \int_0^1 t dt\, J_\nu(j_{\nu,m} t) f(t),$$

so that

$$f(t) = \sum_{m=1}^{\infty} \frac{2 J_\nu(j_{\nu,m} x)}{J_{\nu+1}(j_{\nu,m})^2} g_m.$$

Suppose that f is band-limited in the sense that $g_m = 0$ for $m > M$. Then we have the following fundamental sampling theorem.

$$g_m = \frac{2}{j_{\nu,M}^2} \sum_{k=1}^{M-1} f(\frac{j_{\nu,k}}{j_{\nu,M}}) \frac{J_\nu(j_{\nu,m} j_{\nu,k}/j_{\nu,M})}{J_{\nu+1}(j_{\nu,k})^2}.$$

It is this discrete expression which defines the discrete Hankel transform. 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 a scaling of the fundamental interval, for convenience, so that one take assume the function is defined on the interval $[0, X]$, rather than the unit interval.

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.

30.2 Functions

`gsl_dht *` **gsl_dht_alloc** (`size_t` *size*) Function

This function allocates a Discrete Hankel transform object of size *size*.

`int` **gsl_dht_init** (`gsl_dht *` *t*, `double` *nu*, `double` *xmax*) Function

This function initializes the transform *t* for the given values of *nu* and *x*.

gsl_dht * **gsl_dht_new** (size_t *size*, double *nu*, double *xmax*) Function

This function allocates a Discrete Hankel transform object of size *size* and initializes it for the given values of *nu* and *x*.

void **gsl_dht_free** (gsl_dht * *t*) Function

This function frees the transform *t*.

int **gsl_dht_apply** (const gsl_dht * *t*, double * *f_in*, double * *f_out*) Function

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.

double **gsl_dht_x_sample** (const gsl_dht * *t*, int *n*) Function

This function returns the value of the n'th sample point in the unit interval, $\frac{j_{\nu,n+1}}{j_{\nu,M}} X$. 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*) Function

This function returns the value of the n'th sample point in "k-space", $\frac{j_{\nu,n+1}}{X}$.

30.3 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).

31 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.

31.1 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.

31.2 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 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 go awry, 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.

31.3 Initializing the Solver

`gsl_root_fsolver *` **gsl_root_fsolver_alloc** (`const gsl_root_fsolver_type *` *T*) Function

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*) Function

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*) Function

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*) Function

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*) Function
`void` **gsl_root_fdfsolver_free** (`gsl_root_fdfsolver *` *s*) Function

These functions free all the memory associated with the solver *s*.

`const char *` **gsl_root_fsolver_name** (`const gsl_root_fsolver *` *s*) Function

`const char *` **gsl_root_fdfsolver_name** (`const gsl_root_fdfsolver *` *s*) Function

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`.

31.4 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:

gsl_function Data Type

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:

```
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 following macro,

```
#define GSL_FN_EVAL(F,x)
    (*((F)->function))(x,(F)->params)
```

gsl_function_fdf Data Type

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 following macro,

```
#define GSL_FN_FDF_EVAL_F(FDF,x)
     (*((FDF)->f))(x,(FDF)->params)
```

The derivative $f'(x)$ can be evaluated using the following macro,

```
#define GSL_FN_FDF_EVAL_DF(FDF,x)
     (*((FDF)->df))(x,(FDF)->params)
```

and both the function $y = f(x)$ and its derivative $dy = f'(x)$ can be evaluated at the same time using the following macro,

```
#define GSL_FN_FDF_EVAL_F_DF(FDF,x,y,dy)
     (*((FDF)->fdf))(x,(FDF)->params,(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`.

31.5 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 a 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.

31.6 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*) Function
`int` **gsl_root_fdfsolver_iterate** (`gsl_root_fdfsolver *` *s*) Function

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*) Function
`double` **gsl_root_fdfsolver_root** (`const gsl_root_fdfsolver *` *s*) Function

These functions return the current estimate of the root for the solver *s*.

`double` **gsl_root_fsolver_x_lower** (`const gsl_root_fsolver *` *s*) Function
`double` **gsl_root_fsolver_x_upper** (`const gsl_root_fsolver *` *s*) Function

These functions return the current bracketing interval for the solver *s*.

31.7 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*) Function

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,

$$|a - b| < epsabs + epsrel \min(|a|, |b|)$$

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^*,

$$|r - r^*| < epsabs + epsrel\, r^*$$

assuming that the true root r^* is contained within the interval.

int gsl_root_test_delta (double *x1*, double *x0*, double *epsrel*, double *epsabs*) Function

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,

$$|x_1 - x_0| < epsabs + epsrel\,|x_1|$$

and returns `GSL_CONTINUE` otherwise.

int gsl_root_test_residual (double *f*, double *epsabs*) Function

This function tests the residual value *f* against the absolute error bound *epsabs*. The test returns `GSL_SUCCESS` if the following condition is achieved,

$$|f| < epsabs$$

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.

31.8 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.

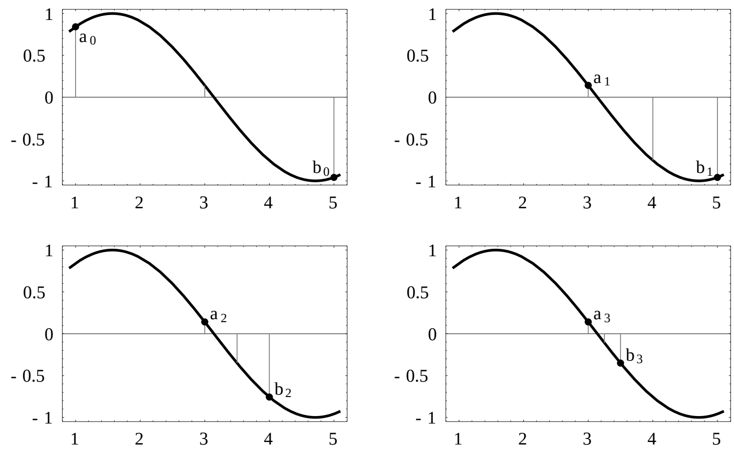
Note that a bracketing algorithm cannot find roots of even degree, since these do not cross the x-axis.

gsl_root_fsolver_bisection Solver

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.



Four iterations of bisection, where a_n is nth position of the beginning of the interval and b_n is the nth position of the end. The midpoint of each interval is also indicated.

gsl_root_fsolver_falsepos Solver

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_brent Solver

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.

31.9 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.

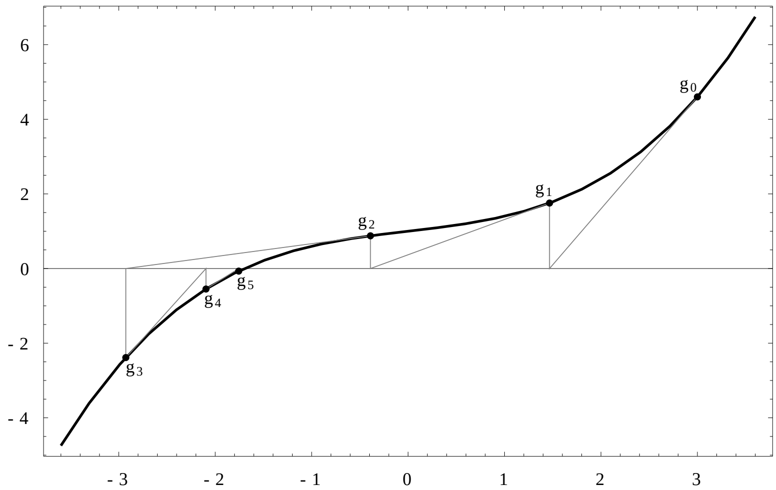
These algorithms make use of both the function and its derivative.

gsl_root_fdfsolver_newton Derivative Solver

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.



Several iterations of Newton's Method, where g_n is the nth guess.

gsl_root_fdfsolver_secant Derivative Solver

The *secant method* is a simplified version of Newton's method 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 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_steffenson Derivative Solver

The *Steffenson Method* 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.

31.10 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);
```

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;
  double c = p->c;

  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>

#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);
  return status;
}
```

Here are the results of the iterations,

```
bash$ ./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,

```
bash$ ./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;
  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);
    return status;
  }
```

Here are the results for Newton's method,

```
bash$ ./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`.

