

C interfaces to GALAHAD BGO

Jari Fowkes and Nick Gould STFC Rutherford Appleton Laboratory Wed May 3 2023

1 GALAHAD C package bgo	1
1.1 Introduction	1
1.1.1 Purpose	1
1.1.2 Authors	1
1.1.3 Originally released	1
1.1.4 Terminology	1
1.1.5 Method	2
1.1.6 References	2
1.2 Call order	3
1.3 Symmetric matrix storage formats	3
1.3.1 Dense storage format	3
1.3.2 Sparse co-ordinate storage format	4
1.3.3 Sparse row-wise storage format	4
2 File Index	5
2.1 File List	5
2.1 File List	Ü
3 File Documentation	7
3.1 galahad_bgo.h File Reference	7
3.1.1 Data Structure Documentation	8
3.1.1.1 struct bgo_control_type	8
3.1.1.2 struct bgo_time_type	9
3.1.1.3 struct bgo_inform_type	9
3.1.2 Function Documentation	10
3.1.2.1 bgo_initialize()	10
3.1.2.2 bgo_read_specfile()	10
3.1.2.3 bgo_import()	10
3.1.2.4 bgo_reset_control()	12
3.1.2.5 bgo_solve_with_mat()	12
3.1.2.6 bgo_solve_without_mat()	14
3.1.2.7 bgo_solve_reverse_with_mat()	17
3.1.2.8 bgo_solve_reverse_without_mat()	21
3.1.2.9 bgo_information()	24
3.1.2.10 bgo_terminate()	25
4 Example Documentation	27
4.1 bgot.c	27
4.2 bgotf.c	34

Chapter 1

GALAHAD C package bgo

1.1 Introduction

1.1.1 Purpose

The bgo package uses a **multi-start trust-region method to find an approximation to the global minimizer** of a differentiable objective function f(x) of n variables x, subject to simple bounds $x^l \le x \le x^u$ on the variables. Here, any of the components of the vectors of bounds x^l and x^u may be infinite. The method offers the choice of direct and iterative solution of the key trust-region subproblems, and is suitable for large problems. First derivatives are required, and if second derivatives can be calculated, they will be exploited—if the product of second derivatives with a vector may be found but not the derivatives themselves, that may also be exploited.

The package offers both random multi-start and local-minimize-and probe methods to try to locate the global minimizer. There are no theoretical guarantees unless the sampling is huge, and realistically the success of the methods decreases as the dimension and nonconvexity increase.

1.1.2 Authors

N. I. M. Gould, STFC-Rutherford Appleton Laboratory, England.

C interface, additionally J. Fowkes, STFC-Rutherford Appleton Laboratory.

Julia interface, additionally A. Montoison and D. Orban, Polytechnique Montréal.

1.1.3 Originally released

July 2016, C interface August 2021.

1.1.4 Terminology

The gradient $\nabla_x f(x)$ of f(x) is the vector whose i-th component is $\partial f(x)/\partial x_i$. The Hessian $\nabla_{xx} f(x)$ of f(x) is the symmetric matrix whose i,j-th entry is $\partial^2 f(x)/\partial x_i \partial x_j$. The Hessian is sparse if a significant and useful proportion of the entries are universally zero.

1.1.5 Method

A choice of two methods is available. In the first, local-minimization-and-probe, approach, local minimization and univariate global minimization are intermixed. Given a current champion x_k^S , a local minimizer x_k of f(x) within the feasible box $x^l \leq x \leq x^u$ is found using the GALAHAD package trb. Thereafter m random directions p are generated, and univariate local minimizer of $f(x_k + \alpha p)$ as a function of the scalar α along each p within the interval $[\alpha^L, \alpha^u]$, where α^L and α^u are the smallest and largest α for which $x^l \leq x_k + \alpha p \leq x^u$, is performed using the GALAHAD package ugo. The point $x_k + \alpha p$ that gives the smallest value of f is then selected as the new champion x_{k+1}^S .

The random directions p are chosen in one of three ways. The simplest is to select the components as

$$p_i = \text{pseudo random} \in \left\{ \begin{array}{ll} \text{[-1,1]} & \text{if} \quad x_i^l < x_{k,i} < x_i^u \\ \text{[0,1]} & \text{if} \quad x_{k,i} = x_i^l \\ \text{[-1,0]} & \text{if} \quad x_{k,i} = x_i^u \end{array} \right.$$

for each $1 \le i \le n$. An alternative is to pick p by partitioning each dimension of the feasible `hypercube' box into m equal segments, and then selecting sub-boxes randomly within this hypercube using GALAHAD's Latin hypercube sampling package, lhs. Each components of p is then selected in its sub-box, either uniformly or pseudo randomly.

The other, random-multi-start, method provided selects m starting points at random, either componentwise pseudo randomly in the feasible box, or by partitioning each component into m equal segments, assigning each to a subbox using Latin hypercube sampling, and finally choosing the values either uniformly or pseudo randomly. Local minimizers within the feasible box are then computed by the GALAHAD package trb, and the best is assigned as the current champion. This process is then repeated until evaluation limits are achieved.

If n=1, the GALAHAD package UGO is called directly.

We reiterate that there are no theoretical guarantees unless the sampling is huge, and realistically the success of the methods decreases as the dimension and nonconvexity increase. Thus the methods used should best be viewed as heuristics.

1.1.6 References

The generic bound-constrained trust-region method is described in detail in

A. R. Conn, N. I. M. Gould and Ph. L. Toint (2000), Trust-region methods. SIAM/MPS Series on Optimization,

the univariate global minimization method employed is an extension of that due to

D. Lera and Ya. D. Sergeyev (2013), 'Acceleration of univariate global optimization algorithms working with Lipschitz functions and Lipschitz first derivatives' SIAM J. Optimization Vol. 23, No. 1, pp. 508–529,

while the Latin-hypercube sampling method employed is that of

B. Beachkofski and R. Grandhi (2002). `'Improved Distributed Hypercube Sampling'', 43rd AIAA structures, structural dynamics, and materials conference, pp. 2002-1274.

1.2 Call order 3

1.2 Call order

To solve a given problem, functions from the bgo package must be called in the following order:

- bgo initialize provide default control parameters and set up initial data structures
- · bgo_read_specfile (optional) override control values by reading replacement values from a file
- · bgo import set up problem data structures and fixed values
- bgo reset control (optional) possibly change control parameters if a sequence of problems are being solved
- · solve the problem by calling one of
 - bgo solve with mat solve using function calls to evaluate function, gradient and Hessian values
 - bgo_solve_without_mat solve using function calls to evaluate function and gradient values and Hessian-vector products
 - bgo_solve_reverse_with_mat solve returning to the calling program to obtain function, gradient and Hessian values, or
 - bgo_solve_reverse_without_mat solve returning to the calling prorgram to obtain function and gradient values and Hessian-vector products
- bgo information (optional) recover information about the solution and solution process
- · bgo_terminate deallocate data structures

See Section 4.1 for examples of use.

1.3 Symmetric matrix storage formats

The symmetric n by n matrix $H = \nabla_{xx} f$ may be presented and stored in a variety of formats. But crucially symmetry is exploited by only storing values from the lower triangular part (i.e, those entries that lie on or below the leading diagonal).

Both C-style (0 based) and fortran-style (1-based) indexing is allowed. Choose control.f_indexing as false for C style and true for fortran style; the discussion below presumes C style, but add 1 to indices for the corresponding fortran version.

Wrappers will automatically convert between 0-based (C) and 1-based (fortran) array indexing, so may be used transparently from C. This conversion involves both time and memory overheads that may be avoided by supplying data that is already stored using 1-based indexing.

1.3.1 Dense storage format

The matrix H is stored as a compact dense matrix by rows, that is, the values of the entries of each row in turn are stored in order within an appropriate real one-dimensional array. Since H is symmetric, only the lower triangular part (that is the part H_{ij} for $0 \le j \le i \le n-1$) need be held. In this case the lower triangle should be stored by rows, that is component i*i/2+j of the storage array H_val will hold the value H_{ij} (and, by symmetry, H_{ji}) for $0 \le j \le i \le n-1$.

1.3.2 Sparse co-ordinate storage format

Only the nonzero entries of the matrices are stored. For the l-th entry, $0 \le l \le ne-1$, of H, its row index i, column index j and value H_{ij} , $0 \le j \le i \le n-1$, are stored as the l-th components of the integer arrays H_row and H_col and real array H_val, respectively, while the number of nonzeros is recorded as H_ne = ne. Note that only the entries in the lower triangle should be stored.

1.3.3 Sparse row-wise storage format

Again only the nonzero entries are stored, but this time they are ordered so that those in row i appear directly before those in row i+1. For the i-th row of H the i-th component of the integer array H_ptr holds the position of the first entry in this row, while H_ptr(n) holds the total number of entries. The column indices j, $0 \le j \le i$, and values H_{ij} of the entries in the i-th row are stored in components I = H_ptr(i), . . ., H_ptr(i+1)-1 of the integer array H_col, and real array H_val, respectively. Note that as before only the entries in the lower triangle should be stored. For sparse matrices, this scheme almost always requires less storage than its predecessor.

