



GALAHAD

BLLS

USER DOCUMENTATION

GALAHAD Optimization Library version 3.3

1 SUMMARY

This package uses a preconditioned, projected-gradient method to solve the **bound-constrained linear least-squares problem**

$$\text{minimize } q(\mathbf{x}) = \frac{1}{2} \|\mathbf{Ax} - \mathbf{b}\|_2^2$$

subject to the simple bound constraints

$$x_j^l \leq x_j \leq x_j^u, \quad j = 1, \dots, n,$$

where the m by n real matrix \mathbf{A} , and the vectors \mathbf{b} , \mathbf{x}^l , \mathbf{x}^u are given. Any of the constraint bounds x_j^l and x_j^u may be infinite. Full advantage is taken of any zero coefficients of the Jacobian matrix \mathbf{A} of the **residuals** $\mathbf{c}(\mathbf{x}) = \mathbf{Ax} - \mathbf{b}$; the matrix need not be provided as there are options to obtain matrix-vector products involving \mathbf{A} and its transpose either by reverse communication or from a user-provided subroutine.

ATTRIBUTES — Versions: GALAHAD_BLLS_single, GALAHAD_BLLS_double. **Uses:** GALAHAD_CPU_time, GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_SBLS, GALAHAD_QPT, GALAHAD_SPECFILE. **Date:** November 2009. **Origin:** N. I. M. Gould, Rutherford Appleton Laboratory. **Language:** Fortran 95 + TR 15581 or Fortran 2003.

2 HOW TO USE THE PACKAGE

Access to the package requires a `USE` statement such as

Single precision version

```
USE GALAHAD_BLLS_single
```

Double precision version

```
USE GALAHAD_BLLS_double
```

If it is required to use both modules at the same time, the derived types `SMT_type`, `QPT_problem_type`, `NLPT_userdata_type`, `BLLS_time_type`, `BLLS_control_type`, `BLLS_inform_type` and `BLLS_data_type` (Section 2.2) and the subroutines `BLLS_initialize`, `BLLS_solve`, `BLLS_terminate`, (Section 2.3) and `BLLS_read_specfile` (Section 2.7) must be renamed on one of the `USE` statements.

2.1 Matrix storage formats

When it is explicitly available, the coefficient matrix \mathbf{A} may be stored in a variety of input formats.

2.1.1 Dense row-wise storage format

The matrix \mathbf{A} 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. Component $n * (i - 1) + j$ of the storage array `A%val` will hold the value $A_{i,j}$ for $i = 1, \dots, m$, $j = 1, \dots, n$.

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2.1.2 Dense column-wise storage format

The matrix \mathbf{A} is stored as a compact dense matrix by columns, that is, the values of the entries of each column in turn are stored in order within an appropriate real one-dimensional array. Component $m * (j - 1) + i$ of the storage array `A%val` will hold the value $\mathbf{A}_{i,j}$ for $i = 1, \dots, m$, $j = 1, \dots, n$.

2.1.3 Sparse co-ordinate storage format

Only the nonzero entries of the matrices are stored. For the l -th entry of \mathbf{A} , its row index i , column index j and value \mathbf{A}_{ij} are stored in the l -th components of the integer arrays `A%row`, `A%col` and real array `A%val`. The order is unimportant, but the total number of entries `A%ne` is required.

2.1.4 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 \mathbf{A} , the i -th component of the integer array `A%ptr` holds the position of the first entry in this row, while `A%ptr (m + 1)` holds the total number of entries plus one. The column indices j and values \mathbf{A}_{ij} of the entries in the i -th row are stored in components $l = \text{A\%ptr}(i), \dots, \text{A\%ptr}(i + 1) - 1$ of the integer array `A%col`, and real array `A%val`, respectively.

2.1.5 Sparse column-wise storage format

Yet again only the nonzero entries are stored, but this time they are ordered so that those in column j appear directly before those in column $j + 1$. For the j -th column of \mathbf{A} , the j -th component of the integer array `A%ptr` holds the position of the first entry in this column, while `A%ptr (n + 1)` holds the total number of entries plus one. The row indices i and values \mathbf{A}_{ij} of the entries in the j -th column are stored in components $l = \text{A\%ptr}(j), \dots, \text{A\%ptr}(j + 1) - 1$ of the integer array `A%row`, and real array `A%val`, respectively.

For sparse matrices, the row- and column-wise storage schemes almost always requires less storage than their predecessor.

2.2 The derived data types

Ten derived data types are accessible from the package.

2.2.1 The derived data type for holding matrices

The derived data type `SMT_TYPE` is used to hold the matrix \mathbf{A} . The components of `SMT_TYPE` used here are:

- `m` is a scalar component of type default `INTEGER`, that holds the number of rows in the matrix.
- `n` is a scalar component of type default `INTEGER`, that holds the number of columns in the matrix.
- `ne` is a scalar variable of type default `INTEGER`, that holds the number of matrix entries.
- `type` is a rank-one allocatable array of type default `CHARACTER`, that is used to indicate the matrix storage scheme used. Its precise length and content depends on the type of matrix to be stored (see §2.2.2).
- `val` is a rank-one allocatable array of type default `REAL` (double precision in `GALAHAD_BLLS_double`) and dimension at least `ne`, that holds the values of the entries. Any duplicated entries that appear in the sparse co-ordinate or row-wise schemes will be summed.