31.11 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

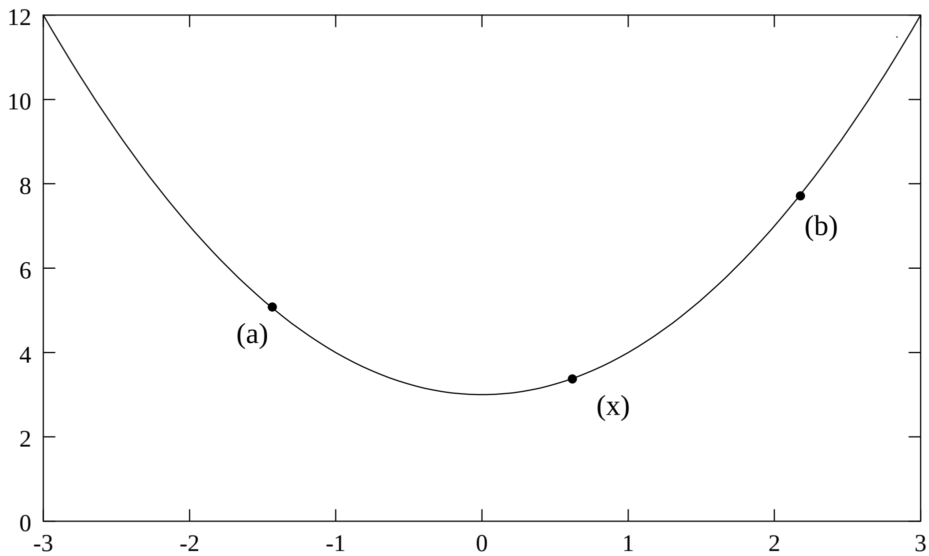
32 One dimensional Minimization

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.

32.1 Overview

The minimization algorithms begin with a bounded region known to contain a minimum. The region is described by an lower bound a and an upper bound b, with an estimate of the location of the minimum x.



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, $f(x') < f(x)$, 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).

32.2 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.

32.3 Initializing the Minimizer

`gsl_min_fminimizer *` **gsl_min_fminimizer_alloc** (`const gsl_min_fminimizer_type *` *T*) Function

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*) Function

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_FAILURE`.

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*) Function

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*) Function

This function frees all the memory associated with the minimizer *s*.

const char * **gsl_min_fminimizer_name** (const gsl_min_fminimizer * *s*) Function

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`.

32.4 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 (see Section 31.4 [Providing the function to solve], page 318).

32.5 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*) Function

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*) Function

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*) Function
double **gsl_min_fminimizer_x_lower** (const gsl_min_fminimizer * *s*) Function

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*) Function
double **gsl_min_fminimizer_f_upper** (const gsl_min_fminimizer **s*) Function
double **gsl_min_fminimizer_f_lower** (const gsl_min_fminimizer **s*) Function

These functions return the value of the function at the current estimate of the minimum and at the upper and lower bounds of interval for the minimizer *s*.

32.6 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*) Function

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,

$$|a - b| < epsabs + epsrel \min(|a|, |b|)$$

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^*,

$$|x_m - x_m^*| < epsabs + epsrel\, x_m^*$$

assuming that the true minimum x_m^* is contained within the interval.

32.7 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.

gsl_min_fminimizer_goldensection Minimizer

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 $(3-\sqrt{5})/2 = 0.3189660\ldots$) 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_brent Minimizer

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.

32.8 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)
{
  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",
          "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 %.7f\n",
                iter, a, b,
                m, m_expected, m - m_expected, b - a);
      }
    while (status == GSL_CONTINUE && iter < max_iter);

    return status;
  }
```

Here are the results of the minimization procedure.

```
bash$ ./a.out
    0 [0.0000000, 6.0000000] 2.0000000 -1.1415927 6.0000000
    1 [2.0000000, 6.0000000] 3.2758640 +0.1342713 4.0000000
    2 [2.0000000, 3.2831929] 3.2758640 +0.1342713 1.2831929
    3 [2.8689068, 3.2831929] 3.2758640 +0.1342713 0.4142862
    4 [2.8689068, 3.2831929] 3.2758640 +0.1342713 0.4142862
    5 [2.8689068, 3.2758640] 3.1460585 +0.0044658 0.4069572
    6 [3.1346075, 3.2758640] 3.1460585 +0.0044658 0.1412565
    7 [3.1346075, 3.1874620] 3.1460585 +0.0044658 0.0528545
    8 [3.1346075, 3.1460585] 3.1460585 +0.0044658 0.0114510
    9 [3.1346075, 3.1460585] 3.1424060 +0.0008133 0.0114510
   10 [3.1346075, 3.1424060] 3.1415885 -0.0000041 0.0077985
Converged:
   11 [3.1415885, 3.1424060] 3.1415927 -0.0000000 0.0008175
```

32.9 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.

33 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.

33.1 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.

33.2 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.

gsl_multiroot_fsolver * **gsl_multiroot_fsolver_alloc** (const gsl_multiroot_fsolver_type * *T*, size_t *n*) — Function

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*) — Function

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*, gsl_vector * *x*) — Function

This function sets, or resets, an existing solver *s* to use the function *f* and the initial guess *x*.

int **gsl_multiroot_fdfsolver_set** (gsl_multiroot_fdfsolver * *s*, gsl_function_fdf * *fdf*, gsl_vector * *x*) — Function

This function sets, or resets, an existing solver *s* to use the function and derivative *fdf* and the initial guess *x*.

void **gsl_multiroot_fsolver_free** (gsl_multiroot_fsolver * *s*) — Function
void **gsl_multiroot_fdfsolver_free** (gsl_multiroot_fdfsolver * *s*) — Function

These functions free all the memory associated with the solver *s*.

`const char *` **gsl_multiroot_fsolver_name** (`const gsl_multiroot_fsolver *` *s*) Function

`const char *` **gsl_multiroot_fdfsolver_name** (`const gsl_multiroot_fdfsolver *` *s*) Function

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`.

33.3 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:

gsl_multiroot_function Data Type

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;
   double A = (params->A);
   double x0 = gsl_vector_get(x,0);
   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.function = &powell;
F.n = 2;
F.params = &params;
```

gsl_multiroot_function_fdf Data Type

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;
   double A = (params->A);
   double x0 = gsl_vector_get(x,0);
   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;
   double A = (params->A);
   double x0 = gsl_vector_get(x,0);
   double x1 = gsl_vector_get(x,1);

   double u0 = exp(-x0);
   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)
   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.

33.4 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*) — Function

`int` **gsl_multiroot_fdfsolver_iterate** (`gsl_multiroot_fdfsolver *` *s*) — Function

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 at all times. This information can be accessed with the following auxiliary functions,

gsl_vector * **gsl_multiroot_fsolver_root** (const gsl_multiroot_fsolver * *s*) Function
gsl_vector * **gsl_multiroot_fdfsolver_root** (const gsl_multiroot_fdfsolver * *s*) Function

These functions return the current estimate of the root for the solver *s*.

gsl_vector * **gsl_multiroot_fsolver_f** (const gsl_multiroot_fsolver * *s*) Function
gsl_vector * **gsl_multiroot_fdfsolver_f** (const gsl_multiroot_fdfsolver * *s*) Function

These functions return the function value $f(x)$ at the current estimate of the root for the solver *s*.

gsl_vector * **gsl_multiroot_fsolver_dx** (const gsl_multiroot_fsolver * *s*) Function
gsl_vector * **gsl_multiroot_fdfsolver_dx** (const gsl_multiroot_fdfsolver * *s*) Function

These functions return the last step *dx* taken by the solver *s*.

33.5 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*) Function

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*) Function

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.

33.6 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.

gsl_multiroot_fdfsolver_hybridsj Derivative Solver

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_hybridj Derivative Solver

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_newton Derivative Solver

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.

gsl_multiroot_fdfsolver_gnewton Derivative Solver

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.

33.7 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 from by finite difference.

gsl_multiroot_fsolver_hybrids Solver

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`.

gsl_multiroot_fsolver_hybrid Solver

This is a finite difference version of the Hybrid algorithm without internal scaling.

gsl_multiroot_fsolver_dnewton Solver

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_broyden Solver

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 not recommended and is included only for demonstration purposes.

33.8 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;

  double x0 = gsl_vector_get (x, 0);
  double x1 = gsl_vector_get (x, 1);

  double y0 = a * (1 - x0);
  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 `hybrids` method.

```
int
main (void)
{
  const gsl_multiroot_fsolver_type *T;
  gsl_multiroot_fsolver *s;

  int status;
  size_t i, iter = 0;

  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),
          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)
{
  double a = ((struct rparams *) params)->a;
  double b = ((struct rparams *) params)->b;

  double x0 = gsl_vector_get (x, 0);

  double df00 = -a;
  double df01 = 0;
  double df10 = -2 * b  * x0;
  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;
}

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;

      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 `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 `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 `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.

33.9 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

34 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.

34.1 Overview

The problem of multidimensional minimization requires finding a point x such that the scalar function,

$$f(x_1, \ldots, x_n)$$

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. All algorithms proceed from an initial guess using a search algorithm which attempts to move in a downhill direction.

All algorithms making use of the gradient of the fuction 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.

The Nelder-Mead Simplex algorithm applies a different strategy. It maintains $n+1$ trial parameter vectors as the vertices of a n-dimensional simplex. In each iteration step it tries to improve the worst vertex by a simple geometrical transformation until the size of the simplex falls below a given tolerance.

Several minimization 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 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-mimisation 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.

34.2 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.

34.3 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.

`gsl_multimin_fdfminimizer *` **gsl_multimin_fdfminimizer_alloc** (`const gsl_multimin_fdfminimizer_type *`*T*, `size_t` *n*) — Function

`gsl_multimin_fminimizer *` **gsl_multimin_fminimizer_alloc** (`const gsl_multimin_fminimizer_type *`*T*, `size_t` *n*) — Function

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*) — Function

This function 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 $p \cdot g < tol|p||g|$.

`int` **gsl_multimin_fminimizer_set** (`gsl_multimin_fminimizer *` *s*, `gsl_multimin_function *`*f*, `const gsl_vector *` *x*, `const gsl_vector *` *step_size*) — Function

This function 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*) — Function

`void` **gsl_multimin_fminimizer_free** (`gsl_multimin_fminimizer *`*s*) — Function

This function frees all the memory associated with the minimizer *s*.

`const char * gsl_multimin_fdfminimizer_name (const gsl_multimin_fdfminimizer * s)` Function

`const char * gsl_multimin_fminimizer_name (const gsl_multimin_fminimizer * s)` Function

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`.

34.4 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 type:

gsl_multimin_function_fdf Data Type

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*.

`int (* 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.

`int (* 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.

gsl_multimin_function Data Type

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*.

`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 paraboloid with two parameters,

