Open Optimization Library

Reference Manual
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The Texinfo source for this manual may be obtained from `http://ool.sourceforge.net`

1 Introduction

The Open Optimization Library (OOL) is a collection of routines for constrained minimization problems, implemented following the GNU Scientific Library (GSL) standards. The routines have been either translated into C or 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 OOL

The library aims to cover a wide range of methods in constrained optimization. Initially, routines are available for minimization of differentiable functions subject to simple bounds on their variables.

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 OOL is Free Software

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

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

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

Also, for our own protection, we must make certain that everyone finds out that there is no warranty for the Open Optimization 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 Open Optimization Library are found in the GNU General Public License (see [GNU General Public License], page 38). 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 OOL

The source code for the library can be obtained in different ways, by copying it from a friend or downloading it from the internet, at the following address

```
http://ool.sourceforge.net/
```

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

1.4 No Warranty

The software described in this manual has no warranty, it is provided "as is". It is your responsibility to validate the behavior of the routines and their accuracy using the source code provided. Consult the GNU General Public license for further details (see [GNU General Public License], page 38).

1.5 Reporting Bugs

A list of known bugs can be found in the '`BUGS`' file included in the OOL 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 `biloti@mat.ufpr.br`.

All bug reports should include:

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

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

2 Using the library

This chapter describes how to compile programs that use OOL, 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 OOL 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 `ool_`, while exported macros have the prefix `OOL_`.

2.2 Compiling and Linking

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

```
#include <ool/ool_conmin.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 '`ool`' directory is '`/usr/local/include/ool`'. A typical compilation command for a source file '`example.c`' with the GNU C compiler `gcc` is,

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

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

The library is installed as a single file, '`libool.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 not only the main library, but also the GSL library, which is required by OOL, 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 example.o -lool -lgsl -lgslcblas -lm
```

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

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

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

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

For more information see "BLAS Support" chapter in the GSL documentation.

The program `ool-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$ ool-config --prefix
/usr/local
```

Further information is available using the command `ool-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, in the Bourne shell (`/bin/sh` or `/bin/bash`), the library path can be set with the following commands:

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

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

```
setenv LD_LIBRARY_PATH /usr/local/lib:$LD_LIBRARY_PATH
```

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

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

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

2.4 Compatibility with C++

The library header files automatically define functions to have `extern "C"` linkage when included in C++ programs.

2.5 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, as well as GSL does. 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.

2.6 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.

3 Quick Start

To impatients, this chapter works out an example on the usage of the library. The code presented, despite its simplicity, can be used to solve real problems with minor modifications.

3.1 Example

Consider the problem

$$\text{minimize } f(x) \equiv \sum_{i=1}^{N} (x_i - a_i)^2$$
$$\text{subject to} \quad \ell \leq x \leq u$$

where a is a given vectors in R^n.

We present a sample code for solving this problem with help of the OOL, and comment it line by line.

```
1: #include <stdio.h>
2: #include <ool/ool_conmin.h>

3: void iteration_echo( ool_conmin_minimizer *M );
```

Line 1 includes the C standard IO header and line 2 includes the header for the OOL library. The last should be included in every program that uses OOL. Line 3 simply defines the prototype of an auxiliary function defined below. The following block defines the objective function. The prototype for objective function should always be like in line 4 and 5. The objective function may have parameters, which are provided by a void pointer params. In this example `params` points to a vector. To be used inside the function, `params` is typecasted to `gsl_vector *` (line 7). For functions depending on several parameters, `params` could points to a structure defined to cluster them all.

```
 4: double
 5: fun( const gsl_vector *X, void* params )
 6: {
 7:    gsl_vector *a = (gsl_vector *) params;
 8:    size_t ii, nn;
 9:    double ai, xi;
10:    double f;

11:    nn = X->size;

12:    f = 0;
13:    for( ii = 0; ii < nn; ii++ )
14:       {
15:          ai = gsl_vector_get( a, ii );
16:          xi = gsl_vector_get( X, ii );
17:          f += (xi - ai)*(xi - ai);
18:       }
19:    return f;
20: }
```

The next block implements functions to evaluate the gradient (lines 21–35), objective function and gradient (simultaneously) (36–53), and the product of Hessian by a given vector (54–66).

```
21: void
22: fun_df( const gsl_vector *X, void* params, gsl_vector *G )
23: {
24:    gsl_vector *a = (gsl_vector *) params;
25:    size_t ii, nn;
26:    double ai, xi, gi;

27:    nn = X->size;

28:    for( ii = 0; ii < nn; ii++ )
29:       {
30:          ai = gsl_vector_get( a, ii );
31:          xi = gsl_vector_get( X, ii );
32:          gi = 2 * ( xi - ai );
33:          gsl_vector_set( G, ii, gi );
34:       }
35: }

36: void
37: fun_fdf( const gsl_vector *X, void* params,
38:          double *f, gsl_vector *G )
39: {
40:    gsl_vector *a = (gsl_vector *) params;
41:    size_t ii, nn;
42:    double ai, xi, gi;

43:    nn = X->size;
44:    (*f) = 0;

45:    for( ii = 0; ii < nn; ii++ )
46:       {
47:          ai = gsl_vector_get( a, ii );
48:          xi = gsl_vector_get( X, ii );
49:          (*f) += (xi - ai)*(xi - ai);
50:          gi = 2 * ( xi - ai );
51:          gsl_vector_set( G, ii, gi );
52:       }
53: }

54: void
55: fun_Hv( const gsl_vector *X, void *params,
56:         const gsl_vector *V, gsl_vector *hv )
57: {
58:    size_t ii, nn;
59:    double hvi;

60:    nn = X->size;

61:    for( ii = 0; ii < nn; ii++ )
62:       {
63:          hvi = 2 * gsl_vector_get( V, ii );
64:          gsl_vector_set( hv, ii, hvi);
65:       }
66: }
```

Finally, comes the main routine which drives the optimization. Lines 69 and 70 define the number of variables of the problem and the limit for the number of iterations, respectively.

```
67: int main( void )
```

```
68: {
69:   size_t nn   = 100;
70:   size_t nmax = 10000;
71:   size_t ii;
72:   int status;
```

The next two lines are the only two lines which are method dependent. They are responsible to select which optimization algorithm will be used, the SPG algorithm, in this example.

```
73:   const ool_conmin_minimizer_type *T = ool_conmin_minimizer_spg;
74:   ool_conmin_spg_parameters P;
```

The next four lines declare variables to hold the objective function, the constraints, the minimizer method, and the initial iterate, respectively.