Chapter 2

File Index

_				
2	1	Fil	ΔI	iet

Here is a list of all files with brief descriptions:	
galahad_bgo.h	

6 File Index

Chapter 3

File Documentation

3.1 galahad bgo.h File Reference

```
#include <stdbool.h>
#include <stdint.h>
#include "galahad_precision.h"
#include "galahad_cfunctions.h"
#include "galahad_trb.h"
#include "galahad_ugo.h"
#include "galahad_lhs.h"
```

Data Structures

- struct bgo_control_type
- struct bgo_time_type
- struct bgo_inform_type

Functions

- void bgo_initialize (void **data, struct bgo_control_type *control, int *status)
- void bgo_read_specfile (struct bgo_control_type *control, const char specfile[])
- void bgo_import (struct bgo_control_type *control, void **data, int *status, int n, const real_wp_ x_[[], const real_wp_ x_u[], const char H_type[], int ne, const int H_row[], const int H_col[], const int H_ptr[])
- void bgo_reset_control (struct bgo_control_type *control, void **data, int *status)
- void bgo_solve_with_mat (void **data, void *userdata, int *status, int n, real_wp_ x[], real_wp_ g[], int ne, int(*eval_f)(int, const real_wp_[], real_wp_ *, const void *), int(*eval_g)(int, const real_wp_[], real_wp_ (], const void *), int(*eval_h)(int, int, const real_wp_[], real_wp_[], const void *), int(*eval_h)(int, const real_wp_[], real_wp_[], real_wp_[], const real_wp_[], const real_wp_[], const real_wp_[], const void *)
- void bgo_solve_without_mat (void **data, void *userdata, int *status, int n, real_wp_ x[], real_wp_ g[], int(*eval_f)(int, const real_wp_[], real_wp_ *, const void *), int(*eval_g)(int, const real_wp_[], real_wp_ [], const void *), int(*eval_hprod)(int, const real_wp_[], real_wp_[], const real_wp_[], bool, const void *), int(*eval_shprod)(int, const real_wp_[], int, const int[], const real_wp_[], int *, int[], real_wp_[], bool, const void *), int(*eval_prec)(int, const real_wp_[], real_wp_[], const real_wp_[], const void *))
- void bgo_solve_reverse_with_mat (void **data, int *status, int *eval_status, int n, real_wp_ x[], real_wp_ f, real_wp_ g[], int ne, real_wp_ H_val[], const real_wp_ u[], real_wp_ v[])
- void bgo_solve_reverse_without_mat (void **data, int *status, int *eval_status, int n, real_wp_ x[], real
 wp f, real_wp_ g[], real_wp_ u[], real_wp_ v[], int index_nz_v[], int *nnz_v, const int index_nz_u[], int
 nnz_u)
- void bgo_information (void **data, struct bgo_inform_type *inform, int *status)
- void bgo_terminate (void **data, struct bgo_control_type *control, struct bgo_inform_type *inform)

3.1.1 Data Structure Documentation

3.1.1.1 struct bgo_control_type

Examples

bgot.c, and bgotf.c.

Data Fields

bool	f_indexing	use C or Fortran sparse matrix indexing
int	error	error and warning diagnostics occur on stream error
int	out	general output occurs on stream out
int	print_level	the level of output required. Possible values are:
		$ullet$ \leq 0 no output,
		1 a one-line summary for every improvement
		2 a summary of each iteration
		$ullet \geq$ 3 increasingly verbose (debugging) output
int	attempts_max	the maximum number of random searches from the best point found so far
int	max_evals	the maximum number of function evaluations made
int	sampling_strategy	sampling strategy used. Possible values are
		1 uniformly spread
		2 Latin hypercube sampling
		3 niformly spread within a Latin hypercube
int	hypercube_discretization	hyper-cube discretization (for sampling stategies 2 and 3)
int	alive_unit	removal of the file alive_file from unit alive_unit terminates execution
char	alive_file[31]	see alive_unit
real_wp_	infinity	any bound larger than infinity in modulus will be regarded as infinite
real_wp_	obj_unbounded	the smallest value the objective function may take before the problem is marked as unbounded
real_wp_	cpu_time_limit	the maximum CPU time allowed (-ve means infinite)
real_wp_	clock_time_limit	the maximum elapsed clock time allowed (-ve means infinite)
bool	random_multistart	perform random-multistart as opposed to local minimize and probe
bool	hessian_available	is the Hessian matrix of second derivatives available or is access only via matrix-vector products?
bool	space_critical	if .space_critical true, every effort will be made to use as little space as possible. This may result in longer computation time
bool	deallocate_error_fatal	if .deallocate_error_fatal is true, any array/pointer deallocation error will terminate execution. Otherwise, computation will continue

Data Fields

char	prefix[31]	all output lines will be prefixed by .prefix(2:LEN(TRIM(.prefix))-1) where .prefix contains the required string enclosed in quotes, e.g. "string" or 'string'
struct ugo_control_type	ugo_control	control parameters for UGO
struct lhs_control_type	lhs_control	control parameters for LHS
struct trb_control_type	trb_control	control parameters for TRB

3.1.1.2 struct bgo_time_type

Data Fields

real_sp_	total	the total CPU time spent in the package
real_sp_	univariate_global	the CPU time spent performing univariate global optimization
real_sp_	multivariate_local	the CPU time spent performing multivariate local optimization
real_wp_	clock_total	the total clock time spent in the package
real_wp_ clock_univariate_global		the clock time spent performing univariate global optimization
real_wp_	clock_multivariate_local	the clock time spent performing multivariate local optimization

3.1.1.3 struct bgo_inform_type

Examples

bgot.c, and bgotf.c.

Data Fields

int	status	return status. See BGO_solve for details
int	alloc_status	the status of the last attempted allocation/deallocation
char	bad_alloc[81]	the name of the array for which an allocation/deallocation error
		occurred
int	f_eval	the total number of evaluations of the objective function
int	g_eval	the total number of evaluations of the gradient of the objective
		function
int	h_eval	the total number of evaluations of the Hessian of the objective
		function
real_wp_	obj	the value of the objective function at the best estimate of the
		solution determined by BGO_solve
real_wp_	norm_pg	the norm of the projected gradient of the objective function at the
		best estimate of the solution determined by BGO_solve
struct bgo_time_type	time	timings (see above)
struct ugo_inform_type	ugo_inform	inform parameters for UGO
struct lhs_inform_type	lhs_inform	inform parameters for LHS
struct trb_inform_type	trb_inform	inform parameters for TRB

3.1.2 Function Documentation

3.1.2.1 bgo_initialize()

Set default control values and initialize private data

Parameters

in,out	data	holds private internal data
out	control	is a struct containing control information (see bgo_control_type)
out	status	is a scalar variable of type int, that gives the exit status from the package. Possible values are (currently):
		0. The import was succesful.

Examples

bgot.c, and bgotf.c.

3.1.2.2 bgo_read_specfile()

Read the content of a specification file, and assign values associated with given keywords to the corresponding control parameters. By default, the spcification file will be named RUNBGO.SPC and lie in the current directory. Refer to Table 2.1 in the fortran documentation provided in \$GALAHAD/doc/bgo.pdf for a list of keywords that may be set.

Parameters

in,out	control	is a struct containing control information (see bgo_control_type)
in	specfile	is a character string containing the name of the specification file

3.1.2.3 bgo_import()

```
void bgo_import (
```

```
struct bgo_control_type * control,
void ** data,
int * status,
int n,
const real_wp_ x_1[],
const real_wp_ x_u[],
const char H_type[],
int ne,
const int H_row[],
const int H_col[],
const int H_ptr[])
```

Import problem data into internal storage prior to solution.

Parameters

in	control	is a struct whose members provide control paramters for the remaining prcedures (see bgo_control_type)
in,out	data	holds private internal data
in,out	status	is a scalar variable of type int, that gives the exit status from the package. Possible values are:
		1. The import was succesful, and the package is ready for the solve phase
		 -1. An allocation error occurred. A message indicating the offending array is written on unit control.error, and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -2. A deallocation error occurred. A message indicating the offending array is written on unit control.error and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -3. The restriction n > 0 or requirement that type contains its relevant string 'dense', 'coordinate', 'sparse_by_rows', 'diagonal' or 'absent' has been violated.
in	n	is a scalar variable of type int, that holds the number of variables.
in	x_I	is a one-dimensional array of size n and type double, that holds the values x^l of the lower bounds on the optimization variables x . The j-th component of x_l, $j=0,\ldots,n-1$, contains x_j^l .
in	x_u	is a one-dimensional array of size n and type double, that holds the values x^u of the upper bounds on the optimization variables x . The j-th component of x_u, $j=0,\ldots,n-1$, contains x_j^u .
in	H_type	is a one-dimensional array of type char that specifies the symmetric storage scheme used for the Hessian. It should be one of 'coordinate', 'sparse_by_rows', 'dense', 'diagonal' or 'absent', the latter if access to the Hessian is via matrix-vector products; lower or upper case variants are allowed.
in	ne	is a scalar variable of type int, that holds the number of entries in the lower triangular part of H in the sparse co-ordinate storage scheme. It need not be set for any of the other three schemes.
in	H_row	is a one-dimensional array of size ne and type int, that holds the row indices of the lower triangular part of H in the sparse co-ordinate storage scheme. It need not be set for any of the other three schemes, and in this case can be NULL
in	H_col	is a one-dimensional array of size ne and type int, that holds the column indices of the lower triangular part of H in either the sparse co-ordinate, or the sparse row-wise storage scheme. It need not be set when the dense or diagonal storage schemes are used, and in this case can be NULL

Parameters

in	H_ptr	is a one-dimensional array of size n+1 and type int, that holds the starting position of
		each row of the lower triangular part of H, as well as the total number of entries, in the
		sparse row-wise storage scheme. It need not be set when the other schemes are used,
		and in this case can be NULL

Examples

bgot.c, and bgotf.c.

3.1.2.4 bgo_reset_control()

Reset control parameters after import if required.

Parameters

in	control	is a struct whose members provide control paramters for the remaining prcedures (see
		bgo_control_type)
in,out	data	holds private internal data
in,out	status	is a scalar variable of type int, that gives the exit status from the package. Possible values are:
		1. The import was succesful, and the package is ready for the solve phase

3.1.2.5 bgo_solve_with_mat()

Find an approximation to the global minimizer of a given function subject to simple bounds on the variables using a multistart trust-region method.

This call is for the case where $H=\nabla_{xx}f(x)$ is provided specifically, and all function/derivative information is available by function calls.

Parameters

in,out	data	holds private internal data
in	userdata	is a structure that allows data to be passed into the function and derivative evaluation programs.
in,out	status	is a scalar variable of type int, that gives the entry and exit status from the package. On initial entry, status must be set to 1. Possible exit are:
		0. The run was succesful
		 -1. An allocation error occurred. A message indicating the offending array is written on unit control.error, and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -2. A deallocation error occurred. A message indicating the offending array is written on unit control.error and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -3. The restriction n > 0 or requirement that type contains its relevant string 'dense', 'coordinate', 'sparse_by_rows', 'diagonal' or 'absent' has been violated.
		 -7. The objective function appears to be unbounded from below
		 -9. The analysis phase of the factorization failed; the return status from the factorization package is given in the component inform.factor_status
		 -10. The factorization failed; the return status from the factorization package is given in the component inform.factor_status.
		 -11. The solution of a set of linear equations using factors from the factorization package failed; the return status from the factorization package is given in the component inform.factor_status.
		-16. The problem is so ill-conditioned that further progress is impossible.
		 -18. Too many iterations have been performed. This may happen if control.maxit is too small, but may also be symptomatic of a badly scaled problem.
		 -19. The CPU time limit has been reached. This may happen if control.cpu_time_limit is too small, but may also be symptomatic of a badly scaled problem.
		 -82. The user has forced termination of solver by removing the file named control.alive_file from unit unit control.alive_unit.
in	n	is a scalar variable of type int, that holds the number of variables
in,out	х	is a one-dimensional array of size n and type double, that holds the values x of the optimization variables. The j-th component of x, j = 0,, n-1, contains x_j .
in,out	g	is a one-dimensional array of size n and type double, that holds the gradient $g=\nabla_x f(x)$ of the objective function. The j-th component of g, j = 0,, n-1, contains g_j .