```
/* Paraboloid centered on (dp[0],dp[1]) */

double
my_f (const gsl_vector *v, void *params)
{
  double x, y;
  double *dp = (double *)params;

  x = gsl_vector_get(v, 0);
  y = gsl_vector_get(v, 1);

  return 10.0 * (x - dp[0]) * (x - dp[0]) +
           20.0 * (y - dp[1]) * (y - dp[1]) + 30.0;
}

/* 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 *dp = (double *)params;

  x = gsl_vector_get(v, 0);
  y = gsl_vector_get(v, 1);

  gsl_vector_set(df, 0, 20.0 * (x - dp[0]));
  gsl_vector_set(df, 1, 40.0 * (y - dp[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;

double p[2] = { 1.0, 2.0 }; /* center at (1,2) */
```

```
my_func.f = &my_f;
my_func.df = &my_df;
my_func.fdf = &my_fdf;
my_func.n = 2;
my_func.params = (void *)p;
```

34.5 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*) — Function

`int` **gsl_multimin_fminimizer_iterate** (`gsl_multimin_fminimizer *`*s*) — Function

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 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*) — Function

`gsl_vector *` **gsl_multimin_fminimizer_x** (`const gsl_multimin_fminimizer *` *s*) — Function

`double` **gsl_multimin_fdfminimizer_minimum** (`const gsl_multimin_fdfminimizer *` *s*) — Function

`double` **gsl_multimin_fminimizer_minimum** (`const gsl_multimin_fminimizer *` *s*) — Function

`gsl_vector *` **gsl_multimin_fdfminimizer_gradient** (`const gsl_multimin_fdfminimizer *` *s*) — Function

`double` **gsl_multimin_fminimizer_size** (`const gsl_multimin_fminimizer *` *s*) — Function

These functions return the current best estimate of the location of the minimum, the value of the function at that point, its gradient, and minimizer specific characteristic size for the minimizer *s*.

`int` **gsl_multimin_fdfminimizer_restart** (`gsl_multimin_fdfminimizer *`*s*) — Function

This function resets the minimizer *s* to use the current point as a new starting point.

34.6 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*) Function

This function tests the norm of the gradient *g* against the absolute tolerance *epsabs*. The gradient of a multidimensional 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*) Function

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.

34.7 Algorithms

There are several minimization methods available. The best choice of algorithm depends on the problem. All of the algorithms uses the value of the function and most of its gradient at each evaluation point, too.

gsl_multimin_fdfminimizer_conjugate_fr Minimizer

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*. At the minimum along this line 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 $p' = g' - \beta g$ where $\beta = -|g'|^2/|g|^2$, and the line minimization is then repeated for the new search direction.

gsl_multimin_fdfminimizer_conjugate_pr Minimizer

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_vector_bfgs Minimizer

This is the vector Broyden-Fletcher-Goldfarb-Shanno (BFGS) conjugate gradient algorithm. It 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.

gsl_multimin_fdfminimizer_steepest_descent Minimizer

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 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.

gsl_multimin_fminimizer_nmsimplex Minimizer

This is the Simplex algorithm by Nelder and Mead. It constructs n vectors p_i from the starting vector x as follows:

$$
\begin{aligned}
p_0 &= x_0, x_1, \cdots, x_n \\
p_1 &= x_0 + step\_size_0, x_1, \cdots, x_n \\
p_2 &= x_0, x_1 + step\_size_1, \cdots, x_n \\
p_n &= x_0, x_1, \cdots, x_n + step\_size_n
\end{aligned}
$$

that form the $n + 1$ vertices of a simplex in n dimensions. In each iteration step the algorithm tries to improve the parameter vector p_i corresponding to the highest, i. e. worst, function value by simple geometrical transformations. These are reflection, reflection followed by expansion, contraction and multiple contraction. Using these transformations the simplex moves through the parameter 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 (getting rid of the worst estimate), every iteration doesn't necessarily improve the current best parameter vector. Usually several iterations are required.

The routine calculates the minimizer specific characteristic size 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`.

34.8 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.

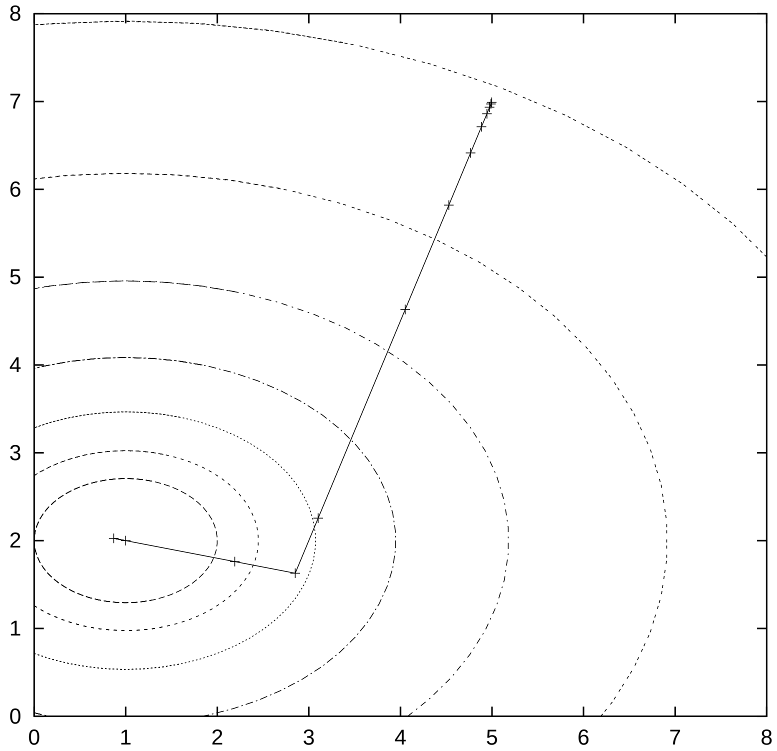
```
int
main (void)
{
  size_t iter = 0;
  int status;

  const gsl_multimin_fdfminimizer_type *T;
  gsl_multimin_fdfminimizer *s;

  /* Position of the minimum (1,2). */
  double par[2] = { 1.0, 2.0 };

  gsl_vector *x;
  gsl_multimin_function_fdf my_func;

  my_func.f = &my_f;
  my_func.df = &my_df;
  my_func.fdf = &my_fdf;
  my_func.n = 2;
  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),
              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.



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)
{
  size_t np = 2;
  double par[2] = {1.0, 2.0};

  const gsl_multimin_fminimizer_type *T =
    gsl_multimin_fminimizer_nmsimplex;
  gsl_multimin_fminimizer *s = NULL;
  gsl_vector *ss, *x;
  gsl_multimin_function minex_func;

  size_t iter = 0, i;
  int rval = GSL_CONTINUE;
  int status = GSL_SUCCESS;
  double ssval;

  /* Initial vertex size vector */

  ss = gsl_vector_alloc (np);

  if (ss == NULL)
```

```
  {
    GSL_ERROR_VAL ("failed to allocate space for ss", GSL_ENOMEM, 0);
  }

gsl_vector_set_all (ss, 1.0);

/* Starting point */

x = gsl_vector_alloc (np);

if (x == NULL)
  {
    gsl_vector_free(ss);
    GSL_ERROR_VAL ("failed to allocate space for x", GSL_ENOMEM, 0);
  }

gsl_vector_set (x, 0, 5.0);
gsl_vector_set (x, 1, 7.0);

/* Initialize method and iterate */

minex_func.f = &my_f;
minex_func.n = np;
minex_func.params = (void *)&par;

s = gsl_multimin_fminimizer_alloc (T, np);
gsl_multimin_fminimizer_set (s, &minex_func, x, ss);

while (rval == GSL_CONTINUE)
  {
    iter++;
    status = gsl_multimin_fminimizer_iterate(s);

    if (status)
      break;

    rval = gsl_multimin_test_size (gsl_multimin_fminimizer_size (s),
                                   1e-2);
    ssval = gsl_multimin_fminimizer_size (s);

    if (rval == GSL_SUCCESS)
      printf ("converged to minimum at\n");

    printf("%5d ", iter);
    for (i = 0; i < np; i++)
      {
        printf ("%10.3e ", gsl_vector_get (s->x, i));
      }
    printf("f() = %-10.3f ssize = %.3f\n", s->fval, ssval);
```