```
75:   ool_conmin_function   F;
76:   ool_conmin_constraint C;
77:   ool_conmin_minimizer *M;
78:   gsl_vector *X;
```

In line 79 a vector is declared to represent the function parameters as in the description of the problem. In the following block, this vector is initialized as $a = (0.1, 0.2, \ldots, 10)^T$.

```
79:   gsl_vector *a;

80:   a = gsl_vector_alloc( nn );
81:   for ( ii = 0; ii < nn; ii++)
82:      gsl_vector_set( a, ii, ((double) ii + 1.0)/10.0 );
```

The function structure is filled in with the number of variables (line 83), pointers to routines to evaluate the objective function and its derivatives (84–87), and a pointer to the function parameters (88).

```
83:   F.n   = nn;
84:   F.f   = &fun;
85:   F.df  = &fun_df;
86:   F.fdf = &fun_fdf;
87:   F.Hv  = &fun_Hv;
88:   F.params = (void *) a;
```

The memory allocation to store the bounds is performed in lines 90 and 91. Further the lower and upper bounds are set to -3 and 3, respectively, to all variables.

```
89:   C.n = nn;
90:   C.L = gsl_vector_alloc( C.n );
91:   C.U = gsl_vector_alloc( C.n );

92:   gsl_vector_set_all( C.L, -3.0 );
93:   gsl_vector_set_all( C.U,  3.0 );
```

These two lines allocate and set the initial iterate.

```
94:   X = gsl_vector_alloc( nn );
95:   gsl_vector_set_all( X, 1.0 );
```

Line 96 allocate the necessary memory for an instance of the optimization algorithm of type `T` (defined in line 73). Line 97 initializes its parameters to default values. If the you want to tune the method by changing the default values to some parameter this should be done between lines 97 and 98.

```
96:   M = ool_conmin_minimizer_alloc( T, nn );

97:   ool_conmin_parameters_default( T, (void*)(&P) );
```

In line 98, everything is put together. It states that this instance of the method `M` is responsible for minimizing function `F`, subject to constraints `C`, starting from point `X`, with parameters `P`.

```
98:   ool_conmin_minimizer_set( M, &F, &C, X, (void*)(&P) );
```

We are now in position to begin iterating. The iteration counter is initialized (line 99) and some information concerning the initial point is displayed (101–102). The iteration loop is repeated while the maximum number of iterations was not reached and the `status` is `OOL_CONTINUE`. Further conditions could also be considered (maximum number of function/gradient evaluation for example). The iteration counter is incremented (104) and one single iteration of the method is performed (105). In line 106 the current iterate is checked for optimality. Finally some information concerning this iteration is displayed.

```
 99:   ii = 0;
100:   status = OOL_CONTINUE;

101:   printf( "%4i : ", ii );
102:   iteration_echo ( M );

103:   while( ii < nmax && status == OOL_CONTINUE ){
104:      ii++;
105:      ool_conmin_minimizer_iterate( M );
106:      status = ool_conmin_is_optimal( M );

107:      printf( "%4i : ", ii );
108:      iteration_echo( M );
109:   }
```

The program ends displaying the convergence status (110–113), number of variables, function and gradient evaluations, the objective function value at the last iterate and the norm of its projected gradient (114–123).

```
110:   if(status == OOL_SUCCESS)
111:      printf("\nConvergence in %i iterations", ii);
112:   else
113:      printf("\nStopped with %i iterations", ii);

114:   printf("\nvariables.............: %6i"
115:    "\nfunction evaluations.....: %6i"
116:    "\ngradient evaluations.....: %6i"
117:    "\nfunction value...........: % .6e"
118:    "\nprojected gradient norm..: % .6e\n",
119:    nn,
120:    ool_conmin_minimizer_fcount( M ),
121:    ool_conmin_minimizer_gcount( M ),
122:    ool_conmin_minimizer_minimum( M ),
123:    ool_conmin_minimizer_size( M ));
```

To finalize, all allocated memory is freed.

```
124:   gsl_vector_free( C.L );
125:   gsl_vector_free( C.U );
126:   gsl_vector_free( X );
127:   gsl_vector_free( a );

128:   ool_conmin_minimizer_free( M );

129:   return OOL_SUCCESS;
130: }
```

This last block codes an auxiliar function to display few elements of the current iterate and the objective value.

```
131: void iteration_echo( ool_conmin_minimizer *M )
132: {
133:   double f = M->f;
134:   size_t ii, nn;

135:   nn = X->size;

136:   printf( "f( " );
137:   for( ii = 0; ii < 3; ii++ )
138:     printf( "%+6.3e, ", gsl_vector_get( M->x, ii ) );
139:   printf( "... ) = %+6.3e\n", f );

140: }
```

This code produces the output:

```
  0 : f( +0.000e+00, +0.000e+00, +0.000e+00, ... ) = +3.384e+03
  1 : f( +1.000e-02, +2.000e-02, +3.000e-02, ... ) = +2.741e+03
  2 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03