Parameters

in	ne	is a scalar variable of type int, that holds the number of entries in the lower triangular part of the Hessian matrix ${\cal H}$.
	eval_f	is a user-supplied function that must have the following signature:
	eval_g	is a user-supplied function that must have the following signature:
	eval_h	is a user-supplied function that must have the following signature: $\inf_{x \in \mathbb{R}^n} \exp \lim_{x \in \mathbb{R}^n} \exp \lim_{x$
	eval_prec	is an optional user-supplied function that may be NULL. If non-NULL, it must have the following signature: $ \begin{array}{l} \text{int eval_prec(int n, const double x[], double u[], const double v[], const } \\ \text{void *userdata)} \\ \hline \text{The product } u = P(x)v \text{ of the user's preconditioner } P(x) \text{ evaluated at } x \text{ with the } \\ \text{vector v} = v, \text{ the result } u \text{ must be retured in u, and the function return value set to 0.} \\ \text{If the evaluation is impossible at x, return should be set to a nonzero value. Data may be passed into eval_prec via the structure userdata.} \\ \hline \end{array} $

Examples

bgot.c, and bgotf.c.

3.1.2.6 bgo_solve_without_mat()

Find an approximation to the global minimizer of a given function subject to simple bounds on the variables using a multistart trust-region method.

This call is for the case where access to $H=\nabla_{xx}f(x)$ is provided by Hessian-vector products, and all function/derivative information is available by function calls.

Parameters

in,out	data	holds private internal data
in	userdata	is a structure that allows data to be passed into the function and derivative evaluation programs.
in,out	status	is a scalar variable of type int, that gives the entry and exit status from the package. On initial entry, status must be set to 1. Possible exit are:
		 0. The run was succesful -1. An allocation error occurred. A message indicating the offending array is written on unit control.error, and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -2. A deallocation error occurred. A message indicating the offending array is written on unit control error and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -3. The restriction n > 0 or requirement that type contains its relevant string 'dense', 'coordinate', 'sparse_by_rows', 'diagonal' or 'absent' has been violated.
		-7. The objective function appears to be unbounded from below
		-9. The analysis phase of the factorization failed; the return status from the factorization package is given in the component inform.factor_status
		-10. The factorization failed; the return status from the factorization package is given in the component inform.factor_status.
		 -11. The solution of a set of linear equations using factors from the factorization package failed; the return status from the factorization package is given in the component inform.factor_status.
		-16. The problem is so ill-conditioned that further progress is impossible.
		 -18. Too many iterations have been performed. This may happen if control.maxit is too small, but may also be symptomatic of a badly scaled problem.
		 -19. The CPU time limit has been reached. This may happen if control.cpu_time_limit is too small, but may also be symptomatic of a badly scaled problem.
		-82. The user has forced termination of solver by removing the file named control.alive_file from unit unit control.alive_unit.
in	n	is a scalar variable of type int, that holds the number of variables
in,out	Х	is a one-dimensional array of size n and type double, that holds the values x of the optimization variables. The j-th component of x, j = 0,, n-1, contains x_j .
in,out	g	is a one-dimensional array of size n and type double, that holds the gradient $g=\nabla_x f(x)$ of the objective function. The j-th component of g, j = 0,, n-1, contains g_j .

Parameters

	eval_f	is a user-supplied function that must have the following signature: int eval_f(int n, const double $x[]$, double $*f$, const void *userdata)
		The value of the objective function $f(x)$ evaluated at $\mathbf{x} = x$ must be assigned to \mathbf{f} ,
		and the function return value set to 0. If the evaluation is impossible at x, return
		should be set to a nonzero value. Data may be passed into ${\tt eval_f}$ via the
		structure userdata.
	eval_g	<pre>is a user-supplied function that must have the following signature: int eval_g(int n, const double x[], double g[], const void *userdata)</pre>
		The components of the gradient $g = \nabla_x f(x)$ of the objective function evaluated at
		x=x must be assigned to g, and the function return value set to 0. If the evaluation
		is impossible at x, return should be set to a nonzero value. Data may be passed
		into eval_g via the structure userdata.
	eval_hprod	<pre>is a user-supplied function that must have the following signature: int eval_hprod(int n, const double x[], double u[], const double v[], bool got_h, const void *userdata)</pre>
		The sum $u + \nabla_{xx} f(x)v$ of the product of the Hessian $\nabla_{xx} f(x)$ of the objective
		function evaluated at x= x with the vector v= v and the vector \$ u must be
		returned in u, and the function return value set to 0. If the evaluation is impossible
		at x, return should be set to a nonzero value. The Hessian has already been
		evaluated or used at x if got_h is true. Data may be passed into eval_hprod via
		the structure userdata.
	eval_shprod	<pre>is a user-supplied function that must have the following signature: int eval_shprod(int n, const double x[], int nnz_v, const int index_nz_v[],</pre>
		bool got_h, const void *userdata)
		The product $u = \nabla_{xx} f(x) v$ of the Hessian $\nabla_{xx} f(x)$ of the objective function
		evaluated at x with the sparse vector $\mathbf{v} = v$ must be returned in \mathbf{u} , and the function
		return value set to 0. Only the components index_nz_v[0:nnz_v-1] of v are
		nonzero, and the remaining components may not have been be set. On exit, the
		user must indicate the nnz_u indices of u that are nonzero in
		index_nz_u[0:nnz_u-1], and only these components of u need be set. If the
		evaluation is impossible at x, return should be set to a nonzero value. The Hessian
		has already been evaluated or used at x if got_h is true. Data may be passed into
		eval_prec via the structure userdata.
	eval_prec	is an optional user-supplied function that may be NULL. If non-NULL, it must have
		the following signature: int eval_prec(int n, const double x[], double u[], const double v[], const void *userdata)
		The product $u=P(x)v$ of the user's preconditioner $P(x)$ evaluated at x with the
		vector $\mathbf{v} = v$, the result u must be retured in \mathbf{u} , and the function return value set to
		0. If the evaluation is impossible at x, return should be set to a nonzero value.
1		Data may be passed into eval_prec via the structure userdata.

Examples

bgot.c, and bgotf.c.

3.1.2.7 bgo_solve_reverse_with_mat()

```
int * eval_status,
int n,
real_wp_ x[],
real_wp_ f,
real_wp_ g[],
int ne,
real_wp_ H_val[],
const real_wp_ u[],
real_wp_ v[])
```

Find an approximation to the global minimizer of a given function subject to simple bounds on the variables using a multistart trust-region method.

This call is for the case where $H=\nabla_{xx}f(x)$ is provided specifically, but function/derivative information is only available by returning to the calling procedure

Parameters

in,out	data	holds private internal data
--------	------	-----------------------------

Parameters

in,out	status	is a scalar variable of type int, that gives the entry and exit status from the package.
		On initial entry, status must be set to 1. Possible exit are:
		0. The run was succesful
		 -1. An allocation error occurred. A message indicating the offending array is written on unit control.error, and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -2. A deallocation error occurred. A message indicating the offending array is written on unit control.error and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -3. The restriction n > 0 or requirement that type contains its relevant string 'dense', 'coordinate', 'sparse_by_rows', 'diagonal' or 'absent' has been violated.
		-7. The objective function appears to be unbounded from below
		 -9. The analysis phase of the factorization failed; the return status from the factorization package is given in the component inform.factor_status
		 -10. The factorization failed; the return status from the factorization package is given in the component inform.factor_status.
		 -11. The solution of a set of linear equations using factors from the factorization package failed; the return status from the factorization package is given in the component inform.factor_status.
		-16. The problem is so ill-conditioned that further progress is impossible.
		 -18. Too many iterations have been performed. This may happen if control.maxit is too small, but may also be symptomatic of a badly scaled problem.
		 -19. The CPU time limit has been reached. This may happen if control.cpu_time_limit is too small, but may also be symptomatic of a badly scaled problem.
		-82. The user has forced termination of solver by removing the file named control.alive_file from unit unit control.alive_unit.

Parameters

status	(continued)
	• 2. The user should compute the objective function value $f(x)$ at the point x indicated in x and then re-enter the function. The required value should be set in f, and eval_status should be set to 0. If the user is unable to evaluate $f(x)$ — for instance, if the function is undefined at x — the user need not set f, but should then set eval_status to a non-zero value.
	• 3. The user should compute the gradient of the objective function $\nabla_x f(x)$ at the point x indicated in x and then re-enter the function. The value of the i-th component of the g radient should be set in g[i], for i = 0,, n-1 and eval_status should be set to 0. If the user is unable to evaluate a component of $\nabla_x f(x)$ — for instance if a component of the gradient is undefined at x -the user need not set g, but should then set eval_status to a non-zero value.
	• 4. The user should compute the Hessian of the objective function $\nabla_{xx}f(x)$ at the point x indicated in x and then re-enter the function. The value I-th component of the Hessian stored according to the scheme input in the remainder of H should be set in H_val[I], for I = 0,, ne-1 and eval_status should be set to 0. If the user is unable to evaluate a component of $\nabla_{xx}f(x)$ — for instance, if a component of the Hessian is undefined at x — the user need not set H_val, but should then set eval_status to a non-zero value.
	• 5. The user should compute the product $\nabla_{xx}f(x)v$ of the Hessian of the objective function $\nabla_{xx}f(x)$ at the point x indicated in x with the vector v , add the result to the vector u and then re-enter the function. The vectors u and v are given in u and v respectively, the resulting vector $u + \nabla_{xx}f(x)v$ should be set in u and eval_status should be set to 0. If the user is unable to evaluate the product— for instance, if a component of the Hessian is undefined at x — the user need not alter u, but should then set eval_status to a non-zero value.
	• 6. The user should compute the product $u=P(x)v$ of their preconditioner $P(x)$ at the point x indicated in x with the vector v and then re-enter the function. The vector v is given in v, the resulting vector $u=P(x)v$ should be set in u and eval_status should be set to 0. If the user is unable to evaluate the product— for instance, if a component of the preconditioner is undefined at x — the user need not set u, but should then set eval_status to a non-zero value.
	 23. The user should follow the instructions for 2 and 3 above before returning.
	 25. The user should follow the instructions for 2 and 5 above before returning.
	 35. The user should follow the instructions for 3 and 5 above before returning.
	 235. The user should follow the instructions for 2, 3 and 5 above before returning.
in,out <i>eval</i> _	tatus is a scalar variable of type int, that is used to indicate if objective function/gradient/Hessian values can be provided (see above)
in <i>n</i>	is a scalar variable of type int, that holds the number of variables
in, out X	is a one-dimensional array of size n and type double, that holds the values x of the optimization variables. The j-th component of x, j = 0,, n-1, contains x_j .
in f	is a scalar variable pointer of type double, that holds the value of the objective function.