```
     }

   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    ssize = 1.082
    2  5.250e+00  4.000e+00 f() = 290.625    ssize = 1.372
    3  5.250e+00  4.000e+00 f() = 290.625    ssize = 1.372
    4  5.500e+00  1.000e+00 f() = 252.500    ssize = 1.372
    5  2.625e+00  3.500e+00 f() = 101.406    ssize = 1.823
    6  3.469e+00  1.375e+00 f() = 98.760     ssize = 1.526
    7  1.820e+00  3.156e+00 f() = 63.467     ssize = 1.105
    8  1.820e+00  3.156e+00 f() = 63.467     ssize = 1.105
    9  1.016e+00  2.812e+00 f() = 43.206     ssize = 1.105
   10  2.041e+00  2.008e+00 f() = 40.838     ssize = 0.645
   11  1.236e+00  1.664e+00 f() = 32.816     ssize = 0.645
   12  1.236e+00  1.664e+00 f() = 32.816     ssize = 0.447
   13  5.225e-01  1.980e+00 f() = 32.288     ssize = 0.447
   14  1.103e+00  2.073e+00 f() = 30.214     ssize = 0.345
   15  1.103e+00  2.073e+00 f() = 30.214     ssize = 0.264
   16  1.103e+00  2.073e+00 f() = 30.214     ssize = 0.160
   17  9.864e-01  1.934e+00 f() = 30.090     ssize = 0.132
   18  9.190e-01  1.987e+00 f() = 30.069     ssize = 0.092
   19  1.028e+00  2.017e+00 f() = 30.013     ssize = 0.056
   20  1.028e+00  2.017e+00 f() = 30.013     ssize = 0.046
   21  1.028e+00  2.017e+00 f() = 30.013     ssize = 0.033
   22  9.874e-01  1.985e+00 f() = 30.006     ssize = 0.028
   23  9.846e-01  1.995e+00 f() = 30.003     ssize = 0.023
   24  1.007e+00  2.003e+00 f() = 30.001     ssize = 0.012
converged to minimum at
   25  1.007e+00  2.003e+00 f() = 30.001     ssize = 0.010
```

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.

34.9 References and Further Reading

A brief description of multidimensional minimization algorithms and further references can be found in the following book,

C.W. Ueberhuber, *Numerical Computation (Volume 2)*, Chapter 14, Section 4.4 "Minimization Methods", p. 325—335, Springer (1997), ISBN 3-540-62057-5.

J.A. Nelder and R. Mead, *A simplex method for function minimization*, Computer Journal vol. 7 (1965), 308—315.

35 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. 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. The functions are declared in the header file 'gsl_fit.h'

35.1 Linear regression

The functions described in this section can be used to perform least-squares fits to a straight line model, $Y = c_0 + c_1 X$. For weighted data the best-fit is found by minimizing the weighted sum of squared residuals, χ^2,

$$\chi^2 = \sum_i w_i (y_i - (c_0 + c_1 x_i))^2$$

for the parameters c_0, c_1. For unweighted data the sum is computed with $w_i = 1$.

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*) Function

This function computes the best-fit linear regression coefficients (*c0*,*c1*) of the model $Y = c_0 + c_1 X$ for the datasets (*x*, *y*), two vectors of length *n* with strides *xstride* and *ystride*. 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*.

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*) Function

This function computes the best-fit linear regression coefficients (*c0*,*c1*) of the model $Y = c_0 + c_1 X$ 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 covariance matrix for the parameters (*c0*, *c1*) is estimated from weighted data 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 *c00*, double *c01*, double *c11*, double **y*, double **y_err*) Function

This function uses the best-fit linear regression coefficients *c0*,*c1* and their estimated 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*.

35.2 Linear fitting 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, $Y = c_1 X$. For weighted data the best-fit is found by minimizing the weighted sum of squared residuals, χ^2,

$$\chi^2 = \sum_i w_i (y_i - c_1 x_i)^2$$

for the parameter c_1. For unweighted data the sum is computed with $w_i = 1$.

`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*) Function

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 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*) Function

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 estimated from the weighted data and returned via the parameters *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` *c11*, `double *`*y*, `double *`*y_err*) Function

This function uses the best-fit linear regression coefficient *c1* and its estimated 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*.

35.3 Multi-parameter fitting

The functions described in this section perform least-squares fits to a general linear model, $y = Xc$ where y is a vector of n observations, X is an n by p matrix of predictor variables, and c are the p unknown best-fit parameters, which are to be estimated.

The best-fit is found by minimizing the weighted sums of squared residuals, χ^2,

$$\chi^2 = (y - Xc)^T W (y - Xc)$$

with respect to the parameters c. The weights are specified by the diagonal elements of the n by n matrix W. For unweighted data W is replaced by the identity matrix.

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 functions described in this section are declared in the header file '`gsl_multifit.h`'.

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.

`gsl_multifit_linear_workspace *` **gsl_multifit_linear_alloc** (`size_t` *n*, `size_t` *p*) Function

This function allocates a workspace for fitting a model to *n* observations using *p* parameters.

`void` **gsl_multifit_linear_free** (`gsl_multifit_linear_workspace *` *work*) Function

This function frees the memory associated with the workspace *w*.

`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*) Function

This function computes the best-fit parameters *c* of the model $y = Xc$ for the observations *y* and the matrix of predictor variables *X*. The variance-covariance matrix of the model parameters *cov* is estimated from the scatter of the observations about the best-fit. The sum of squares of the residuals from the best-fit, χ^2, is returned in *chisq*.

The best-fit is found by singular value decomposition of the matrix X using the preallocated workspace provided in *work*. The modified Golub-Reinsch SVD algorithm is used, 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_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*) Function

This function computes the best-fit parameters *c* of the model $y = Xc$ for the observations *y* and the matrix of predictor variables *X*. The covariance matrix of the model parameters *cov* is estimated from the weighted data. The weighted sum of squares of the residuals from the best-fit, χ^2, is returned in *chisq*.

The best-fit is found by singular value decomposition of the matrix X using the preallocated workspace provided in *work*. Any components which have zero singular value (to machine precision) are discarded from the fit.

35.4 Examples

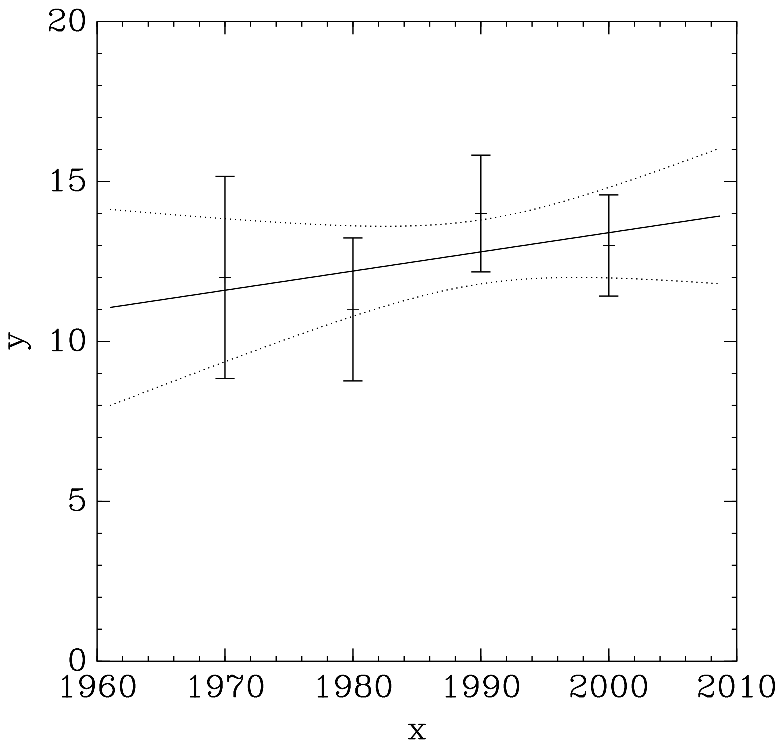
The following program computes a least squares straight-line fit to a simple (fictitious) dataset, and outputs the best-fit line and its associated one standard-deviation error bars.