Convergence in 2 iterations
variables.................:    100
function evaluations.....:      3
gradient evaluations.....:      3
function value...........:  1.167950e+03
projected gradient norm..:  8.881784e-16
```

4 Brief Theoretical Introduction

This chapter furnishes a brief description of the theory regarding constrained minimization.

4.1 Theory Overview

The problem considered in the CONMIN library is the minimization of a smooth function $f : R^n \to R$ subject to $x \in \Omega$. The set Ω defined by the constraints is called *feasile set*. Briefly, our aim is to solve

$$\min f(x), \text{ s.t. } x \in \Omega$$

where, by this, we mean to find a *local minimizer*, that is, a point x^* such that

$$f(x^*) \leq f(x), \text{ for all } x \in \Omega \text{ near } x^*.$$

4.2 Optimality Conditions

The most general situation for the feasible set is when

$$\Omega = \{x \in R^n \mid g(x) \leq 0,\ h(x) = 0,\ \ell \leq x \leq u\},$$

where $g : R^n \to R^{n_g}$ and $h : R^n \to R^{n_h}$. In this case, the Karush-Kuhn-Tucker (KKT) first order optimality conditions states that, if x^* is a local minimum, then there exist λ_i, , for $i = 1, \ldots, n_h$, and μ_i, , for $i = 1, \ldots, n_g$, such that

$$\nabla f(x^*) + \sum_{i=1}^{n_h} \lambda_i \nabla h_i(x^*) + \sum_{i=1}^{n_g} \mu_i \nabla g_i(x^*) \ = \ 0$$

$$x^* \in \Omega$$

$$\mu_i \geq 0, \text{ for } i = 1, \ldots, n_g$$

We say that x^* is a *critical point* if x^* solves the system above. Therefore, the critical points are candidates for the local minimum.

4.2.1 Convex Case

Instead of finding the critical points by solving the KKT system above, methods for minimization subject to general constraints often may be built based on combinations of methods for minimization with simpler constraints. For instance, when Ω is convex and f is a smooth function, the necessary optimality condition is that the *projected gradient* given by

$$g_P(x) = P_\Omega(x - \nabla f(x)) - x,$$

is the ortogonal projection onto Ω. This can be seen as a particular form of the KKT optimality conditions. The critical points x^*, in this case, are those such that $g_P(x^*) = 0$.

4.2.2 Box Constraints

The simplest convex case, regarding the constraints, is when the feasible set Ω is given by

$$\Omega = \{x \in R^n \mid \ell \leq x \leq u\}.$$

4.3 General Method Structure

4.3.1 Line Search

A common component of optimization methods are *line search* strategies. By this we mean that once given the current point x_c and a descent direction d, we look for λ such that

$$f(x_c + \lambda d) \leq f(x_c).$$

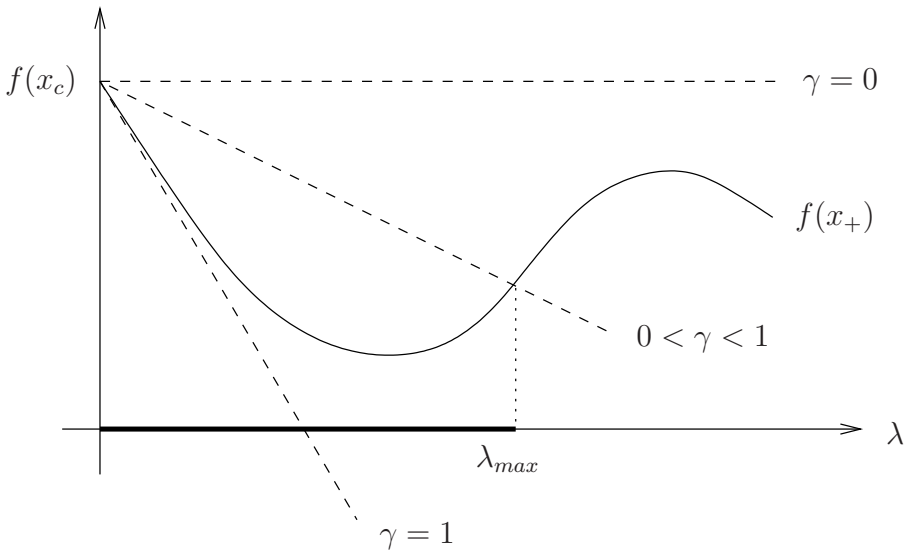
However, if the decreasing achieved at the inequality above for some λ is too small, it is not possible to guarantee convergence to a local minimum. To prevent this, we require that the trial λ to satisfy the *Armijo "sufficient decrease"* condition given by

$$f(x_c + \lambda d) \leq f(x_c) + \lambda\gamma\nabla f(x_c)^T d,$$

where $\gamma \in (0, 1)$. It says that we must choose a λ such that $f(x_+)$ for the trial point $x_+ = x_c + \lambda d$ is smaller than the damped linear model. In the figure below, the interval for λ where the condition holds is $[0, \lambda_{max}]$. Clearly, we can rewrite it alternatively as

$$f(x_+) \leq f(x_c) + \gamma\nabla f(x_c)^T (x_+ - x_c),$$

where we avoid explicitly writing λ and d.



The *nonmonotone Armijo* condition to accept a trial point x_+ is

$$f(x_+) \leq \max_{0 \leq j \leq \min\{k, M-1\}} f(x_{k-j}) + \gamma\nabla f(x_k)^T (x_+ - x_k),$$

where M is an integer greater than zero. If x_+ is rejected, the steplength is redefined as

$$\bar{\lambda} = \max\{\sigma_1\lambda,\ \min\{\sigma_2\lambda,\ \lambda^*\}\},$$

where λ^* minimizes a quadratic model.

4.4 References and Further Reading

An introductory description of constrained minimization algorithms and further references can be found in the following references.

D.P. Bertsekas, *Nonlinear Programming*, Athena Scientific, 1999.

D.P. Bertsekas, *Constrained Optimization and Lagrange Multiplier Methods*, Athena Scientific, 1982.

R. Fletcher, *Practical Methods for Optimization*, John Wiley and Sons, 2nd ed., 1987.

C.T. Kelley, *Iterative Methods for Optimization*, Frontiers in Applied Mathematics, SIAM, Philadelphia, 1999.

5 Constrained Optimization

This chapter describes the common interfaces for constrained minimization of arbitrary multidimensional functions. The library provides implementations and reimplementations of methods published in well known optimization and applied mathematics journals. The library follows, as close as possible, the GSL standards and tries to use the GSL routines, specially those ones for optimization, described at chapters 31, 32, 33, 34, 35 and 36 of the GSL Reference Manual, version 1.4.

In order to fit the same standards of the GSL multidimensional minimization, only one iteration, for each method, is implemented. This means that in case of reimplemented codes, to obtain the same results of the original version, the user must provide a main routine that calls the OOL method and checks for optimality, as well as for stopping criteria, exactly as in the original implementation.

The header file '`ool_conmin.h`' contains prototypes for the minimization functions and related declarations.

5.1 Choosing the Minimization Method

Initially the user must define two variables: T indicates the method used and P stands for its parameters. For example, if you choose to use the Projected Gradient Methods (`pgrad`), the code lines are