Parameters

in,out	g	is a one-dimensional array of size n and type double, that holds the gradient $g=\nabla_x f(x)$ of the objective function. The j-th component of g, j = 0, , n-1, contains g_j .
in	ne	is a scalar variable of type int, that holds the number of entries in the lower triangular part of the Hessian matrix ${\cal H}.$
in	H_val	is a one-dimensional array of size ne and type double, that holds the values of the entries of the lower triangular part of the Hessian matrix ${\cal H}$ in any of the available storage schemes.
in	и	is a one-dimensional array of size n and type double, that is used for reverse communication (see above for details)
in,out	V	is a one-dimensional array of size n and type double, that is used for reverse communication (see above for details)

Examples

bgot.c, and bgotf.c.

3.1.2.8 bgo_solve_reverse_without_mat()

```
void bgo_solve_reverse_without_mat (
    void ** data,
    int * status,
    int * eval_status,
    int n,
    real_wp_ x[],
    real_wp_ f,
    real_wp_ g[],
    real_wp_ u[],
    real_wp_ v[],
    int index_nz_v[],
    int * nnz_v,
    const int index_nz_u[],
    int nnz_u)
```

Find an approximation to the global minimizer of a given function subject to simple bounds on the variables using a multistart trust-region method.

This call is for the case where access to $H=\nabla_{xx}f(x)$ is provided by Hessian-vector products, but function/derivative information is only available by returning to the calling procedure.

Parameters

in,out	data	holds private internal data
111,000	uaia	noise private internal data

Parameters

in,out	status	is a scalar variable of type int, that gives the entry and exit status from the package.
		On initial entry, status must be set to 1. Possible exit are:
		0. The run was succesful
		 -1. An allocation error occurred. A message indicating the offending array is written on unit control.error, and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -2. A deallocation error occurred. A message indicating the offending array is written on unit control.error and the returned allocation status and a string containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.
		 -3. The restriction n > 0 or requirement that type contains its relevant string 'dense', 'coordinate', 'sparse_by_rows', 'diagonal' or 'absent' has been violated.
		 -7. The objective function appears to be unbounded from below
		 -9. The analysis phase of the factorization failed; the return status from the factorization package is given in the component inform.factor_status
		 -10. The factorization failed; the return status from the factorization package is given in the component inform.factor_status.
		 -11. The solution of a set of linear equations using factors from the factorization package failed; the return status from the factorization package is given in the component inform.factor_status.
		-16. The problem is so ill-conditioned that further progress is impossible.
		 -18. Too many iterations have been performed. This may happen if control.maxit is too small, but may also be symptomatic of a badly scaled problem.
		 -19. The CPU time limit has been reached. This may happen if control.cpu_time_limit is too small, but may also be symptomatic of a badly scaled problem.
		 -82. The user has forced termination of solver by removing the file named control.alive_file from unit unit control.alive_unit.

Parameters

	status	(continued)
		• 2. The user should compute the objective function value $f(x)$ at the point x indicated in x and then re-enter the function. The required value should be set in f, and eval_status should be set to 0. If the user is unable to evaluate $f(x)$ — for instance, if the function is undefined at x — the user need not set f, but should then set eval_status to a non-zero value.
		• 3. The user should compute the gradient of the objective function $\nabla_x f(x)$ at the point x indicated in x and then re-enter the function. The value of the i-th component of the g radient should be set in g[i], for i = 0,, n-1 and eval_status should be set to 0. If the user is unable to evaluate a component of $\nabla_x f(x)$ — for instance if a component of the gradient is undefined at x -the user need not set g, but should then set eval_status to a non-zero value.
		• 5. The user should compute the product $\nabla_{xx}f(x)v$ of the Hessian of the objective function $\nabla_{xx}f(x)$ at the point x indicated in x with the vector v , add the result to the vector u and then re-enter the function. The vectors u and v are given in u and v respectively, the resulting vector $u + \nabla_{xx}f(x)v$ should be set in u and eval_status should be set to 0. If the user is unable to evaluate the product— for instance, if a component of the Hessian is undefined at x — the user need not alter u, but should then set eval_status to a non-zero value.
		• 6. The user should compute the product $u=P(x)v$ of their preconditioner $P(x)$ at the point x indicated in x with the vector v and then re-enter the function. The vector v is given in v, the resulting vector $u=P(x)v$ should be set in u and eval_status should be set to 0. If the user is unable to evaluate the product— for instance, if a component of the preconditioner is undefined at x — the user need not set u, but should then set eval_status to a non-zero value.
		• 7. The user should compute the product $u=\nabla_{xx}f(x)v$ of the Hessian of the objective function $\nabla_{xx}f(x)$ at the point x indicated in x with the sparse vector $\mathbf{v}=v$ and then re-enter the function. The nonzeros of v are stored in $\mathbf{v}[\text{index_nz_v}[0:\text{nnz_v-1}]]$ while the nonzeros of v should be returned in $\mathbf{v}[\text{index_nz_u}[0:\text{nnz_u-1}]]$; the user must set $\mathbf{nnz_u}$ and $\mathbf{index_nz_u}$ accordingly, and set \mathbf{v} eval_status to 0. If the user is unable to evaluate the product— for instance, if a component of the Hessian is undefined at v —the user need not alter v , but should then set v eval_status to a non-zero value.
		 23. The user should follow the instructions for 2 and 3 above before returning.
		 25. The user should follow the instructions for 2 and 5 above before returning.
		 35. The user should follow the instructions for 3 and 5 above before returning.
		 235. The user should follow the instructions for 2, 3 and 5 above before returning.
in,out	eval_status	is a scalar variable of type int, that is used to indicate if objective function/gradient/Hessian values can be provided (see above)
in	n	is a scalar variable of type int, that holds the number of variables
in,out	Х	is a one-dimensional array of size n and type double, that holds the values x of the optimization variables. The j-th component of x, j = 0,, n-1, contains x_j .

Parameters

in	f	is a scalar variable pointer of type double, that holds the value of the objective function.
in,out	g	is a one-dimensional array of size n and type double, that holds the gradient $g=\nabla_x f(x)$ of the objective function. The j-th component of g, j = 0,, n-1, contains g_j .
in,out	и	is a one-dimensional array of size n and type double, that is used for reverse communication (see status=5,6,7 above for details)
in,out	V	is a one-dimensional array of size n and type double, that is used for reverse communication (see status=5,6,7 above for details)
in,out	index_nz↔ _v	is a one-dimensional array of size n and type int, that is used for reverse communication (see status=7 above for details)
in,out	nnz_v	is a scalar variable of type int, that is used for reverse communication (see status=7 above for details)
in	index_nz↔ _u	s a one-dimensional array of size n and type int, that is used for reverse communication (see status=7 above for details)
in	nnz_u	is a scalar variable of type int, that is used for reverse communication (see status=7 above for details). On initial (status=1) entry, nnz_u should be set to an (arbitrary) nonzero value, and nnz_u=0 is recommended

Examples

bgot.c, and bgotf.c.

3.1.2.9 bgo_information()

Provides output information

Parameters

in,out	data	holds private internal data
out	inform	is a struct containing output information (see bgo_inform_type)
out	status	is a scalar variable of type int, that gives the exit status from the package. Possible values are (currently):
		0. The values were recorded succesfully

Examples

bgot.c, and bgotf.c.

3.1.2.10 bgo_terminate()

Deallocate all internal private storage

Parameters

in,out	data	holds private internal data
out	control	is a struct containing control information (see bgo_control_type)
out	inform	is a struct containing output information (see bgo_inform_type)

Examples

bgot.c, and bgotf.c.

Chapter 4

Example Documentation

4.1 bgot.c

This is an example of how to use the package to find an approximation to the global minimum of a given function within a bounded region. A variety of supported Hessian and constraint matrix storage formats are shown.