```
#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 next 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*.

```
#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);
  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);
    }
    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);
    }
  return 0;
}
```

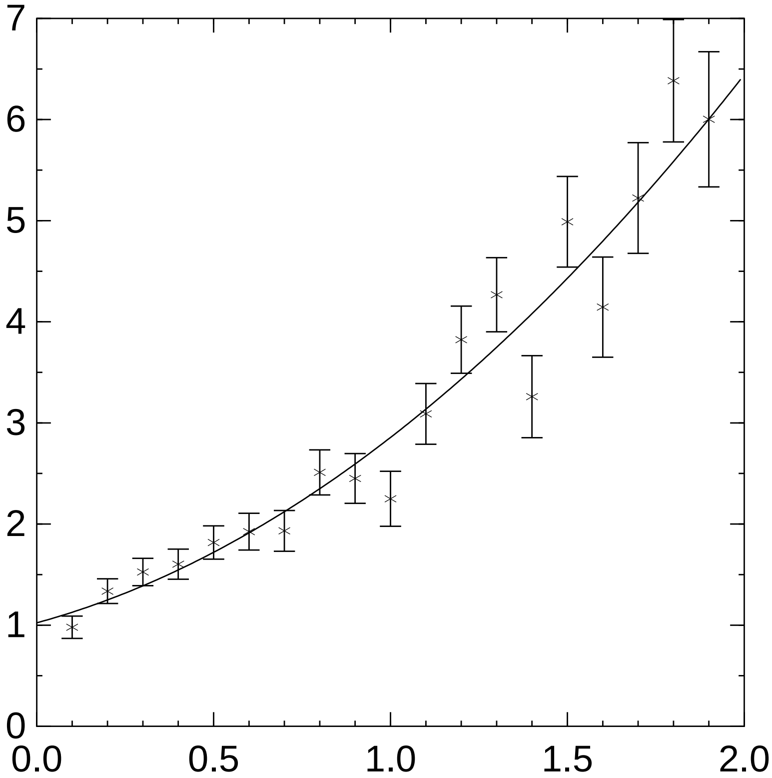
The data can be prepared by running the resulting executable program,

```
$ ./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.



35.5 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`.

36 Nonlinear Least-Squares Fitting

This chapter describes functions for multidimensional nonlinear least-squares fitting. 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_multifit_nlin.h`' contains prototypes for the multidimensional nonlinear fitting functions and related declarations.

36.1 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,

$$\Phi(x) = \frac{1}{2}\sum_{i=1}^{n} f_i(x_1,\ldots,x_p)^2 = \frac{1}{2}||F(x)||^2$$

All algorithms proceed from an initial guess using the linearization,

$$\psi(p) = ||F(x+p)|| \approx ||F(x) + Jp\,||$$

where x is the initial point, p is the proposed step and J is the Jacobian matrix $J_{ij} = \partial f_i/\partial x_j$. Additional strategies are used to enlarge the region of convergence. These include requiring a decrease in the norm $||F||$ on each step or using a trust region to avoid steps which fall outside the linear regime.

36.2 Initializing the Solver

gsl_multifit_fsolver * **gsl_multifit_fsolver_alloc** (const gsl_multifit_fsolver_type * T, size_t n, size_t p) — Function

This function returns a pointer to a newly allocated instance of a solver of type T for n observations and p parameters.

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_fdfsolver * **gsl_multifit_fdfsolver_alloc** (const gsl_multifit_fdfsolver_type * T, size_t n, size_t p) — Function

This function returns a pointer to a newly allocated instance of a derivative solver of type T for n observations and p parameters. For example, the following code creates an instance of a Levenberg-Marquardt solver for 100 data points and 3 parameters,

```
const gsl_multifit_fdfsolver_type * T
    = gsl_multifit_fdfsolver_lmder;
gsl_multifit_fdfsolver * s
    = gsl_multifit_fdfsolver_alloc (T, 100, 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`.

`int` **gsl_multifit_fsolver_set** (`gsl_multifit_fsolver *` *s*, `gsl_multifit_function *` *f*, `gsl_vector *` *x*) — Function

This function initializes, or reinitializes, an existing solver *s* to use the function *f* and the initial guess *x*.

`int` **gsl_multifit_fdfsolver_set** (`gsl_multifit_fdfsolver *` *s*, `gsl_function_fdf *` *fdf*, `gsl_vector *` *x*) — Function

This function initializes, or reinitializes, an existing solver *s* to use the function and derivative *fdf* and the initial guess *x*.

`void` **gsl_multifit_fsolver_free** (`gsl_multifit_fsolver *` *s*) — Function

`void` **gsl_multifit_fdfsolver_free** (`gsl_multifit_fdfsolver *` *s*) — Function

These functions free all the memory associated with the solver *s*.

`const char *` **gsl_multifit_fsolver_name** (`const gsl_multifit_fdfsolver *` *s*) — Function

`const char *` **gsl_multifit_fdfsolver_name** (`const gsl_multifit_fdfsolver *` *s*) — Function

These functions return a pointer to the name of the solver. For example,

```
printf("s is a '%s' solver\n",
       gsl_multifit_fdfsolver_name (s));
```

would print something like `s is a 'lmder' solver`.

36.3 Providing the Function to be Minimized

You must provide *n* functions of *p* variables for the minimization algorithms to operate on. In order to allow for general parameters the functions are defined by the following data types:

gsl_multifit_function — Data Type

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 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 vectors *x*

`void *` *params*
: a pointer to the parameters of the function

gsl_multifit_function_fdf — Data Type

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-p 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 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 vectors x

`void * params`
: a pointer to the parameters of the function

36.4 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_multifit_fsolver_iterate** (gsl_multifit_fsolver * *s*) — Function
int **gsl_multifit_fdfsolver_iterate** (gsl_multifit_fdfsolver * *s*) — Function

These functions perform a single iteration of the solver *s*. If the iteration encounters an unexpected problem then an error code will be returned. The solver maintains a current estimate of the best-fit parameters at all times. This information can be accessed with the following auxiliary functions,

gsl_vector * **gsl_multifit_fsolver_position** (const gsl_multifit_fsolver * *s*) — Function
gsl_vector * **gsl_multifit_fdfsolver_position** (const gsl_multifit_fdfsolver * *s*) — Function

These functions return the current position (i.e. best-fit parameters) of the solver *s*.

36.5 Search 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 functions below allow the user to test the current estimate of the best-fit parameters in several standard ways.

`int` **gsl_multifit_test_delta** (`const gsl_vector *` *dx*, `const gsl_vector *` *x*, `double` *epsabs*, `double` *epsrel*) Function

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_multifit_test_gradient** (`const gsl_vector *` *g*, `double` *epsabs*) Function

This function tests the residual gradient *g* against the absolute error bound *epsabs*. Mathematically, the gradient should be exactly zero at the minimum. The test returns `GSL_SUCCESS` if the following condition is achieved,

$$\sum_i |g_i| < epsabs$$

and returns `GSL_CONTINUE` otherwise. This criterion is suitable for situations where the precise location of the minimum, x, is unimportant provided a value can be found where the gradient is small enough.

`int` **gsl_multifit_gradient** (`const gsl_matrix *` *J*, `const gsl_vector *` *f*, `gsl_vector *` *g*) Function

This function computes the gradient g of $\Phi(x) = (1/2)||F(x)||^2$ from the Jacobian matrix J and the function values *f*, using the formula $g = J^T f$.

36.6 Minimization Algorithms using Derivatives

The minimization algorithms described in this section make use of both the function and its derivative. They require an initial guess for the location of the minimum. 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 minimum for it to work.

gsl_multifit_fdfsolver_lmsder Derivative Solver

This is a robust and efficient version of the Levenberg-Marquardt algorithm as implemented in the scaled LMDER routine in MINPACK. Minpack was written by Jorge J. Moré, Burton S. Garbow and Kenneth E. Hillstrom.

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 attempts to minimize the linear system $|F + Jp|$ subject to the constraint $|Dp| < \Delta$. The solution to this constrained linear system is found using the Levenberg-Marquardt method.

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, and follows the predicted behavior of the function within the trust region. then it is accepted and size of the trust region is increased. If the proposed step fails to improve the solution, or differs significantly from the expected behavior within the trust region, then the size of the trust region is decreased and another trial step is computed.

The algorithm also monitors the progress of the solution and returns an error if the changes in the solution are smaller than the machine precision. The possible error codes are,

`GSL_ETOLF`
: the decrease in the function falls below machine precision

`GSL_ETOLX`
: the change in the position vector falls below machine precision

`GSL_ETOLG`
: the norm of the gradient, relative to the norm of the function, falls below machine precision

These error codes indicate that further iterations will be unlikely to change the solution from its current value.

gsl_multifit_fdfsolver_lmder — Derivative Solver

This is an unscaled version of the LMDER algorithm. The elements of the diagonal scaling matrix D are set to 1. This algorithm may be useful in circumstances where the scaled version of LMDER converges too slowly, or the function is already scaled appropriately.

36.7 Minimization Algorithms without Derivatives

There are no algorithms implemented in this section at the moment.

36.8 Computing the covariance matrix of best fit parameters

`int` **gsl_multifit_covar** (`const gsl_matrix *` *J*, `double` *epsrel*, `gsl_matrix *` *covar*) — Function

This function uses the Jacobian matrix J to compute the covariance matrix of the best-fit parameters, *covar*. The parameter *epsrel* is used to remove linear-dependent columns when J is rank deficient.

The covariance matrix is given by,

$$C = (J^T J)^{-1}$$

and is computed by QR decomposition of J with column-pivoting. 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).