```
/* Method structs */
const ool_conmin_minimizer_type *T = ool_conmin_minimizer_pgrad;
ool_conmin_pgrad_parameters P;
```

5.2 Initialization and Finalization

The following function initializes a multidimensional constrained minimizer. The minimizer itself depends only on the dimension of the problem and the algorithm and can be reused for different problems.

`ool_conmin_minimizer * ool_conmin_minimizer_alloc (const ool_conmin_minimizer_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 `OOL_ENOMEM`.

`void ool_conmin_parameters_default (const ool_conmin_minimizer_type * T, void * P)` [Function]

This function initializes the parameters P with its default values, for algorithm T.

`int` **ool_conmin_minimizer_set** (`ool_conmin_minimizer * M, ool_conmin_function *fdf, ool_conmin_constraint * C, const gsl_vector * x, void * P`) [Function]

This function initializes the minimizer M to minimize the function *fdf* subject to the constraints C, starting from the initial point x. The parameters for the method M are given in P. Note that for some methods, the initial point x must be feasible.

`void` **ool_conmin_minimizer_free** (`ool_conmin_minimizer *M`) [Function]

This function frees all the memory associated to the minimizer M.

`const char *` **ool_conmin_minimizer_name** (`const ool_conmin_minimizer * M`) [Function]

This function returns a pointer to the name of the minimizer. For example,

```
printf ("s is a '%s' minimizer\n",
        ool_conmin_minimizer_name (s));
```

would print something like `s is a 'pgrad' minimizer`.

5.3 Providing a function to minimize

You must provide a parametric function of n variables for the minimizer 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. Some methods may require a routine to calculate the Hessian times a given vector. In order to allow for general parameters the functions are defined by the following data type:

ool_conmin_function [Data Type]

This data type defines a general function of n variables with parameters and the corresponding gradient vector of derivatives, as well as the product of the Hessian matrix by a vector.

`size_t n` the dimension of the system, i.e. the number of components of the vectors x.

`double (* f) (const gsl_vector * x, const void * params)`
This function should return the result $f(x, params)$ for argument x and parameters *params*.

`void (* df) (const gsl_vector * x, const void * params, gsl_vector * g)`
This function should store the n-dimensional gradient $g_i = \partial f(x, params)/\partial x_i$ in the vector g for argument x and parameters *params*, returning an appropriate error code if the function cannot be computed.

`void (* fdf) (const gsl_vector * x, const 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 gradient at the same time.

`void (* Hv) (const gsl_vector *x, const void * params, const gsl_vector * V, gsl_vector * hv )`

This function should return the value *hv* of the Hessian matrix times the vector *v*, for arguments *x* and parameters *params*. *For some methods, this routine may be required.*

`void * params`

A pointer to the parameters of the function.

The following example function defines a simple quadratic with parameters,

```
double
quadratic( const gsl_vector *X, void* params )
{
  size_t ii, nn;
  double f, x;

  nn = X->size;

  f = 0;

  for( ii = 0; ii < nn; ii++ )
    {
      x  = gsl_vector_get( X, ii );
      f += (ii+1) * gsl_pow_2( x );
    }

  return f;
}

void
quadratic_df( const gsl_vector *X, void* params, gsl_vector *G )
{
  size_t ii, nn;
  double xx, gg;

  nn = X->size;

  for( ii = 0; ii < nn; ii++ )
    {
      xx = gsl_vector_get( X, ii );
      gg = 2.0 * (ii+1) * xx;
      gsl_vector_set( G, ii, gg );
    }
}

void
quadratic_fdf( const gsl_vector *X, void* params,
       double *f, gsl_vector *G )
```

```
{
  size_t ii, ip1, nn;
  double xx, gg;

  nn = X->size;
  (*f) = 0;

  for( ii = 0; ii < nn; ii++ )
    {
      ip1 = ii + 1;

      xx = gsl_vector_get( X, ii );

      (*f) += ip1 * gsl_pow_2( xx );
      gg = 2.0 * ip1 * xx;

      gsl_vector_set( G, ii, gg );
    }
}

void
quadratic_Hv( const gsl_vector *X, void *params,
      const gsl_vector *V, gsl_vector *hv )
{
  size_t ii, nn;
  double aux;

  nn = X->size;

  for( ii = 0; ii < nn; ii++ )
    {
      aux = 2.0 * (ii+1) * gsl_vector_get( V, ii );
      gsl_vector_set( hv, ii, aux );
    }
}
```

The function structure can be initialized using the following code,

```
ool_conmin_function F;

F.n   = nn;
F.f   = &quadratic;
F.df  = &quadratic_df;
F.fdf = &quadratic_fdf;
F.Hv  = &quadratic_Hv;
F.params = NULL;
```

5.4 Providing the constraints

You must provide the lower and upper bound of the box constraints for the minimizers to operate on.

ool_conmin_constraint [Data Type]

This data type defines a general simple bound constraints for n variables.

`size_t n` the dimension of the system, i.e. the number of components of the vectors x.

`gsl_vector * L`
`gsl_vector * U`
box constraints.

The constraints can be initialized using the following code,

```
ool_conmin_constraint  C;
C.n  = nn;

C.L = gsl_vector_alloc( nn );
C.U = gsl_vector_alloc( nn );