Notice that C-style indexing is used, and that this is flaggeed by setting control.f_indexing to false.

```
/* bgot.c */
/\star Full test for the BGO C interface using C sparse matrix indexing \star/
#include <stdio.h>
#include <math.h>
#include "galahad_precision.h"
#include "galahad_cfunctions.h"
#include "galahad_bgo.h"
// Custom userdata struct
struct userdata_type {
   real_wp_ p;
   real_wp_ freq;
   real_wp_ mag;
};
// Function prototypes
int fun( int n, const real_wp_ x[], real_wp_ *f, const void * );
int grad( int n, const real_wp_ x[], real_wp_ g[], const void * );
int hess( int n, int ne, const real_wp_ x[], real_wp_ hval[], const void * );
int hess_dense( int n, int ne, const real_wp_ x[], real_wp_ hval[], const void * );
int hessprod( int n, const real_wp_ x[], real_wp_ u[], const real_wp_ v[],
                 bool got_h, const void * );
int shessprod( int n, const real_wp_ x[], int nnz_v, const int index_nz_v[],
                  const real_wp_ v[], int *nnz_u, int index_nz_u[], real_wp_ u[],
bool got_h, const void * );
int prec(int n, const real_wp_ x[], real_wp_ u[], const real_wp_ v[], const void \star );
int fun_diag(int n, const real_wp_ x[], real_wp_ *f, const void * );
int grad_diag(int n, const real_wp_ x[], real_wp_ g[], const void * );
int hess_diag(int n, int ne, const real_wp_ x[], real_wp_ hval[], const void * );
int hessprod_diag( int n, const real_wp_ x[], real_wp_ u[], const real_wp_ v[],
                       bool got_h, const void * );
int shessprod_diag( int n, const real_wp_ x[], int nnz_v, const int index_nz_v[],
                         const real_wp_ v[], int *nnz_u, int index_nz_u[],
                         real_wp_ u[], bool got_h, const void * );
int main(void) {
     // Derived types
     void *data;
     struct bgo_control_type control;
     struct bgo_inform_type inform;
     // Set user data
     struct userdata_type userdata;
     userdata.p = 4.0;
     userdata.freq = 10;
userdata.mag = 1000;
    // Set problem data
int n = 3; // dimension
int ne = 5; // Hesssian elements
real_wp_ x_1[] = {-10,-10,-10};
real_wp_ x_u[] = {0.5,0.5,0.5};
```

```
int H_{row[]} = \{0, 1, 2, 2, 2\}; // Hessian H
int H_col[] = {0, 1, 0, 1, 2}; // NB lower triangle int H_ptr[] = {0, 1, 2, 5}; // row pointers
// Set storage
real_wp_ g[n]; // gradient
char st:
int status;
printf(" C sparse matrix indexing\n\n");
printf(" tests options for all-in-one storage format\n\n");
for(int d=1; d <= 5; d++) {
     // Initialize BGO</pre>
   bgo initialize ( &data, &control, &status );
    // Set user-defined control options
    control.f_indexing = false; // C sparse matrix indexing
    control.attempts_max = 10000;
    control.max_evals = 20000;
   control.sampling_strategy = 3;
control.trb_control.maxit = 100;
    //control.print_level = 1;
    // Start from 0
    real_wp_ x[] = \{0,0,0\};
    switch(d) {
       case 1: // sparse co-ordinate storage
    st = 'C';
            bgo_import( &control, &data, &status, n, x_1, x_u,
                        "coordinate", ne, H_row, H_col, NULL );
            bgo_solve_with_mat( &data, &userdata, &status, n, x, g,
                                ne, fun, grad, hess, hessprod, prec );
           break;
        case 2: // sparse by rows
st = 'R';
            bgo_solve_with_mat( &data, &userdata, &status, n, x, g,
                                ne, fun, grad, hess, hessprod, prec );
            break;
       case 3: // dense
st = 'D';
            bgo_import( &control, &data, &status, n, x_1, x_u,
            "dense", ne, NULL, NULL, NULL);
bgo_solve_with_mat( &data, &userdata, &status, n, x, g,
                                ne, fun, grad, hess_dense, hessprod, prec );
           break:
        case 4: // diagonal st = 'I';
            bgo_import( &control, &data, &status, n, x_l, x_u,
            hessprod_diag, prec );
           break;
        case 5: // access by products
            st = 'P';
            fun, grad, hessprod, shessprod, prec );
    // Record solution information
   bgo_information( &data, &inform, &status );
if(inform.status == 0){
       printf("%c:%6i evaluations. Optimal objective value = %5.2f"
          " status = %1i\n", st, inform.f_eval, inform.obj, inform.status);
    }else{
       printf("%c: BGO_solve exit status = %li\n", st, inform.status);
    //printf("x: ");
    //for(int i = 0; i < n; i++) printf("%f ", x[i]);
    //printf("\n");
    //printf("gradient: ");
    //for(int i = 0; i < n; i++) printf("%f ", g[i]);
    //printf("\n");
    // Delete internal workspace
    bgo_terminate( &data, &control, &inform );
printf("\n tests reverse-communication options\n\n");\\
// reverse-communication input/output
int eval_status, nnz_u, nnz_v;
real_wp_ f = 0.0;
real_wp_ u[n], v[n];
int index_nz_u[n], index_nz_v[n];
real_wp_ H_val[ne], H_dense[n*(n+1)/2], H_diag[n];
for (int d=1; d <= 5; d++) {</pre>
    // Initialize BGO
   bgo_initialize( &data, &control, &status );
```

GALAHAD 4.0

4.1 bgot.c 29

```
// Set user-defined control options
control.f_indexing = false; // C sparse matrix indexing
control.attempts_max = 10000;
control.max_evals = 20000;
control.sampling_strategy = 3;
control.trb_control.maxit = 100;
//control.print_level = 1;
// Start from 0
real_wp_ x[] = \{0,0,0\};
switch(d){
    case 1: // sparse co-ordinate storage
         st = 'C';
         bgo_import( &control, &data, &status, n, x_l, x_u,
                       "coordinate", ne, H_row, H_col, NULL );
         while (true) { // reverse-communication loop
             break;
              }else if(status < 0){ // error exit</pre>
                  break;
              }else if(status == 2){ // evaluate f
              eval_status = fun( n, x, &f, &userdata ); } else if(status == 3) { // evaluate g
                  eval_status = grad( n, x, q, &userdata );
              }else if(status == 4) { // evaluate H
                   eval_status = hess( n, ne, x, H_val, &userdata );
              }else if(status == 5){ // evaluate Hv product
                   eval_status = hessprod( n, x, u, v, false, &userdata );
              }else if(status == 6){ // evaluate the product with P
    eval_status = prec( n, x, u, v, &userdata );
}else if(status == 23){ // evaluate f and g
                   eval_status = fun( n, x, &f, &userdata );
              eval_status = grad( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
    eval_status = fun( n, x, &f, &userdata );
              eval_status = hessprod( n, x, u, v, false, &userdata );
}else if(status == 35){ // evaluate g and Hv product
                   eval_status = grad( n, x, g, &userdata );
              eval_status = hesprod( n, x, u, v, false, &userdata }else if(status == 235){ // evaluate f, g and Hv product
                   eval_status = fun( n, x, &f, &userdata );
                   eval_status = grad( n, x, g, &userdata );
                   eval_status = hessprod( n, x, u, v, false, &userdata );
                  printf(" the value %1i of status should not occur\n",
                          status );
                  break:
              }
         break;
    case 2: // sparse by rows
         st = 'R';
         while(true){ // reverse-communication loop
              bgo_solve_reverse_with_mat( &data, &status, &eval_status,
                                               n, x, f, g, ne, H_val, u, v);
              if(status == 0){ // successful termination
                  break;
              }else if(status < 0){ // error exit</pre>
                  break;
              }else if(status == 2){ // evaluate f
              eval_status = fun( n, x, &f, &userdata );
}else if(status == 3){ // evaluate g
                   eval_status = grad( n, x, g, &userdata );
              }else if(status == 4){ // evaluate H
                   eval_status = hess( n, ne, x, H_val, &userdata );
              }else if(status == 5){ // evaluate Hv product
                   eval_status = hessprod( n, x, u, v, false, &userdata );
              }else if(status == 6){ // evaluate the product with P
              eval_status = prec( n, x, u, v, &userdata );
}else if(status == 23){ // evaluate f and g
  eval_status = fun( n, x, &f, &userdata );
              eval_status = grad( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
                   eval_status = fun( n, x, &f, &userdata );
                   eval_status = hessprod( n, x, u, v, false, &userdata );
              }else if(status == 35){ // evaluate g and Hv product
                   eval\_status = grad(n, x, g, &userdata);
              eval_status = prau( n, x, y, auserdata /, eval_status = hessprod( n, x, u, v, false, &userdata ); }else if(status == 235){ // evaluate f, g and Hv product
                   eval_status = fun( n, x, &f, &userdata );
                   eval_status = grad( n, x, g, &userdata );
                   eval_status = hessprod( n, x, u, v, false, &userdata );
              }else{
                   printf(" the value %1i of status should not occur\n",
```

```
status);
            break;
        }
    break:
case 3: // dense
st = 'D';
    bgo_import( &control, &data, &status, n, x_1, x_u,
                 "dense", ne, NULL, NULL, NULL );
    while(true){ // reverse-communication loop
        bgo_solve_reverse_with_mat( &data, &status, &eval_status, n, x, f, g, n*(n+1)/2,
                                       H_dense, u, v);
         if(status == 0){ // successful termination
         }else if(status < 0){ // error exit</pre>
            break:
         }else if(status == 2){ // evaluate f
            eval_status = fun( n, x, &f, &userdata );
         }else if(status == 3){ // evaluate g
             eval_status = grad( n, x, g, &userdata );
         }else if(status == 4){ // evaluate H
             eval_status = hess_dense( n, n*(n+1)/2, x, H_dense,
                                         &userdata ):
         }else if(status == 5){ // evaluate Hv product
            eval_status = hessprod( n, x, u, v, false, &userdata );
         }else if(status == 6){ // evaluate the product with P
         eval_status = prec( n, x, u, v, &userdata );
}else if(status == 23){ // evaluate f and g
             eval_status = fun( n, x, &f, &userdata );
         eval_status = grad( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
             eval_status = fun( n, x, &f, &userdata );
             eval\_status = hessprod(n, x, u, v, false, &userdata);
         }else if(status == 35){ // evaluate g and Hv product
             eval_status = grad( n, x, g, &userdata );
         eval_status = hessprod(n, x, u, v, false, &userdata);
}else if(status == 235){ // evaluate f, g and Hv product
             eval_status = fun( n, x, &f, &userdata );
             eval_status = grad( n, x, g, &userdata );
             eval_status = hessprod( n, x, u, v, false, &userdata );
         lelse(
            printf(" the value %1i of status should not occur\n",
                   status);
             break;
    break;
case 4: // diagonal
    st = 'I';
    bgo_import( &control, &data, &status, n, x_1, x_u,
                 "diagonal", ne, NULL, NULL, NULL);
    while(true) { // reverse-communication loop
        break;
         }else if(status < 0){ // error exit</pre>
            break;
         }else if(status == 2){ // evaluate f
             eval\_status = fun\_diag(n, x, &f, &userdata);
         }else if(status == 3) { // evaluate g
            eval_status = grad_diag( n, x, g, &userdata );
         }else if(status == 4){ // evaluate H
             eval_status = hess_diag( n, n, x, H_diag, &userdata );
         }else if(status == 5){ // evaluate Hv product
             eval_status = hessprod_diag( n, x, u, v, false,
                                            &userdata );
         }else if(status == 6) { // evaluate the product with P
         eval_status = prec( n, x, u, v, &userdata );
}else if(status == 23){ // evaluate f and g
             eval\_status = fun\_diag(n, x, &f, &userdata);
         eval_status = grad_diag( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
             eval_status = fun_diag( n, x, &f, &userdata );
             eval_status = hessprod_diag( n, x, u, v, false,
                                            &userdata );
         }else if(status == 35){ // evaluate g and Hv product
             eval\_status = grad\_diag(n, x, g, &userdata);
             eval_status = hessprod_diag( n, x, u, v, false,
                                            &userdata );
         }else if(status == 235) { // evaluate f, g and Hv product
             eval_status = fun_diag( n, x, &f, &userdata );
             eval_status = grad_diag( n, x, g, &userdata );
             eval\_status = hessprod\_diag(n, x, u, v, false,
                                            &userdata ):
         }else{
```