36.9 Examples

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,

$$f_i = ((A\exp(-\lambda t_i) + b) - y_i)/\sigma_i$$

where we have chosen $t_i = i$. 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 $x_2 = b$.

```
#include <stdlib.h>
#include <stdio.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_multifit_nlin.h>

struct data {
  size_t n;
  double * y;
  double * sigma;
};

int
expb_f (const gsl_vector * x, void *params,
        gsl_vector * f)
{
  size_t n = ((struct data *)params)->n;
  double *y = ((struct data *)params)->y;
  double *sigma = ((struct data *) params)->sigma;

  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 * i) + b */
      double t = i;
      double Yi = A * exp (-lambda * t) + b;
      gsl_vector_set (f, i, (Yi - y[i])/sigma[i]);
    }

  return GSL_SUCCESS;
}

int
expb_df (const gsl_vector * x, void *params,
         gsl_matrix * J)
{
  size_t n = ((struct data *)params)->n;
  double *sigma = ((struct data *) params)->sigma;

  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 * i) + b  */
      /* and the xj are the parameters (A,lambda,b) */
      double t = i;
      double s = sigma[i];
      double e = exp(-lambda * t);
      gsl_matrix_set (J, i, 0, e/s);
      gsl_matrix_set (J, i, 1, -t * A * e/s);
      gsl_matrix_set (J, i, 2, 1/s);


    }
  return GSL_SUCCESS;
}

int
expb_fdf (const gsl_vector * x, void *params,
          gsl_vector * f, gsl_matrix * J)
{
  expb_f (x, params, f);
```

```
  expb_df (x, params, J);

  return GSL_SUCCESS;
}
```

The main part of the program sets up a Levenberg-Marquardt solver and some simulated random data. The data uses the known parameters (1.0,5.0,0.1) combined with gaussian noise (standard deviation = 0.1) over a range of 40 timesteps. The initial guess for the parameters is chosen as (0.0, 1.0, 0.0).

```
#define N 40

int
main (void)
{
  const gsl_multifit_fdfsolver_type *T;
  gsl_multifit_fdfsolver *s;

  int status;
  size_t i, iter = 0;

  const size_t n = N;
  const size_t p = 3;

  gsl_matrix *covar = gsl_matrix_alloc (p, p);

  double y[N], sigma[N];

  struct data d = { n, y, sigma};

  gsl_multifit_function_fdf f;

  double x_init[3] = { 1.0, 0.0, 0.0 };

  gsl_vector_view x = gsl_vector_view_array (x_init, p);

  const gsl_rng_type * type;
  gsl_rng * r;

  gsl_rng_env_setup();

  type = gsl_rng_default;
  r = gsl_rng_alloc (type);

  f.f = &expb_f;
  f.df = &expb_df;
  f.fdf = &expb_fdf;
  f.n = n;
  f.p = p;
  f.params = &d;
```

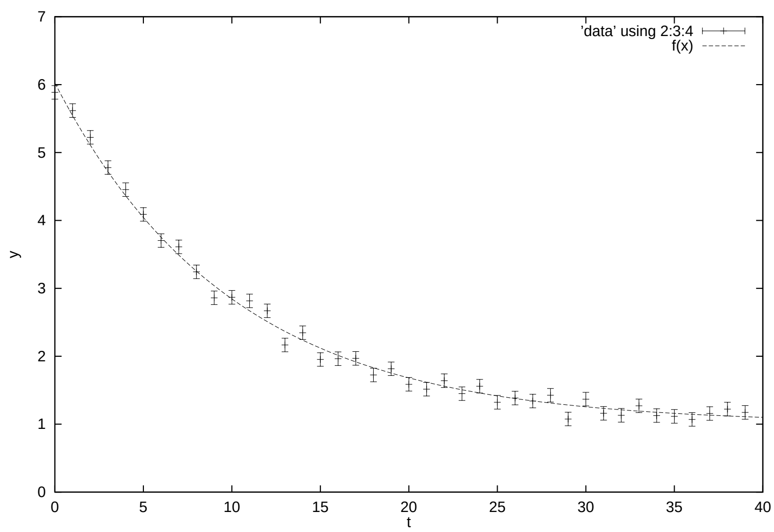
```
  /* This is the data to be fitted */

  for (i = 0; i < n; i++)
    {
      double t = i;
      y[i] = 1.0 + 5 * exp (-0.1 * t)
                 + gsl_ran_gaussian(r, 0.1);
      sigma[i] = 0.1;
      printf("data: %d %g %g\n", i, y[i], sigma[i]);
    };


  T = gsl_multifit_fdfsolver_lmsder;
  s = gsl_multifit_fdfsolver_alloc (T, n, p);
  gsl_multifit_fdfsolver_set (s, &f, &x.vector);

  print_state (iter, s);

  do
    {
      iter++;
      status = gsl_multifit_fdfsolver_iterate (s);

      printf ("status = %s\n", gsl_strerror (status));

      print_state (iter, s);

      if (status)
        break;

      status = gsl_multifit_test_delta (s->dx, s->x,
                                        1e-4, 1e-4);
    }
  while (status == GSL_CONTINUE && iter < 500);

  gsl_multifit_covar (s->J, 0.0, covar);

  gsl_matrix_fprintf (stdout, covar, "%g");

#define FIT(i) gsl_vector_get(s->x, i)
#define ERR(i) sqrt(gsl_matrix_get(covar,i,i))

  printf("A      = %.5f +/- %.5f\n", FIT(0), ERR(0));
  printf("lambda = %.5f +/- %.5f\n", FIT(1), ERR(1));
  printf("b      = %.5f +/- %.5f\n", FIT(2), ERR(2));

  printf ("status = %s\n", gsl_strerror (status));

  gsl_multifit_fdfsolver_free (s);
```

```
  return 0;
}

int
print_state (size_t iter, gsl_multifit_fdfsolver * s)
{
  printf ("iter: %3u x = % 15.8f % 15.8f % 15.8f "
          "|f(x)| = %g\n",
          iter,
          gsl_vector_get (s->x, 0),
          gsl_vector_get (s->x, 1),
          gsl_vector_get (s->x, 2),
          gsl_blas_dnrm2 (s->f));
}
```

The iteration terminates when the change in x is smaller than 0.0001, as both an absolute and relative change. Here are the results of running the program,

```
iter: 0 x = 1.00000000 0.00000000 0.00000000 |f(x)| = 118.574
iter: 1 x = 1.64919392 0.01780040 0.64919392 |f(x)| = 77.2068
iter: 2 x = 2.86269020 0.08032198 1.45913464 |f(x)| = 38.0579
iter: 3 x = 4.97908864 0.11510525 1.06649948 |f(x)| = 10.1548
iter: 4 x = 5.03295496 0.09912462 1.00939075 |f(x)| = 6.4982
iter: 5 x = 5.05811477 0.10055914 0.99819876 |f(x)| = 6.33121
iter: 6 x = 5.05827645 0.10051697 0.99756444 |f(x)| = 6.33119
iter: 7 x = 5.05828006 0.10051819 0.99757710 |f(x)| = 6.33119

A      = 5.05828 +/- 0.05983
lambda = 0.10052 +/- 0.00309
b      = 0.99758 +/- 0.03944
status = success
```

The approximate values of the parameters are found correctly. The errors on the parameters are given by the square roots of the diagonal elements of the covariance matrix.



36.10 References and Further Reading

The MINPACK algorithm is described in the following article,

J.J. Moré, *The Levenberg-Marquardt Algorithm: Implementation and Theory*, Lecture Notes in Mathematics, v630 (1978), ed G. Watson.

The following paper is also relevant to the algorithms described in this section,

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

37 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 MKS system (meters, kilograms, seconds) and the CGS system (centimeters, grams, seconds), which is commonly used in Astronomy.

The definitions of constants in the MKS system are available in the file 'gsl_const_mks.h'. The constants in the CGS system are defined in 'gsl_const_cgs.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.

37.1 Fundamental Constants

GSL_CONST_MKS_SPEED_OF_LIGHT
: The speed of light in vacuum, c.

GSL_CONST_MKS_VACUUM_PERMEABILITY
: The permeability of free space, μ_0

GSL_CONST_MKS_VACUUM_PERMITTIVITY
: The permittivity of free space, ϵ_0.

GSL_CONST_NUM_AVOGADRO
: Avogadro's number, N_a.

GSL_CONST_MKS_FARADAY
: The molar charge of 1 Faraday.

GSL_CONST_MKS_BOLTZMANN
: The Boltzmann constant, k.

GSL_CONST_MKS_MOLAR_GAS
: The molar gas constant, R_0.

GSL_CONST_MKS_STANDARD_GAS_VOLUME
: The standard gas volume, V_0.

GSL_CONST_MKS_GAUSS
: The magnetic field of 1 Gauss.

GSL_CONST_MKS_MICRON
: The length of 1 micron.

GSL_CONST_MKS_HECTARE
: The area of 1 hectare.

GSL_CONST_MKS_MILES_PER_HOUR
: The speed of 1 mile per hour.

GSL_CONST_MKS_KILOMETERS_PER_HOUR
: The speed of 1 kilometer per hour.

37.2 Astronomy and Astrophysics

GSL_CONST_MKS_ASTRONOMICAL_UNIT
The length of 1 astronomical unit (mean earth-sun distance), au.