gsl_vector_set_all( C.L,   1.0 );
gsl_vector_set_all( C.U,  10.0 );
```

5.5 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` **ool_conmin_minimizer_iterate** (`ool_conmin_minimizer *M`) [Function]

The function performs a single iteration of the minimizer M. If the iteration encounters an unexpected problem then an error code will be returned.

`int` **ool_conmin_minimizer_restart** (`ool_conmin_minimizer *M`) [Function]

This function resets the minimizer M to use the current point as a new starting point.

The method parameters can be changed between the iterations, using the functions

`void` **ool_conmin_parameters_get** (`const ool_conmin_minimizer *M, void *param_view`) [Function]

`int` **ool_conmin_parameters_set** (`ool_conmin_minimizer *M, void *new_param`) [Function]

The first one returns the parameters *param_view* used in the previous iteration, and the second one sets the new parameters *new_param*.

The minimizer maintains a current best estimate of the minimum at all times. This information can be accessed through the following auxiliary functions,

`gsl_vector * ool_conmin_minimizer_x (const ool_conmin_minimizer * M)` [Function]
`gsl_vector * ool_conmin_minimizer_dx (const ool_conmin_minimizer * M)` [Function]
`double ool_conmin_minimizer_minimum (const ool_conmin_minimizer * M)` [Function]
`gsl_vector * ool_conmin_minimizer_gradient (const ool_conmin_minimizer * M)` [Function]
`double ool_conmin_minimizer_size (const ool_conmin_minimizer * M)` [Function]

These functions return the current best estimate of the location of the minimum, the last step, the value of the function at that point, its gradient, and minimizer specific characteristic size for the minimizer M, respectively.

5.6 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.
- An error has occurred.

The handling of these conditions is under user control. The functions below permit the user to test the precision of the current result.

`int ool_conmin_is_optimal (ool_conmin_minimizer * M)` [Function]

This functions checks for optimality and is method dependent. The test returns `OOL_SUCCESS` if the following condition is achieved, and `OOL_CONTINUE` otherwise.

`size_t ool_conmin_minimizer_fcount (const ool_conmin_minimizer * M)` [Function]
`size_t ool_conmin_minimizer_gcount (const ool_conmin_minimizer * M)` [Function]
`size_t ool_conmin_minimizer_hcount (const ool_conmin_minimizer * M)` [Function]

These functions return, respectively, the number of objective function, gradient and product Hessian-vector evaluations.

5.7 Algorithms

Presently, there are only algorithms for simple bound constraints. They use the value of the function and most of its gradient at each evaluation point, too.

ool_conmin_minimizer_pgrad [Minimizer]

This is a natural extension of the steepest descent algorithm to bound constraints problems. In each step, a line search is perfomed along the projected gradient direction.

ool_conmin_minimizer_spg [Minimizer]
This is the classical projected gradient method extended to a include nonmonotone line search strategy and the spectral steplength, which greatly improves the convergence rate of the method.

ool_conmin_minimizer_gencan [Minimizer]
This is a active-set method for smooth box-constrained minimization. The algorithm combines an unconstrained method, including a line search which aims to add many constraints to the working set at a single iteration, with a technique (spectral projected gradient) for dropping constraints from the working set.

5.8 References and Further Reading

A brief description of constrained minimization algorithms and further references can be found in the following references.

D.P. Bertsekas, *Nonlinear Programming*, Athena Scientific, 1999.

D.P. Bertsekas, *Constrained Optimization and Lagrange Multiplier Methods*, Athena Scientific, 1982.

R. Fletcher, *Practical Methods for Optimization*, John Wiley and Sons, 1987.

C.T. Kelley, *Iterative Methods for Optimization*, Frontiers in Applied Mathematics, SIAM, 1999.

6 Projected Gradient Method

This chapter describes the routine PGRAD, for constrained minimization of differentiable multidimensional functions, which implements the Projected Gradient Method.

6.1 Overview

The problem solved by PGRAD is the minimization of a smooth function with bounds on the variables (see Chapter 4 [Brief Theoretical Introduction], page 11 and Section 4.2.2 [Box Constraints], page 11).

The Projected Gradient method is a natural extension of the Steepest Descent method for unconstrained minimization. At each step a line search is performed over direction of projected gradient. This method is not inteded to be used for production. For further details, see the reference at the end of this section.

6.2 Parameters

Inside PGRAD, there are few parameters which can be choosen to improve the minimizing efforts. The parameter list, together with the default values are given below.

`double` **tol** `= 1.0e-4` [Parameter]
Tolerance on infinite norm of the projected gradient for optimality check.

`double` **fmin** `= -1e+99` [Parameter]
Value to declare f as unbounded.

`double` **alpha** `= 1.0e-4` [Parameter]
Constant for the *sufficient decrease* condition

$$f(x(\lambda)) - f(x) \leq -\frac{\alpha}{\lambda}||x - x(\lambda)||^2.$$

`double` **sigma1** `= 0.1` [Parameter]
`double` **sigma2** `= 0.9` [Parameter]
Bounds to the redution of the steplength.

6.3 Stopping Criteria

The algorithm declares convergence whenever the infinite norm of projected gradient is less than or equal to a given tolerance.

The infinite norm of the projected gradient at the current iterate can be retrieved by calling `ool_conmin_minimizer_size()` function.

6.4 Example

For an example of PGRAD, see Chapter 3 [Quick Start], page 6, replacing lines 73 and 75 of that code by

```
const ool_conmin_minimizer_type *T = ool_conmin_minimizer_pgrad;
ool_conmin_pgrad_parameters P;
```

The output of the program is shown below.

```
 0 : f( +0.000e+00, +0.000e+00, +0.000e+00, ... ) = +3.384e+03
 1 : f( +2.000e-01, +4.000e-01, +6.000e-01, ... ) = +1.190e+03
 2 : f( +1.800e-01, +3.600e-01, +5.400e-01, ... ) = +1.182e+03
 3 : f( +1.640e-01, +3.280e-01, +4.920e-01, ... ) = +1.177e+03
 4 : f( +1.512e-01, +3.024e-01, +4.536e-01, ... ) = +1.174e+03
 5 : f( +1.410e-01, +2.819e-01, +4.229e-01, ... ) = +1.172e+03
 6 : f( +1.328e-01, +2.655e-01, +3.983e-01, ... ) = +1.170e+03
 7 : f( +1.262e-01, +2.524e-01, +3.786e-01, ... ) = +1.169e+03
 8 : f( +1.210e-01, +2.419e-01, +3.629e-01, ... ) = +1.169e+03
 9 : f( +1.168e-01, +2.336e-01, +3.503e-01, ... ) = +1.169e+03
10 : f( +1.134e-01, +2.268e-01, +3.403e-01, ... ) = +1.168e+03
11 : f( +1.107e-01, +2.215e-01, +3.322e-01, ... ) = +1.168e+03
12 : f( +1.086e-01, +2.172e-01, +3.258e-01, ... ) = +1.168e+03
13 : f( +1.069e-01, +2.137e-01, +3.206e-01, ... ) = +1.168e+03
14 : f( +1.055e-01, +2.110e-01, +3.165e-01, ... ) = +1.168e+03
15 : f( +1.044e-01, +2.088e-01, +3.132e-01, ... ) = +1.168e+03
16 : f( +1.035e-01, +2.070e-01, +3.106e-01, ... ) = +1.168e+03
17 : f( +1.028e-01, +2.056e-01, +3.084e-01, ... ) = +1.168e+03
18 : f( +1.023e-01, +2.045e-01, +3.068e-01, ... ) = +1.168e+03
19 : f( +1.018e-01, +2.036e-01, +3.054e-01, ... ) = +1.168e+03
20 : f( +1.014e-01, +2.029e-01, +3.043e-01, ... ) = +1.168e+03
21 : f( +1.012e-01, +2.023e-01, +3.035e-01, ... ) = +1.168e+03
22 : f( +1.009e-01, +2.018e-01, +3.028e-01, ... ) = +1.168e+03
23 : f( +1.007e-01, +2.015e-01, +3.022e-01, ... ) = +1.168e+03
24 : f( +1.006e-01, +2.012e-01, +3.018e-01, ... ) = +1.168e+03
25 : f( +1.005e-01, +2.009e-01, +3.014e-01, ... ) = +1.168e+03
26 : f( +1.004e-01, +2.008e-01, +3.011e-01, ... ) = +1.168e+03
27 : f( +1.003e-01, +2.006e-01, +3.009e-01, ... ) = +1.168e+03
28 : f( +1.002e-01, +2.005e-01, +3.007e-01, ... ) = +1.168e+03
29 : f( +1.002e-01, +2.004e-01, +3.006e-01, ... ) = +1.168e+03
30 : f( +1.002e-01, +2.003e-01, +3.005e-01, ... ) = +1.168e+03
31 : f( +1.001e-01, +2.002e-01, +3.004e-01, ... ) = +1.168e+03
32 : f( +1.001e-01, +2.002e-01, +3.003e-01, ... ) = +1.168e+03
33 : f( +1.001e-01, +2.002e-01, +3.002e-01, ... ) = +1.168e+03
34 : f( +1.001e-01, +2.001e-01, +3.002e-01, ... ) = +1.168e+03
35 : f( +1.001e-01, +2.001e-01, +3.002e-01, ... ) = +1.168e+03
36 : f( +1.000e-01, +2.001e-01, +3.001e-01, ... ) = +1.168e+03
37 : f( +1.000e-01, +2.001e-01, +3.001e-01, ... ) = +1.168e+03
38 : f( +1.000e-01, +2.001e-01, +3.001e-01, ... ) = +1.168e+03
```