4.1 bgot.c 31

printf(" the value %1i of status should not occur $\n"$,

```
status);
                             break:
                       }
                   break:
              case 5: // access by products
                   st = 'P';
                   bgo_import( &control, &data, &status, n, x_l, x_u,
                                  "absent", ne, NULL, NULL, NULL);
                   nnz u = 0:
                   while(true){ // reverse-communication loop
                       bgo_solve_reverse_without_mat( &data, &status, &eval_status, n, x, f, g, u, v, index_nz_v, &nnz_v, index_nz_u, nnz_u );
                        if(status == 0){ // successful termination
                            break:
                        }else if(status < 0){ // error exit</pre>
                            break;
                        }else if(status == 2){ // evaluate f
                        eval_status = fun( n, x, &f, &userdata );
}else if(status == 3){ // evaluate g
                             eval\_status = grad(n, x, g, &userdata);
                        }else if(status == 5) { // evaluate Hv product
                            eval_status = hessprod( n, x, u, v, false, &userdata );
                        }else if(status == 6){ // evaluate the product with P
                             eval_status = prec( n, x, u, v, &userdata );
                        }else if(status == 7){ // evaluate sparse Hess-vect product
                             eval_status = shessprod( n, x, nnz_v, index_nz_v, v,
                                                           &nnz_u, index_nz_u, u,
                        false, &userdata );
}else if(status == 23){ // evaluate f and g
                             eval_status = fun( n, x, &f, &userdata );
                        eval_status = grad( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
    eval_status = fun( n, x, &f, &userdata );
                        eval_status = hessprod( n, x, u, v, false, &userdata );
}else if(status == 35){ // evaluate g and Hv product
                             eval_status = grad( n, x, g, &userdata );
                        eval_status = hesprod( n, x, u, v, false, &userdata }else if(status == 235){ // evaluate f, g and Hv product
                             eval_status = fun( n, x, &f, &userdata );
                             eval_status = grad( n, x, g, &userdata );
                             eval_status = hessprod( n, x, u, v, false, &userdata );
                            printf(" the value %1i of status should not occur\n",
                                    status);
                             break:
                        }
                   break;
         // Record solution information
         bgo_information( &data, &inform, &status );
         if (inform.status == 0) {
              printf("%c:%6i evaluations. Optimal objective value = %5.2f"
                  status = %1i\n", st, inform.f_eval, inform.obj, inform.status);
              printf("%c: BGO_solve exit status = %li\n", st, inform.status);
         //printf("x: "):
         //for(int i = 0; i < n; i++) printf("%f ", x[i]);
         //printf("\n");
          //printf("gradient: ");
          //for(int i = 0; i < n; i++) printf("%f ", g[i]);
          //printf("\n");
          // Delete internal workspace
         bgo_terminate( &data, &control, &inform );
// Objective function
int fun( int n,
          const real_wp_ x[],
          real_wp_ *f,
const void *userdata ) {
    struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ p = myuserdata->p;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
     \begin{array}{lll} \text{Teal\_wp\_ mag - myuserdata-/mag;} \\ \text{*f = pow}(x[0] + x[2] + p, 2) + pow(x[1] + x[2], 2) + mag * cos(freq*x[0]) \\ & + x[0] + x[1] + x[2]; \end{array} 
    return 0;
// Gradient of the objective
int grad( int n,
            const real_wp_ x[],
            real_wp_ g[],
```

```
const void *userdata ) {
     struct userdata_type *myuserdata = (struct userdata_type *) userdata;
     real_wp_ p = myuserdata->p;
    real_wp_ freq = myuserdata->freq;

real_wp_ mag = myuserdata->mag;

g[0] = 2.0 * (x[0] + x[2] + p) - mag * freq * sin(freq*x[0]) + 1;

g[1] = 2.0 * (x[1] + x[2]) + 1;
     g[2] = 2.0 * (x[0] + x[2] + p) + 2.0 * (x[1] + x[2]) + 1;
     return 0;
}
// Hessian of the objective
int hess( int n,
            int ne,
            const real_wp_ x[],
            real_wp_ hval[],
           const void *userdata ){
     struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
     hval[0] = 2.0 - mag * freq * freq * cos(freq*x[0]);
    hval[1] = 2.0;
hval[2] = 2.0;
     hval[3] = 2.0;
     hval[4] = 4.0;
    return 0;
// Dense Hessian
int hess_dense( int n,
                   int ne.
                   const real_wp_ x[],
                   real_wp_ hval[],
const void *userdata ){
     struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
     hval[0] = 2.0 - mag * freq * freq * cos(freq*x[0]);
     hval[1] = 0.0;
     hval[2] = 2.0;
     hval[3] = 2.0;
    hval[4] = 2.0;

hval[5] = 4.0;
     return 0;
// Hessian-vector product
int hessprod( int n,
                const real_wp_ x[],
                real_wp_ u[],
                const real_wp_ v[],
                bool got_h,
    const void *userdata ) {
struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
     u[0] = u[0] + 2.0 * (v[0] + v[2])
    return 0;
// Sparse Hessian-vector product
int nnz_v,
const int index_nz_v[],
                  const real_wp_ v[],
                  int *nnz u.
                  int index_nz_u[],
                  real_wp_ u[],
                  bool got_h,
     const void *userdata ) {
struct userdata_type *myuserdata = (struct userdata_type *) userdata;
     real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
real_wp_ p[] = {0., 0., 0.};
     bool used[] = {false, false, false};
     for(int i = 0; i < nnz_v; i++) {
   int j = index_nz_v[i];</pre>
         switch(j){
              case 0:
                   p[0] = p[0] + 2.0 * v[0] - mag * freq * freq * cos(freq*x[0]) * v[0];
                   used[0] = true;
                   p[2] = p[2] + 2.0 * v[0];
used[2] = true;
                   break:
```

4.1 bgot.c 33

```
case 1:
                     p[1] = p[1] + 2.0 * v[1];
                     used[1] = true;
p[2] = p[2] + 2.0 * v[1];
used[2] = true;
                     break:
                case 2:
                     p[0] = p[0] + 2.0 * v[2];
                     used[0] = true;
                     used[0] - true;
p[1] = p[1] + 2.0 * v[2];
used[1] = true;
p[2] = p[2] + 4.0 * v[2];
used[2] = true;
          }
     *nnz_u = 0;
for(int j = 0; j < 3; j++){</pre>
          if(used[j]){
          u[j] = p[j];
*nnz_u = *nnz_u + 1;
          index_nz_u[*nnz_u-1] = j;
     return 0;
// Apply preconditioner
int prec( int n,
            const real_wp_ x[],
            real_wp_ u[],
const real_wp_ v[],
const void *userdata ){
   u[0] = 0.5 * v[0];
u[1] = 0.5 * v[1];
   u[2] = 0.25 * v[2];
   return 0;
// Objective function
int fun_diag( int n,
                 const real_wp_ x[],
     real_wp_ *f,
    const void *userdata ) {
struct userdata_type *myuserdata = (struct userdata_type *) userdata;
     real_wp_ p = myuserdata->p;
     real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
*f = pow(x[2] + p, 2) + pow(x[1], 2) + mag * cos(freq*x[0])
          + x[0] + x[1] + x[2];
     return 0:
// Gradient of the objective
int grad_diag( int n,
                   const real_wp_ x[],
     real_wp_ p = myuserdata->p;
     real_wp_ freq = myuserdata->freq;
    real_wp_ mag = myuserdata->mag;

g[0] = -mag * freq * sin(freq*x[0]) + 1;

g[1] = 2.0 * x[1] + 1;

g[2] = 2.0 * (x[2] + p) + 1;
     return 0;
// Hessian of the objective
int hess_diag( int n,
                   int ne,
                    const real_wp_ x[],
                   real_wp_ hval[],
const void *userdata ){
     struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
hval[0] = -mag * freq * freq * cos(freq*x[0]);
hval[1] = 2.0;
     hval[2] = 2.0;
     return 0;
// Hessian-vector product
int hessprod_diag( int n,
                         const real_wp_ x[],
                         real_wp_ u[],
                         const real_wp_ v[],
                         bool got_h,
     const void *userdata ) {
struct userdata_type *myuserdata = (struct userdata_type *) userdata;
     real_wp_ freq = myuserdata->freq;
```

```
real_wp_ mag = myuserdata->mag;
     u[0] = u[0] + -mag * freq * freq * cos(freq*x[0]) * v[0];
u[1] = u[1] + 2.0 * v[1];
u[2] = u[2] + 2.0 * v[2];
     return 0:
// Sparse Hessian-vector product
int shessprod_diag( int n,
                           const real_wp_ x[],
                          int nnz_v,
const int index_nz_v[],
                           const real_wp_ v[],
                           int *nnz u,
                           int index_nz_u[],
                           real_wp_ u[],
     struct userdata_type *myuserdata = (:
real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
real_wp_ p[] = {0., 0., 0.);
bool used[] = {false, false, false};
for(int i = 0; i < nnz_v; i++) {
   int j = index_nz_v[i];
   switch(i);</pre>
          switch(j){
              case 0:
                     p[0] = p[0] - mag * freq * freq * cos(freq*x[0]) * v[0];
                     used[0] = true;
                     break;
                case 1:
                     p[1] = p[1] + 2.0 * v[1];
                     used[1] = true;
                     break;
                case 2:
                     p[2] = p[2] + 2.0 * v[2];
used[2] = true;
                     break;
          }
     *nnz_u = 0;
     for(int j = 0; j < 3; j++){
          if(used[j]){
          u[j] = p[j];
*nnz_u = *nnz_u + 1;
          index_nz_u[*nnz_u-1] = j;
     return 0;
```

4.2 bgotf.c

This is the same example, but now fortran-style indexing is used.

```
/\star Full test for the BGO C interface using Fortran sparse matrix indexing \star/
#include <stdio.h>
#include <math.h>
#include "galahad_precision.h"
#include "galahad_cfunctions.h"
#include "galahad_bgo.h"
// Custom userdata struct
struct userdata_type {
  real_wp_ p;
   real_wp_ freq;
  real_wp_ mag;
};
// Function prototypes
int fun( int n, const real_wp_ x[], real_wp_ *f, const void * );
int hessprod( int n, const real_wp_ x[], real_wp_ u[], const real_wp_ v[],
              bool got_h, const void * );
int shessprod( int n, const real_wp_ x[], int nnz_v, const int index_nz_v[],
               const real_wp_ v[], int *nnz_u, int index_nz_u[], real_wp_ u[],
bool got_h, const void * );
int prec( int n, const real_wp_ x[], real_wp_ u[], const real_wp_ v[], const void * );
int fun_diag( int n, const real_wp_ x[], real_wp_ *f, const void * );
```