GSL_CONST_MKS_GRAVITATIONAL_CONSTANT
The gravitational constant, G.

GSL_CONST_MKS_LIGHT_YEAR
The distance of 1 light-year, ly.

GSL_CONST_MKS_PARSEC
The distance of 1 parsec, pc.

GSL_CONST_MKS_GRAV_ACCEL
The standard gravitational acceleration on Earth, g.

GSL_CONST_MKS_SOLAR_MASS
The mass of the Sun.

37.3 Atomic and Nuclear Physics

GSL_CONST_MKS_ELECTRON_CHARGE
The charge of the electron, e.

GSL_CONST_MKS_ELECTRON_VOLT
The energy of 1 electron volt, eV.

GSL_CONST_MKS_UNIFIED_ATOMIC_MASS
The unified atomic mass, amu.

GSL_CONST_MKS_MASS_ELECTRON
The mass of the electron, m_e.

GSL_CONST_MKS_MASS_MUON
The mass of the muon, m_μ.

GSL_CONST_MKS_MASS_PROTON
The mass of the proton, m_p.

GSL_CONST_MKS_MASS_NEUTRON
The mass of the neutron, m_n.

GSL_CONST_NUM_FINE_STRUCTURE
The electromagnetic fine structure constant α.

GSL_CONST_MKS_RYDBERG
The Rydberg constant, Ry, in units of energy. This is related to the Rydberg inverse wavelength R by $Ry = hcR$.

GSL_CONST_MKS_BOHR_RADIUS
The Bohr radius, a_0.

GSL_CONST_MKS_ANGSTROM
The length of 1 angstrom.

GSL_CONST_MKS_BARN
: The area of 1 barn.

GSL_CONST_MKS_BOHR_MAGNETON
: The Bohr Magneton, μ_B.

GSL_CONST_MKS_NUCLEAR_MAGNETON
: The Nuclear Magneton, μ_N.

GSL_CONST_MKS_ELECTRON_MAGNETIC_MOMENT
: The absolute value of the magnetic moment of the electron, μ_e. The physical magnetic moment of the election is negative.

GSL_CONST_MKS_PROTON_MAGNETIC_MOMENT
: The magnetic moment of the proton, μ_p.

37.4 Measurement of Time

GSL_CONST_MKS_MINUTE
: The number of seconds in 1 minute.

GSL_CONST_MKS_HOUR
: The number of seconds in 1 hour.

GSL_CONST_MKS_DAY
: The number of seconds in 1 day.

GSL_CONST_MKS_WEEK
: The number of seconds in 1 week.

37.5 Imperial Units

GSL_CONST_MKS_INCH
: The length of 1 inch.

GSL_CONST_MKS_FOOT
: The length of 1 foot.

GSL_CONST_MKS_YARD
: The length of 1 yard.

GSL_CONST_MKS_MILE
: The length of 1 mile.

GSL_CONST_MKS_MIL
: The length of 1 mil (1/1000th of an inch).

37.6 Nautical Units

GSL_CONST_MKS_NAUTICAL_MILE
: The length of 1 nautical mile.

GSL_CONST_MKS_FATHOM
: The length of 1 fathom.

`GSL_CONST_MKS_KNOT`
The speed of 1 knot.

37.7 Printers Units

`GSL_CONST_MKS_POINT`
The length of 1 printer's point (1/72 inch).

`GSL_CONST_MKS_TEXPOINT`
The length of 1 TeX point (1/72.27 inch).

37.8 Volume

`GSL_CONST_MKS_ACRE`
The area of 1 acre.

`GSL_CONST_MKS_LITER`
The volume of 1 liter.

`GSL_CONST_MKS_US_GALLON`
The volume of 1 US gallon.

`GSL_CONST_MKS_CANADIAN_GALLON`
The volume of 1 Canadian gallon.

`GSL_CONST_MKS_UK_GALLON`
The volume of 1 UK gallon.

`GSL_CONST_MKS_QUART`
The volume of 1 quart.

`GSL_CONST_MKS_PINT`
The volume of 1 pint.

37.9 Mass and Weight

`GSL_CONST_MKS_POUND_MASS`
The mass of 1 pound.

`GSL_CONST_MKS_OUNCE_MASS`
The mass of 1 ounce.

`GSL_CONST_MKS_TON`
The mass of 1 ton.

`GSL_CONST_MKS_METRIC_TON`
The mass of 1 metric ton (1000 kg).

`GSL_CONST_MKS_UK_TON`
The mass of 1 UK ton.

`GSL_CONST_MKS_TROY_OUNCE`
The mass of 1 troy ounce.

`GSL_CONST_MKS_CARAT`
The mass of 1 carat.

`GSL_CONST_MKS_GRAM_FORCE`
The force of 1 gram weight.

`GSL_CONST_MKS_POUND_FORCE`
The force of 1 pound weight.

`GSL_CONST_MKS_KILOPOUND_FORCE`
The force of 1 kilopound weight.

`GSL_CONST_MKS_POUNDAL`
The force of 1 poundal.

37.10 Thermal Energy and Power

`GSL_CONST_MKS_CALORIE`
The energy of 1 calorie.

`GSL_CONST_MKS_BTU`
The energy of 1 British Thermal Unit, *btu*.

`GSL_CONST_MKS_THERM`
The energy of 1 Therm.

`GSL_CONST_MKS_HORSEPOWER`
The power of 1 horsepower.

37.11 Pressure

`GSL_CONST_MKS_BAR`
The pressure of 1 bar.

`GSL_CONST_MKS_STD_ATMOSPHERE`
The pressure of 1 standard atmosphere.

`GSL_CONST_MKS_TORR`
The pressure of 1 torr.

`GSL_CONST_MKS_METER_OF_MERCURY`
The pressure of 1 meter of mercury.

`GSL_CONST_MKS_INCH_OF_MERCURY`
The pressure of 1 inch of mercury.

`GSL_CONST_MKS_INCH_OF_WATER`
The pressure of 1 inch of water.

`GSL_CONST_MKS_PSI`
The pressure of 1 pound per square inch.

37.12 Viscosity

`GSL_CONST_MKS_POISE`
: The dynamic viscosity of 1 poise.

`GSL_CONST_MKS_STOKES`
: The kinematic viscosity of 1 stokes.

37.13 Light and Illumination

`GSL_CONST_MKS_STILB`
: The luminance of 1 stilb.

`GSL_CONST_MKS_LUMEN`
: The luminous flux of 1 lumen.

`GSL_CONST_MKS_LUX`
: The illuminance of 1 lux.

`GSL_CONST_MKS_PHOT`
: The illuminance of 1 phot.

`GSL_CONST_MKS_FOOTCANDLE`
: The illuminance of 1 footcandle.

`GSL_CONST_MKS_LAMBERT`
: The luminance of 1 lambert.

`GSL_CONST_MKS_FOOTLAMBERT`
: The luminance of 1 footlambert.

37.14 Radioactivity

`GSL_CONST_MKS_CURIE`
: The activity of 1 curie.

`GSL_CONST_MKS_ROENTGEN`
: The exposure of 1 roentgen.

`GSL_CONST_MKS_RAD`
: The absorbed dose of 1 rad.

37.15 Force and Energy

`GSL_CONST_MKS_NEWTON`
: The SI unit of force, 1 Newton.

`GSL_CONST_MKS_DYNE`
: The force of 1 Dyne = 10^{-5} Newton.

`GSL_CONST_MKS_JOULE`
: The SI unit of energy, 1 Joule.

`GSL_CONST_MKS_ERG`
: The energy 1 erg = 10^{-7} Joule.

37.16 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}

37.17 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 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 MKS 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_mks.h>

int
main (void)
{
  double c  = GSL_CONST_MKS_SPEED_OF_LIGHT;
  double au = GSL_CONST_MKS_ASTRONOMICAL_UNIT;
  double minutes = GSL_CONST_MKS_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);

  return 0;
}
```

Here is the output from the program,

```
light travel time from Earth to Mars:
minimum = 4.3 minutes
maximum = 21.0 minutes
```

37.18 References and Further Reading

Further information on the values of physical constants is available from the NIST website,

`http://www.physics.nist.gov/cuu/Constants/index.html`

38 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'.

38.1 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,

$$(-1)^s (1 \cdot fffff \ldots) 2^E$$

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,

$$(-1)^s (0 \cdot fffff \ldots) 2^{E_{min}}$$

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*) Function
void **gsl_ieee_fprintf_double** (FILE * *stream*, const double * *x*) Function

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*) Function
`void` **gsl_ieee_printf_double** (`const double *` *x*) Function
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 */

  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.

38.2 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 way of accessing them. For example, the Linux kernel provides the function `__setfpucw` (*set-fpu-control-word*) to set IEEE modes, while HP-UX and Solaris use the functions `fpsetround` and `fpsetmask`. 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`.

`void` **gsl_ieee_env_setup** () Function

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
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`.

The following 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.

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,

$$e = 1 + \frac{1}{2!} + \frac{1}{3!} + \frac{1}{4!} + \ldots = 2.71828182846...$$

```
#include <math.h>
#include <stdio.h>
#include <gsl/gsl_ieee_utils.h>

int
main (void)
{
  double x = 1, oldsum = 0, sum = 0;
  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 series no longer converges (the reason is that when we add each term to the sum the final result is always rounded up. This is guaranteed to increase the sum by at least one tick on each iteration). 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.