```
 39 : f( +1.000e-01, +2.000e-01, +3.001e-01, ... ) = +1.168e+03
 40 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03
 41 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03
 42 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03
 43 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03
 44 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03
 45 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03
 46 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03
 47 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03
 48 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03

Convergence in 48 iterations
variables.............:    100
function evaluations.....:     96
gradient evaluations.....:     49
function value...........:  1.167950e+03
projected gradient norm..:  8.362779e-05
```

6.5 References and Further Reading

The projected gradient method appears in several books. This implementation was based on the book

C. T. Kelley, *Iterative Methods of Optimization*, SIAM, Philadelphia, 1999.

7 Spectral Projected Gradient Method

This chapter describes the routine SPG for constrained minimization of differentiable multidimensional functions on convex sets.

7.1 Overview

The Spectral Projected Gradient Method is designed to minimize differentiable function on convex sets. The SPG Method is similar to the Projected Gradient Method, differing only by the choice of the spectral steplength, which accelerates the convergence of the method. Despite this similarity, it can be shown that the SPG Method is related to the quasi-Newton family of methods.

This implementation deals with box constrained (see Chapter 4 [Brief Theoretical Introduction], page 11 and Section 4.2.2 [Box Constraints], page 11).

The SPG routine implements the version SPG2 of the Nonmonotone Spectral Projected Gradient Method, as published in Birgin *et al.* (2000), which differs from the classical SPG method by the nonmonotone Armijo sufficient decrease condition to accept a trial point x_+ (see Section 4.3.1 [Line Search], page 12). This method is a competitive option for large problems, since it has low memory requirements.

7.2 Parameters

Inside SPG, there is a set of parameters which can be changed to improve the minimizing efforts. The parameter list, together with the default values are given below.

`double` **fmin** `= -1.0e+99` [Parameter]
: Value to declare f as unbounded.

`double` **tol** `= -1.0e-4` [Parameter]
: Tolerance on the infinite norm of the projected gradient to declare convergence.

`size_t` **M** `= 10` [Parameter]
: Nonmonotonicity parameter. Setting M to 1 turns the method monotone.

`double` **alphamax** `= 1.0e+30` [Parameter]
: Upper bound to spectral step size.

`double` **alphamin** `= 1.0e-30` [Parameter]
: Lower bound to spectral step size.

`double` **gamma** `= 1.0e-4` [Parameter]
: Sufficient decrease parameter ($0 < \gamma < 1$).

`double` **sigma1** `= 0.1` [Parameter]
`double` **sigma2** `= 0.9` [Parameter]
: Bounds to the redution of the steplength.

7.3 Stopping Criteria

The method declares convergence whenever the function value is equal to or less than a prescribed value, through the *fmin* parameter, or the inifinte norm of projected gradient is less than the tolerance defined in *tol* parameter.

The infinite norm of the projected gradient at the current iterate can be retrieved by calling `ool_conmin_minimizer_size()` function.

7.4 Example

See Chapter 3 [Quick Start], page 6, for an example program which employs SPG.

7.5 References and Further Reading

The Nonmonotone Spectral Projected Gradient Method was published in the following paper, where a full description and further references can be found.

E.G. Birgin, J.M. Martínez, and M. Raydan, *Nonmonotone Spectral Projected Gradient Methods on Convex Sets*, SIAM Journal on Optimization 10:1196–1211, 2000.

8 Gencan Method

This chapter describes the routine GENCAN for constrained minimization of arbitrary multidimensional functions.

8.1 Overview

The problem solved by GENCAN is the minimization of a smooth function with bounds on the variables (see Chapter 4 [Brief Theoretical Introduction], page 11 and Section 4.2.2 [Box Constraints], page 11).

Suppose that an iterate x is inside a given face of Ω (the feasible set) and consider $g_I(x)$ to be the projection of $g_P(x)$ inside this face. The main algorithm then performs the test $||g_I(x)|| \leq (1-\eta)||g_P(x)||$, where $\eta \in (0,1)$. If false, the new point must remain in the face and an iteration of a truncated Newton method is performed (only for the free variables). However, if that condition holds, some constraint must be abandoned and the new point is computed doing one iteration of the "Spectral Projected Gradient" method. For further details, see the reference at the end of this section.

8.2 Parameters

Inside GENCAN, there is a set of parameters which can be changed to improve the minimizing efforts. The parameter list, together with the default values are given below.

`double` **epsgpen** `= 1.0e-5` [Parameter]
: Tolerance on euclidean norm of the projected gradient to declare convergence.

`double` **epsgpsn** `= 1.0e-5` [Parameter]
: Tolerance on infinite norm of the projected gradient to declare convergence.

`double` **fmin** `= -1.0e+99` [Parameter]
: Function value to declare f as unbounded.

`double` **udelta0** `= -1` [Parameter]
: Initial trust-region radius for Conjugate Gradient subalgorithm. The default value max(`delmin`, 0.1 $*$ max(1, $|x|$)) is used if `udelta0` is non-positive.

`int` **ucgmia** `= -1` [Parameter]
`int` **ucgmib** `= -1` [Parameter]
: Maximum number of iterations allowed for each call of the Conjugate Gradient subalgorithm. If `ucgmia` and `ucgmib` are both set to positive values, the maximum number of iterations is set as max(1, `ucgmia * nind + ucgmib`), where `nind` states for the number of variables of the subproblem. Otherwise, thr default value for the maximum number of iterations is a linear function of the infinite norm of the projected gradient, which ranges from max(1, 10 * log(`nind`)) to `nind`, as the current iterate gets closer to the solution.