4.2 bgotf.c 35

```
int hessprod_diag( int n, const real_wp_ x[], real_wp_ u[], const real_wp_ v[],
const real_wp_ v[], int *nnz_u, int index_nz_u[],
                      real_wp_ u[], bool got_h, const void * );
int main(void) {
    // Derived types
    void *data:
    struct bgo_control_type control;
struct bgo_inform_type inform;
    // Set user data
    struct userdata_type userdata;
    userdata.p = 4.0;
userdata.freq = 10;
userdata.mag = 1000;
   // Set problem data
int n = 3; // dimension
int ne = 5; // Hesssian elements
real_wp_ x_1[] = {-10,-10,-10};
real_wp_ x_u[] = {0.5,0.5,0.5};
int H_row[] = {1, 2, 3, 3, 3}; // Hessian H
int H_col[] = {1, 2, 1, 2, 3}; // NB lower triangle
int H ptr[] = {1, 2, 3, 6}; // row pointers
    // Set storage
    real_wp_ g[n]; // gradient
    char st:
    int status:
    printf("Fortran sparse matrix indexing\n^{n});
printf("tests options for all-in-one storage format\n^{n});
    for(int d=1; d <= 5; d++) {
         // Initialize BGO
        bgo_initialize( &data, &control, &status );
        // Set user-defined control options control.f_indexing = true; // Fortran sparse matrix indexing
         control.attempts_max = 10000;
         control.max_evals = 20000;
        control.sampling_strategy = 3;
control.trb_control.maxit = 100;
        //control.print_level = 1;
         // Start from 0
        real_wp_ x[] = \{0,0,0\};
         switch(d){
             case 1: // sparse co-ordinate storage
    st = 'C';
                 bgo_import( &control, &data, &status, n, x_1, x_u,
                               "coordinate", ne, H_row, H_col, NULL );
                 bgo_solve_with_mat( &data, &userdata, &status, n, x, g,
                                       ne, fun, grad, hess, hessprod, prec );
                 break;
             case 2: // sparse by rows
st = 'R';
                 bgo_solve_with_mat( &data, &userdata, &status, n, x, g,
                                       ne, fun, grad, hess, hessprod, prec );
             break;
case 3: // dense
st = 'D';
                 bgo_import( &control, &data, &status, n, x_l, x_u,
                 "dense", ne, NULL, NULL, NULL);
bgo_solve_with_mat( &data, &userdata, &status, n, x, g,
                                       ne, fun, grad, hess_dense, hessprod, prec );
             break;
case 4: // diagonal
st = 'I';
                 ne, fun_diag, grad_diag, hess_diag,
                                        hessprod_diag, prec );
                 break;
             case 5: // access by products
                 st = 'P';
                 fun, grad, hessprod, shessprod, prec );
                 break;
         // Record solution information
        bgo_information( &data, &inform, &status );
         if(inform.status == 0){
             printf("%c:%6i evaluations. Optimal objective value = %5.2f"
```

```
" status = %1i\n", st, inform.f_eval, inform.obj, inform.status);
    }else{
        printf("%c: BGO_solve exit status = %li\n", st, inform.status);
    //printf("x: "):
    //for(int i = 0; i < n; i++) printf("%f ", x[i]);
    //printf("\n");
    //printf("gradient: ");
     //for(int i = 0; i < n; i++) printf("%f ", g[i]);
    //printf("\n");
    // Delete internal workspace
    bgo_terminate( &data, &control, &inform );
printf("\n tests reverse-communication options\n\n");
// reverse-communication input/output
int eval_status, nnz_u, nnz_v;
real_wp_ f = 0.0;
real_wp_ u[n], v[n];
int index_nz_u[n], index_nz_v[n];
real_wp_ H_val[ne], H_dense[n*(n+1)/2], H_diag[n];
for(int d=1; d <= 5; d++) {
    // Initialize BGO
    bgo initialize ( &data, &control, &status );
    // Set user-defined control options
    control.f_indexing = true; // Fortran sparse matrix indexing
    control.attempts_max = 10000;
    control.max_evals = 20000;
    control.sampling_strategy = 3;
control.trb_control.maxit = 100;
    //control.print_level = 1;
    // Start from 0
    real_wp_ x[] = \{0,0,0\};
    switch(d) {
        case 1: // sparse co-ordinate storage
    st = 'C';
             bgo_import( &control, &data, &status, n, x_1, x_u,
                           "coordinate", ne, H_row, H_col, NULL );
             while(true){ // reverse-communication loop
                  bgo_solve_reverse_with_mat( &data, &status, &eval_status,
                                                 n, x, f, g, ne, H_val, u, v);
                  if(status == 0) { // successful termination
                      break:
                  }else if(status < 0){ // error exit</pre>
                      break;
                  }else if(status == 2){ // evaluate f
                  eval_status = fun( n, x, &f, &userdata );
}else if(status == 3){ // evaluate g
                      eval_status = grad( n, x, g, &userdata );
                  }else if(status == 4){ // evaluate H
                      eval_status = hess( n, ne, x, H_val, &userdata );
                  }else if(status == 5){ // evaluate Hv product
                      eval\_status = hessprod(n, x, u, v, false, &userdata);
                  }else if(status == 6){ // evaluate the product with P
    eval_status = prec( n, x, u, v, &userdata );
}else if(status == 23){ // evaluate f and g
                      eval_status = fun( n, x, &f, &userdata );
                  eval_status = grad( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
                      eval_status = fun( n, x, &f, &userdata );
                  eval_status = hessprod( n, x, u, v, false, &userdata );
}else if(status == 35){ // evaluate g and Hv product
                      eval_status = grad( n, x, g, &userdata );
                  eval_status = hesprod( n, x, u, v, false, &userdata }else if(status == 235) { // evaluate f, g and Hv product
                      eval\_status = fun(n, x, &f, &userdata);
                      eval_status = grad( n, x, g, &userdata );
eval_status = hessprod( n, x, u, v, false, &userdata );
                  }else{
                      printf(" the value %1i of status should not occur\n",
                             status );
                      break;
                  }
             break;
         case 2: // sparse by rows
             st = 'R';
             bgo_solve_reverse_with_mat( &data, &status, &eval_status,
                                                  n, x, f, g, ne, H_val, u, v);
                  if(status == 0) { // successful termination
                      break;
                  }else if(status < 0){ // error exit</pre>
                      break:
                  }else if(status == 2){ // evaluate f
```

GALAHAD 4.0

4.2 bgotf.c 37

```
eval_status = fun( n, x, &f, &userdata );
}else if(status == 3){ // evaluate g
              eval_status = grad( n, x, g, &userdata );
         }else if(status == 4){ // evaluate H
         eval_status = hess( n, ne, x, H_val, &userdata );
}else if(status == 5){ // evaluate Hv product
              eval_status = hessprod( n, x, u, v, false, &userdata );
         }else if(status == 6){ // evaluate the product with P
         eval_status = prec( n, x, u, v, &userdata );
}else if(status == 23){ // evaluate f and g
              eval_status = fun( n, x, &f, &userdata );
         eval_status = grad( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
              eval_status = fun( n, x, &f, &userdata );
              eval_status = hessprod( n, x, u, v, false, &userdata );
         }else if(status == 35){ // evaluate g and Hv product
              eval_status = grad( n, x, g, &userdata );
         eval_status = hessprod(n, x, u, v, false, &userdata);

}else if(status == 235){ // evaluate f, g and Hv product
              eval_status = fun( n, x, &f, &userdata );
              eval_status = grad( n, x, g, &userdata );
              eval_status = hessprod( n, x, u, v, false, &userdata );
         lelse(
              printf(" the value %1i of status should not occur\n",
                     status);
    break;
case 3: // dense
st = 'D';
    bgo_import( &control, &data, &status, n, x_1, x_u,
                   "dense", ne, NULL, NULL, NULL);
    while(true){ // reverse-communication loop
         \label{eq:bgo_solve_reverse_with_mat} bgo\_solve\_reverse\_with\_mat( &data, &status, &eval\_status, \\ n, x, f, g, n*(n+1)/2,
                                           H dense, u, v );
         if(status == 0){ // successful termination
              break;
         }else if(status < 0){ // error exit</pre>
              break:
         }else if(status == 2){ // evaluate f
         eval_status = fun( n, x, &f, &userdata );
}else if(status == 3){ // evaluate g
              eval_status = grad( n, x, g, &userdata );
         }else if(status == 4){ // evaluate H
              eval_status = hess_dense( n, n*(n+1)/2, x, H_dense,
                                             &userdata );
         }else if(status == 5) { // evaluate Hv product
              eval_status = hessprod( n, x, u, v, false, &userdata );
         }else if(status == 6){ // evaluate the product with P
         eval_status = prec( n, x, u, v, &userdata );
}else if(status == 23){ // evaluate f and g
              eval_status = fun( n, x, &f, &userdata );
         eval_status = grad( n, x, g, &userdata );
eval_status = grad( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
              eval_status = fun( n, x, &f, &userdata );
              eval_status = hessprod( n, x, u, v, false, &userdata );
         }else if(status == 35){ // evaluate g and Hv product
              eval\_status = grad(n, x, g, &userdata);
         eval_status = hesprod(n, x, u, v, false, &userdata);
}else if(status == 235){ // evaluate f, g and Hv product
              eval_status = fun( n, x, &f, &userdata );
              eval_status = grad( n, x, g, &userdata );
              eval_status = hessprod( n, x, u, v, false, &userdata );
         }else{
              printf(" the value %1i of status should not occur\n",
              status);
break;
         }
    break;
case 4: // diagonal
   st = 'I';
    while(true){ // reverse-communication loop
         bgo_solve_reverse_with_mat( &data, &status, &eval_status,
          n, \ x, \ f, \ g, \ n, \ H\_diag, \ u, \ v \ ); \\  \mbox{if(status == 0){ // successful termination} } 
             break;
         }else if(status < 0){ // error exit</pre>
              break;
         }else if(status == 2){ // evaluate f
              eval\_status = fun\_diag(n, x, &f, &userdata);
         }else if(status == 3){ // evaluate g
              eval_status = grad_diag( n, x, g, &userdata );
```

```
}else if(status == 4){ // evaluate H
                   eval_status = hess_diag( n, n, x, H_diag, &userdata );
              }else if(status == 5) { // evaluate Hv product
                   eval_status = hessprod_diag( n, x, u, v, false,
                                                      &userdata );
              }else if(status == 6) { // evaluate the product with P
              eval_status = prec( n, x, u, v, &userdata );
}else if(status == 23){ // evaluate f and g
                   eval_status = fun_diag( n, x, &f, &userdata );
              eval_status = grad_diag( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
                   eval_status = fun_diag( n, x, &f, &userdata );
                   eval_status = hessprod_diag( n, x, u, v, false,
                                                      &userdata );
              }else if(status == 35){ // evaluate g and Hv product
                   eval_status = grad_diag( n, x, g, &userdata );
eval_status = hessprod_diag( n, x, u, v, false,
                                                      &userdata );
              }else if(status == 235){ // evaluate f, g and Hv product
                   eval_status = fun_diag( n, x, &f, &userdata );
                   eval_status = grad_diag( n, x, g, &userdata );
                   eval_status = hessprod_diag( n, x, u, v, false,
                                                      &userdata );
                   printf(" the value %1i of status should not occur\n",
                          status);
                   break:
         break:
    case 5: // access by products
    st = 'P';
         bgo_import( &control, &data, &status, n, x_1, x_u,
                        "absent", ne, NULL, NULL, NULL);
         nnz_u = 0;
         while(true){ // reverse-communication loop
              bgo_solve_reverse_without_mat( &data, &status, &eval_status, n, x, f, g, u, v, index_nz_v, &nnz_v, index_nz_u, nnz_u );
              if(status == 0){ // successful termination
                   break;
              }else if(status < 0){ // error exit</pre>
                  break:
              }else if(status == 2){ // evaluate f
              eval_status = fun( n, x, &f, &userdata );
}else if(status == 3){ // evaluate g
              eval_status = grad( n, x, g, &userdata );
}else if(status == 5) { // evaluate Hv product
                   eval_status = hessprod( n, x, u, v, false, &userdata );
              }else if(status == 6){ // evaluate the product with P
                   eval_status = prec( n, x, u, v, &userdata );
              }else if(status == 7) { // evaluate sparse Hess-vect product
                   eval_status = shessprod( n, x, nnz_v, index_nz_v, v,
                                                  &nnz_u, index_nz_u, u,
              false, &userdata );
}else if(status == 23){ // evaluate f and g
                   eval_status = fun( n, x, &f, &userdata );
              eval_status = grad( n, x, g, &userdata );
}else if(status == 25){ // evaluate f and Hv product
                   eval_status = fun( n, x, &f, &userdata );
              eval_status = hessprod( n, x, u, v, false, &userdata );
}else if(status == 35){ // evaluate g and Hv product
                   eval_status = grad( n, x, g, &userdata );
              eval_status = hesprod( n, x, u, v, false, &userdata }else if(status == 235) { // evaluate f, g and Hv product
                   eval\_status = fun(n, x, &f, &userdata);
                   eval_status = grad( n, x, g, &userdata );
eval_status = hessprod( n, x, u, v, false, &userdata );
              }else{
                  printf(" the value %li of status should not occur\n",
                          status);
                   break;
              }
         break;
// Record solution information
bgo_information( &data, &inform, &status );
if (inform.status == 0) {
    printf("%c:%6i evaluations. Optimal objective value = %5.2f"
        'status = 1i\n'', st, inform.f_eval, inform.obj, inform.status);
   printf("%c: BGO_solve exit status = %li\n", st, inform.status);
//printf("x: ");
//for(int i = 0; i < n; i++) printf("%f ", x[i]);
//printf("\n");
```