38.3 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 paper "What Every Computer Scientist Should Know About Floating-Point Arithmetic".

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.

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

Appendix A Debugging Numerical Programs

This chapter describes some tips and tricks for debugging numerical programs which use GSL.

A.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 variable 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`,

```
bash$ 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",
    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`.

A.2 Examining floating point registers

The contents of floating point registers can be examined using the command `info float` (not available on all 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
    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
```

A.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 see Chapter 38 [IEEE floating-point arithmetic], page 391.

```
(gdb) set env GSL_IEEE_MODE=double-precision
```

A.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
  -Wtraditional -Wconversion -Wshadow
  -Wpointer-arith -Wcast-qual -Wcast-align
  -Wwrite-strings -Wnested-externs
  -fshort-enums -fno-common -Dinline= -g -O4
```

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.

`-O4`
: Turn on optimization. The warnings for uninitialized variables in `-Wall` rely on the optimizer to analyze the code. If there is no optimization then the 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.

`-Wtraditional`
: This warns about certain constructs that behave differently in traditional and ANSI C. Whether the traditional or ANSI interpretation is used might be unpredictable on other compilers.

`-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 an 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.

A.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

Appendix B 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 and eigensystems.

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.

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
Write the routines for generating combinations

Appendix C Autoconf Macros

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
```

Appendix D 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 Section 12.3 [BLAS References and Further Reading], page 126).

D.1 Level 1

float **cblas_sdsdot** (const int *N*, const float *alpha*, const float **x*, const int *incx*, const float **y*, const int *incy*) — Function

double **cblas_dsdot** (const int *N*, const float **x*, const int *incx*, const float **y*, const int *incy*) — Function

float **cblas_sdot** (const int *N*, const float **x*, const int *incx*, const float **y*, const int *incy*) — Function

double **cblas_ddot** (const int *N*, const double **x*, const int *incx*, const double **y*, const int *incy*) — Function

void **cblas_cdotu_sub** (const int *N*, const void **x*, const int *incx*, const void **y*, const int *incy*, void **dotu*) — Function

void **cblas_cdotc_sub** (const int *N*, const void **x*, const int *incx*, const void **y*, const int *incy*, void **dotc*) — Function

void **cblas_zdotu_sub** (const int *N*, const void **x*, const int *incx*, const void **y*, const int *incy*, void **dotu*) — Function

void **cblas_zdotc_sub** (const int *N*, const void **x*, const int *incx*, const void **y*, const int *incy*, void **dotc*) — Function

float **cblas_snrm2** (const int *N*, const float **x*, const int *incx*) — Function

float **cblas_sasum** (const int *N*, const float **x*, const int *incx*) — Function

double **cblas_dnrm2** (const int *N*, const double **x*, const int *incx*) — Function

double **cblas_dasum** (const int *N*, const double **x*, const int *incx*) — Function

float **cblas_scnrm2** (const int *N*, const void **x*, const int *incx*) — Function

float **cblas_scasum** (const int *N*, const void **x*, const int *incx*) — Function

double **cblas_dznrm2** (const int *N*, const void **x*, const int *incx*) — Function double **cblas_dzasum** (const int *N*, const void **x*, const int *incx*) Function

CBLAS_INDEX **cblas_isamax** (const int *N*, const float **x*, const int *incx*) Function

CBLAS_INDEX **cblas_idamax** (const int *N*, const double **x*, const int *incx*) Function

CBLAS_INDEX **cblas_icamax** (const int *N*, const void **x*, const int *incx*) Function

CBLAS_INDEX **cblas_izamax** (const int *N*, const void **x*, const int *incx*) Function

void **cblas_sswap** (const int *N*, float **x*, const int *incx*, float **y*, const int *incy*) Function

void **cblas_scopy** (const int *N*, const float **x*, const int *incx*, float **y*, const int *incy*) Function

void **cblas_saxpy** (const int *N*, const float *alpha*, const float **x*, const int *incx*, float **y*, const int *incy*) Function

void **cblas_dswap** (const int *N*, double **x*, const int *incx*, double **y*, const int *incy*) Function

void **cblas_dcopy** (const int *N*, const double **x*, const int *incx*, double **y*, const int *incy*) Function

void **cblas_daxpy** (const int *N*, const double *alpha*, const double **x*, const int *incx*, double **y*, const int *incy*) Function

void **cblas_cswap** (const int *N*, void **x*, const int *incx*, void **y*, const int *incy*) Function

void **cblas_ccopy** (const int *N*, const void **x*, const int *incx*, void **y*, const int *incy*) Function

void **cblas_caxpy** (const int *N*, const void **alpha*, const void **x*, const int *incx*, void **y*, const int *incy*) Function

void **cblas_zswap** (const int *N*, void **x*, const int *incx*, void **y*, const int *incy*) Function

void **cblas_zcopy** (const int *N*, const void **x*, const int *incx*, void **y*, const int *incy*) Function

void **cblas_zaxpy** (const int *N*, const void **alpha*, const void **x*, const int *incx*, void **y*, const int *incy*) Function void **cblas_srotg** (float **a*, float **b*, float **c*, float **s*) Function

void **cblas_srotmg** (float **d1*, float **d2*, float **b1*, const float *b2*, float **P*) Function

void **cblas_srot** (const int *N*, float **x*, const int *incx*, float **y*, const int *incy*, const float *c*, const float *s*) Function

void **cblas_srotm** (const int *N*, float **x*, const int *incx*, float **y*, const int *incy*, const float **P*) Function

void **cblas_drotg** (double **a*, double **b*, double **c*, double **s*) Function

void **cblas_drotmg** (double **d1*, double **d2*, double **b1*, const double *b2*, double **P*) Function

void **cblas_drot** (const int *N*, double **x*, const int *incx*, double **y*, const int *incy*, const double *c*, const double *s*) Function

void **cblas_drotm** (const int *N*, double **x*, const int *incx*, double **y*, const int *incy*, const double **P*) Function

void **cblas_sscal** (const int *N*, const float *alpha*, float **x*, const int *incx*) Function

void **cblas_dscal** (const int *N*, const double *alpha*, double **x*, const int *incx*) Function

void **cblas_cscal** (const int *N*, const void **alpha*, void **x*, const int *incx*) Function

void **cblas_zscal** (const int *N*, const void **alpha*, void **x*, const int *incx*) Function

void **cblas_csscal** (const int *N*, const float *alpha*, void **x*, const int *incx*) Function

void **cblas_zdscal** (const int *N*, const double *alpha*, void **x*, const int *incx*) Function

D.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*) Function 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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function 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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function 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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function 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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function 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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function 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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function 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*) Function

D.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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function 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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function

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*) Function 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*) — Function

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*) — Function

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*) — Function

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*) — Function

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*) — Function

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*) — Function

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*) — Function

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*) — Function

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*) — Function 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*) Function

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*) Function

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*) Function

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*) Function

void **cblas_xerbla** (int *p*, const char **rout*, const char **form*, ...) Function

D.4 Examples

The following program computes the product of two matrices using the Level-3 BLAS function SGEMM,

$$\begin{pmatrix} 0.11 & 0.12 & 0.13 \\ 0.21 & 0.22 & 0.23 \end{pmatrix} \begin{pmatrix} 1011 & 1012 \\ 1021 & 1022 \\ 1031 & 1031 \end{pmatrix} = \begin{pmatrix} 367.76 & 368.12 \\ 674.06 & 674.72 \end{pmatrix}$$

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 };
```

```
  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 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,

```
$ ./a.out
[ 367.76, 368.12
  674.06, 674.72 ]
```

Appendix E Reporting Bugs

A list of known bugs can be found in the 'BUGS' file included in the GSL distribution. 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 behaviour
- A short program which exercises the bug

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

Thank you.

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```
one line to give the program's name and a brief idea of what it does.
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Boston, MA 02111-1307, USA.
```

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```
Gnomovision version 69, Copyright (C) 19yy  name of author
Gnomovision comes with ABSOLUTELY NO WARRANTY; for details
type 'show w'.  This is free software, and you are welcome
to redistribute it under certain conditions; type 'show c'
for details.
```

The hypothetical commands '`show w`' and '`show c`' should show the appropriate parts of the General Public License. Of course, the commands you use may be called something other than '`show w`' and '`show c`'; they could even be mouse-clicks or menu items—whatever suits your program.

You should also get your employer (if you work as a programmer) or your school, if any, to sign a "copyright disclaimer" for the program, if necessary. Here is a sample; alter the names:

```
Yoyodyne, Inc., hereby disclaims all copyright interest in
the program 'Gnomovision' (which makes passes at compilers)
written by James Hacker.

signature of Ty Coon, 1 April 1989
```

```
Ty Coon, President of Vice
```

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