`int` **cg_scre** = `1` [Parameter]
`double` **cg_gpnf** = `epsgpen` [Parameter]
`double` **cg_epsi** = `1.0e-1` [Parameter]
`double` **cg_epsf** = `1.0e-5` [Parameter]

`cg_scre` states for Conjugate Gradient Stopping Criterion Relation, and `cg_gpnf` states for Conjugate Gradient Projected Gradient Final Norm. Both are related to a stopping criterion of Conjugate Gradients. This stopping criterion depends on the norm of the residual of the linear system. The norm of the residual should be less or equal than a *small* quantity which decreases as the iterate gets closer to the solution of the minimization problem. Then, the log of the required accuracy requested to Conjugate Gradient has a linear dependence on the log of the norm of the continuous projected gradient. This linear relation uses the squared Euclidian norm of the projected gradient if `cg_scre` is equal to 1 and uses the infinite norm if `cg_scre` is equal to 2. In addition, the precision required to CG is equal to `cg_epsi` (conjugate gradient initial epsilon) at the initial iterate and `cg_epsf` (conjugate gradient final epsilon) when the Euclidian- or infinite norm of the projected gradient is equal to `cg_gpnf` (conjugate gradients projected gradient final norm) which is an estimation of the value of the Euclidian- or infinite norm of the projected gradient at the solution. In case `cg_scre` is equal to 2, one suggests that `cg_gpnf` be equal to `epsgpsn`.

`double` **cg_epsnqmp** = `1.0e-4` [Parameter]
`size_t` **maxitnqmp** = `5` [Parameter]

Both parameters are used for a stopping criterion of the Conjugate Gradients subalgorithm. If the progress in the quadratic model is smaller than fraction `epsnqmp` of the best progress during `maxitnqmp` consecutive iterations then CG is stopped declaring "not enough progress of the quadratic model".

`int` **nearlyq** = `0` [Parameter]

Use `nearlyq` = 1 if the objective function is nearly quadratic. When an iteration of the CG finds a direction d such that $d^T H d \leq 0$ then, depending on `nearlyq`, CG does: if `nearlyq`=0, it stops at current point or if `nearly`=1 it takes the direction d and tries to go to the boundary choosing the best among the two points at the boundary and the current one.

`double` **nint** = `2.0` [Parameter]

Constant for the interpolation. See the description of `sigma1` and `sigma2`. Sometimes we take as a new trial step the previous one divided by `nint`.

`double` **next** = `2.0` [Parameter]

Constant for the extrapolation when extrapolating we try $\alpha_{new} = \alpha$ next.

`size_t` **mininterp** = `4` [Parameter]

Constant for testing if, after having made at least `mininterp` interpolations, the steplength is too small. In that case, failure of the line search is declared. It is possible that the direction is not a descent direction due to an error in the gradient calculations.

`size_t` **maxextrap** = `100` [Parameter]

Constant to limit the number of extrapolations in the Truncated Newton direction.

`int` **trtype** = `0` [Parameter]
Type of trust-region radius: `trtype` = 0 means Euclidian norm trust-region and `trtype` = 1 means infinite-norm trust-region.

`double` **eta** = `0.9` [Parameter]
Constant for deciding abandon the current face or not. We abandon the current face if the norm of the internal gradient (here, internal components of the continuous projected gradient) is smaller than (1-`eta`) times the norm of the continuous projected gradient. Using the default value is a rather conservative strategy in the sense that internal iterations are preferred over SPG iterations.

`double` **delmin** = `0.1` [Parameter]
Minimum "trust region" to compute the *Truncated Newton* direction.

`double` **lspgmi** = `1.0e-10` [Parameter]
`double` **lspgma** = `1.0e+10` [Parameter]
The spectral steplength, called λ, is projected inside the box [`lspgmi`,`lspgma`].

`double` **theta** = `1.0e-6` [Parameter]
Constant for the angle condition, i.e., at iteration k we need a direction d_k such that $\langle g_k, d_k\rangle \leq -\theta||g||_2||d_k||_2$, where $g_k = \nabla f(x_k)$.

`double` **gamma** = `1.0e-4` [Parameter]
Constant for the Armijo condition.

`double` **beta** = `0.5` [Parameter]
Constant for the beta condition $\langle d_k, g(x_k+d_k)\rangle \geq$ `beta` $\langle d_k, g_k\rangle$. If (x_k+d_k) satisfies the Armijo condition but does not satisfy the beta condition then the point is accepted, but if it satisfied the Armijo condition and also satisfies the beta condition then we know that there is the possibility for a successful extrapolation.

`double` **sigma1** = `0.1` [Parameter]
`double` **sigma2** = `0.9` [Parameter]
Constants for the safeguarded interpolation. If $\alpha_{new} \notin [\text{sigma1}, \sigma\alpha]$, then we take $\alpha_{new} = \alpha/$`nint`.

`double` **epsrel** = `1.0e-7` [Parameter]
`double` **epsabs** = `1.0e-10` [Parameter]
`double` **infrel** = `1.0e+20` [Parameter]
`double` **infabs** = `1.0e+99` [Parameter]
These constants mean a "relative small number", "an absolute small number", "relative infinite number", "absolute infinite number", respectively.

8.3 Stopping Criteria

In the original paper, some criteria are used to detect if the iteration process should stop. They are (in the same order they appear)

- Test whether the *Euclidean norm of the continuous projected gradient* is small enough to declare convergence.

- Test whether the *infinite norm of the continuous projected gradient* is small enough to declare convergence.
- Test whether it was performed too many iterations without a satisfactory decreasing of the *objective function value*.
- Test whether it was performed too many iterations without a satisfactory decreasing of the *Euclidean norm of the projected gradient*.

The infinite norm of the projected gradient at the current iterate can be retrieved by calling `ool_conmin_minimizer_size()` function.

8.4 Example

See Chapter 3 [Quick Start], page 6, for an example program, replacing lines 73 and 75 of that code by

```
const ool_conmin_minimizer_type *T = ool_conmin_minimizer_gencan;
ool_conmin_gencan_parameters P;
```

The output of the program is shown below.