GALAHAD 4.0

4.2 bgotf.c 39

```
//printf("gradient: ");
         //for(int i = 0; i < n; i++) printf("%f ", g[i]);
//printf("\n");
         // Delete internal workspace
         bgo_terminate( &data, &control, &inform );
// Objective function
int fun( int n,
          const real_wp_ x[],
          real_wp_ *f,
          const void *userdata ) {
    struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ p = myuserdata->p;
    real_wp_ freq = myuserdata->freq;
    real_wp_ mag = myuserdata->mag;

*f = pow(x[0] + x[2] + p, 2) + pow(x[1] + x[2], 2) + mag * cos(freq*x[0]) + x[0] + x[1] + x[2];
// Gradient of the objective
int grad( int n,
           const real_wp_ x[],
           real_wp_ g[],
const void *userdata ) {
    struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ p = myuserdata->p;
    real_wp_ freq = myuserdata->freq;

real_wp_ mag = myuserdata->freq;

real_wp_ mag = myuserdata->mag;

g[0] = 2.0 * (x[0] + x[2] + p) - mag * freq * sin(freq*x[0]) + 1;

g[1] = 2.0 * (x[1] + x[2]) + 1;
    g[2] = 2.0 * (x[0] + x[2] + p) + 2.0 * (x[1] + x[2]) + 1;
    return 0;
// Hessian of the objective
int hess( int n,
           int ne,
           const real_wp_ x[],
           real_wp_ hval[],
           const void *userdata ) {
    struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
    hval[0] = 2.0 - mag * freq * freq * cos(freq*x[0]);
    hval[1] = 2.0;
    hval[2] = 2.0;
    hval[3] = 2.0;
    hval[4] = 4.0;
    return 0;
// Dense Hessian
int hess_dense( int n,
                  int ne,
                  const real_wp_ x[],
                  real_wp_ hval[],
const void *userdata ){
    struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
    hval[0] = 2.0 - mag * freq * freq * cos(freq*x[0]);
    hval[1] = 0.0;
    hval[2] = 2.0;
    hval[3] = 2.0;
    hval[4] = 2.0;
hval[5] = 4.0;
    return 0:
// Hessian-vector product
int hessprod( int n,
                const real_wp_ x[],
                real_wp_ u[],
                const real_wp_ v[],
                bool got h,
                const void *userdata ) {
    struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
    u[0] = u[0] + 2.0 * (v[0] + v[2])
    return 0;
// Sparse Hessian-vector product
```

```
int shessprod( int n,
                      const real_wp_ x[],
                      int nnz_v,
const int index_nz_v[],
                      const real_wp_ v[],
                      int *nnz_u,
int index_nz_u[],
                      real_wp_ u[],
                      bool got_h,
                      const void *userdata ){
     struct userdata_type *myuserdata = (struct userdata_type *) userdata;
     real_wp_ freq = myuserdata->freq;
     real_wp_ freq = myuserdata->ireq;
real_wp_ mag = myuserdata->mag;
real_wp_ p[] = {0., 0., 0.);
bool used[] = {false, false, false};
for(int i = 0; i < nnz_v; i++) {
   int j = index_nz_v[i];
   owitch(i);</pre>
           switch(j){
                 case 1:
                      p[0] = p[0] + 2.0 * v[0]
                       - mag * freq * freq * cos(freq*x[0]) * v[0];
used[0] = true;
                       p[2] = p[2] + 2.0 * v[0];
used[2] = true;
                       break;
                  case 2:
                       p[1] = p[1] + 2.0 * v[1];
                       used[1] = true;
                       p[2] = p[2] + 2.0 * v[1];
used[2] = true;
                       break:
                  case 3:
                      p[0] = p[0] + 2.0 * v[2];
                       used[0] = true;
                       used[0] - true;
p[1] = p[1] + 2.0 * v[2];
used[1] = true;
p[2] = p[2] + 4.0 * v[2];
used[2] = true;
                       break;
           }
     *nnz u = 0;
     for(int j = 0; j < 3; j++) {
           if(used[j]){
           u[j] = p[j];
*nnz_u = *nnz_u + 1;
           index_nz_u[*nnz_u-1] = j+1;
           }
     }
     return 0;
// Apply preconditioner
int prec( int n,
              const real_wp_ x[],
              real_wp_ u[],
const real_wp_ v[],
const void *userdata ) {
    u[0] = 0.5 * v[0];
    u[1] = 0.5 * v[1];
    u[2] = 0.25 * v[2];
    return 0;
// Objective function
int fun_diag( int n,
                    const real_wp_ x[],
                    real_wp_ *f,
     const void *userdata ) {
struct userdata_type *myuserdata = (struct userdata_type *) userdata;
     real_wp_ p = myuserdata->p;
     real_wp_ freq = myuserdata->freq;
     real_wp_ mag = myuserdata->mag;

*f = pow(x[2] + p, 2) + pow(x[1], 2) + mag * cos(freq*x[0])
            + x[0] + x[1] + x[2];
     return 0:
// Gradient of the objective
int grad_diag( int n,
                      const real_wp_ x[],
     real_wp_ g[],
    const void *userdata ) {
struct userdata_type *myuserdata = (struct userdata_type *) userdata;
     struct userdata_type *myuserdata = (structureal_wp_ p = myuserdata->p;
real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
g[0] = -mag * freq * sin(freq*x[0]) + 1;
g[1] = 2.0 * x[1] + 1;
g[2] = 2.0 * (x[2] + p) + 1;
```

GALAHAD 4.0

4.2 bgotf.c 41

```
return 0;
// Hessian of the objective
int hess_diag( int n,
                 int ne,
                  const real_wp_ x[],
                  real_wp_ hval[],
                  const void *userdata ) {
    struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
hval[0] = -mag * freq * freq * cos(freq*x[0]);
hval[1] = 2.0;
    hval[2] = 2.0;
    return 0;
// Hessian-vector product
int hessprod_diag( int n,
                      const real_wp_ x[],
                       real_wp_ u[],
                       const real_wp_ v[],
    bool got_h,
const void *userdata ) {
struct userdata_type *myuserdata = (struct userdata_type *) userdata;
    real_wp_ freq = myuserdata->freq;
real_wp_ mag = myuserdata->mag;
    u[0] = u[0] + -mag * freq * freq * cos(freq*x[0]) * v[0];

u[1] = u[1] + 2.0 * v[1];

u[2] = u[2] + 2.0 * v[2];
    return 0;
// Sparse Hessian-vector product
int shessprod_diag( int n, const real_wp_ x[],
                        int nnz_v,
const int index_nz_v[],
                        const real_wp_ v[],
                        int *nnz_u,
                        int index_nz_u[],
                        real_wp_ u[],
    bool used[] = {false, false, false};
for(int i = 0; i < nnz_v; i++) {
   int j = index_nz_v[i];</pre>
         switch(j){
             case 1:
                   p[0] = p[0] - mag * freq * freq * cos(freq*x[0]) * v[0];
                   used[0] = true;
                   break;
              case 2:
                   p[1] = p[1] + 2.0 * v[1];
                   used[1] = true;
                   break;
              case 3:
p[2] = p[2] + 2.0 * v[2];
                   used[2] = true;
                   break;
         }
     *nnz_u = 0;
    for(int j = 0; j < 3; j++){
         if(used[j]){
         u[j] = p[j];
*nnz_u = *nnz_u + 1;
         index_nz_u[*nnz_u-1] = j+1;
    return 0;
```