```
 0 : f( +0.000e+00, +0.000e+00, +0.000e+00, ... ) = +3.384e+03
 1 : f( +1.200e-01, +2.400e-01, +3.600e-01, ... ) = +1.170e+03
 2 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.169e+03
 3 : f( +1.000e-01, +2.000e-01, +3.000e-01, ... ) = +1.168e+03

Convergence in 3 iterations
variables.............:    100
function evaluations.....:     15
gradient evaluations.....:      5
function value...........:  1.167950e+03
projected gradient norm..:  0.000000e+00
```

8.5 References and Further Reading

The GENCAN algorithm was published in the following paper, where a full description and further references can be found.

E.G. Birgin and J.M. Martínez, *Large-Scale Active-Set Box-Constrained Optimization Method with Spectral Projected Gradients*, Computational Optimization and Applications, 23:101–125, 2002.

9 Tools

This chapter describes some extra frequently useful tools.

9.1 Numerical Gradient and Hessian

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

The numerical evaluation of the gradient and the Hessian can be done with the following functions.

`int` **ool_diff_g** (`double(* f) (const gsl_vector*, void*), gsl_vector * X, void * fparam, gsl_vector * G, const double eps`) [Function]

This function numerically evaluates the gradient G of f at the point X. The derivatives are approximated by centered differences with step *eps*, i.e.,

$$\frac{\partial f}{\partial x_i}(x) = \frac{f(x + \varepsilon\, e_i) - f(x - \varepsilon\, e_i)}{2\varepsilon} + \mathcal{O}(\varepsilon^2),$$

where e_i is the i-th canonical vector. A suitable choice for *eps* is $\varepsilon_f^{1/3}||x||_\infty$, where ε_f states for the function evaluation accuracy. Typically, for ε_f near 10^{-16}, the machine roundoff, and $||x||_\infty$ with order near 1, *eps* should be 10^{-5}.

`int` **ool_diff_g_auto** (`double(* f) (const gsl_vector*, void*), gsl_vector * X, void * fparam, gsl_vector * G`) [Function]

This function numerically evaluates the gradient G of f at the point X, selecting the stepsize discretization automatically.

`int` **ool_diff_Hv** (`const ool_diff_Hv_accel * a, void(* df) (const gsl_vector*, void*, gsl_vector*), gsl_vector * X, void * fparam, const gsl_vector * V, gsl_vector * Hv, const double eps`) [Function]

This function numerically evaluates the product Hv of the Hessian of f, at the point X, by a given vector V, which is numerically approximated by

$$[H(x)v]_i = \left(\frac{\nabla f(x + \varepsilon\, e_i) - \nabla f(x - \varepsilon\, e_i)}{2\varepsilon}\right)^T v.$$

The routine requires a function *df* that evaluates the gradient. Optionally, to speed up the numerical evaluation, we suggest to provide an accelerator *a*. If not provided, in case *a* receives `NULL`, the routine itself takes care of the required memory allocation and deallocation, each time it is called.

`ool_diff_Hv_accel *` **ool_diff_Hv_accel_alloc** (`size_t n`) [Function]

This function returns a pointer to an accelerator object, which avoids memory allocations and deallocations, throughout the repetitive calls to function `ool_diff_Hv`.

`void` **ool_diff_Hv_accel_free** (`ool_diff_Hv_accel * a`) [Function]

This routine frees memory associated to an accelerator object.

9.2 References and Further Reading

For further references concerning numerical evaluation of gradient and Hessian, please, refer to

C.T. Kelley, *Iterative Methods for Optimization*, Frontiers in Applied Mathematics, SIAM, Philadelphia, 1999.

Appendix A Contributors to OOL

(See the AUTHORS file in the distribution for up-to-date information.)

Ricardo Biloti
: Conceived OOL, wrote the design document. Wrote the codes for the SPG method and the numerical evaluation tools, as well as their documentation.

Luis Alberto D'Afonseca
: Wrote all the codes in the C/GSL format. Wrote the CONMIN library.

Sergio Ventura
: Wrote the documentation, as well as the html page. Converted GENCAN from Fortran 77 to C.

Iara da Cunha
: Wrote the codes for the projected gradient method.

Appendix B Reporting Constants

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

`OOL_UNBOUNDEDF`
: Lower unbounded function.

`OOL_INFEASIBLE`
: Infeasible point

`OOL_FINNERIT`
: Too many inner iterations

`OOL_FLSEARCH`
: Line search failed

`OOL_FDDIR`
: Unable to find a descent direction

Appendix C 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)
```

It is important to check for `libm` and `libgslcblas` before `libgsl`, otherwise the tests will fail. Assuming the libraries are found the output during the configure stage looks like this,

```
checking for 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++.

To test for `inline` the following test should be placed in your '`configure.in`' file,

```
AC_C_INLINE

if test "$ac_cv_c_inline" != no ; then
  AC_DEFINE(HAVE_INLINE,1)
  AC_SUBST(HAVE_INLINE)
fi
```

and the macro will then be defined in the compilation flags or by including the file 'config.h' before any library headers.

The following autoconf test will check for extern inline,

```
dnl Check for "extern inline", using a modified version
dnl of the test for AC_C_INLINE from acspecific.mt
dnl
AC_CACHE_CHECK([for extern inline], ac_cv_c_extern_inline,
[ac_cv_c_extern_inline=no
AC_TRY_COMPILE([extern $ac_cv_c_inline double foo(double x);
extern $ac_cv_c_inline double foo(double x) { return x+1.0; };
double foo (double x) { return x + 1.0; };],
[  foo(1.0)  ],
[ac_cv_c_extern_inline="yes"])
])

if test "$ac_cv_c_extern_inline" != no ; then
  AC_DEFINE(HAVE_INLINE,1)
  AC_SUBST(HAVE_INLINE)
fi
```

The substitution of portability functions can be made automatically if you use autoconf. For example, to test whether the BSD function hypot is available you can include the following line in the configure file 'configure.in' for your application,

```
AC_CHECK_FUNCS(hypot)
```

and place the following macro definitions in the file 'config.h.in',

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

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

The application source files can then use the include command #include <config.h> to substitute gsl_hypot for each occurrence of hypot when hypot is not available.

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The following article was written by Richard Stallman, founder of the GNU Project.

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```
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```

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```
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