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- `row` is a rank-one allocatable array of type default `INTEGER`, and dimension at least `ne`, that may hold the row indices of the entries. (see §2.1.3 and §2.1.5).
- `col` is a rank-one allocatable array of type default `INTEGER`, and dimension at least `ne`, that may hold the column indices of the entries (see §2.1.3–2.1.4).
- `ptr` is a rank-one allocatable array of type default `INTEGER`, and dimension at least `m + 1`, that may hold the pointers to the first entry in each row (see §2.1.4). or dimension at least `n + 1`, that may hold the pointers to the first entry in each column (see §2.1.5).

2.2.2 The derived data type for holding the problem

The derived data type `QPT_problem_type` is used to hold the problem. The components of `QPT_problem_type` are:

- `n` is a scalar variable of type default `INTEGER`, that holds the number of optimization variables, n .
- `m` is a scalar variable of type default `INTEGER`, that holds the number of residuals, m .
- `A` is scalar variable of type `SMT_TYPE` that holds the Jacobian matrix **A** of the residuals (if it is available). The following components are used here:

`A%type` is an allocatable array of rank one and type default `CHARACTER`, that is used to indicate the storage scheme used. If the dense row-wise storage scheme (see Section 2.1.1) is used, the first thirteen components of `A%type` must contain the string `DENSE_BY_ROW`, while if the column-wise scheme (see Section 2.1.2) is used, the sixteen components of `A%type` must contain the string `DENSE_BY_COLUMN`. For the sparse co-ordinate scheme (see Section 2.1.3), the first ten components of `A%type` must contain the string `COORDINATE`, for the sparse row-wise storage scheme (see Section 2.1.4), the first fourteen components of `A%type` must contain the string `SPARSE_BY_ROWS`. and for the sparse column-wise storage scheme (see Section 2.1.5), the first seventeen components of `A%type` must contain the string `SPARSE_BY_COLUMNS`.

For convenience, the procedure `SMT_put` may be used to allocate sufficient space and insert the required keyword into `A%type`. For example, if `nlp` is of derived type `BLLS_problem_type` and involves a Jacobian we wish to store using the co-ordinate scheme, we may simply

```
CALL SMT_put( nlp%A%type, 'COORDINATE' )
```

See the documentation for the GALAHAD package `SMT` for further details on the use of `SMT_put`.

- `A%ne` is a scalar variable of type default `INTEGER`, that holds the number of entries in **J** in the sparse co-ordinate storage scheme (see Section 2.1.3). It need not be set for any of the other three schemes.
- `A%val` is a rank-one allocatable array of type default `REAL` (double precision in `GALAHAD-BLLS_double`), that holds the values of the entries of the Jacobian matrix **A** in any of the storage schemes discussed in Section 2.1.
- `A%row` is a rank-one allocatable array of type default `INTEGER`, that holds the row indices of **A** in the sparse co-ordinate storage scheme (see Section 2.1.3). It need not be allocated for any of the other three schemes.
- `A%col` is a rank-one allocatable array variable of type default `INTEGER`, that holds the column indices of **A** in either the sparse co-ordinate (see Section 2.1.3), or the sparse row-wise (see Section 2.1.4) storage scheme. It need not be allocated when the dense or column-wise storage schemes are used.
- `A%row` is a rank-one allocatable array variable of type default `INTEGER`, that holds the row indices of **A** in either the sparse co-ordinate (see Section 2.1.3), or the sparse column-wise (see Section 2.1.5) storage scheme. It need not be allocated when the dense or row-wise storage schemes are used.

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- `A%ptr` is a rank-one allocatable array and type default `INTEGER`, that must be of dimension $m+1$ and hold the starting position of each row of \mathbf{A} , as well as the total number of entries plus one, in the sparse row-wise storage scheme (see Section 2.1.4). If the sparse column-wise storage scheme (see Section 2.1.5) is used, it must instead be of dimension $n+1$ and hold the starting position of each column of \mathbf{A} , as well as the total number of entries plus one. It need not be allocated when the other schemes are used.
- `B` is a rank-one allocatable array of dimension m and type default `REAL` (double precision in `GALAHAD_BLLS_`-double), that holds the constant term \mathbf{b} in the residuals. The i -th component of `B`, $i = 1, \dots, m$, contains \mathbf{b}_i .
- `C` is a rank-one allocatable array of dimension m and type default `REAL` (double precision in `GALAHAD_BLLS_`-double), that holds the residuals, $\mathbf{c}(\mathbf{x}) = \mathbf{Ax} - \mathbf{b}$, at the point \mathbf{x} . The i -th component of `C`, $i = 1, \dots, m$, contains $\mathbf{c}_i(\mathbf{x})$.
- `G` is a rank-one allocatable array of dimension n and type default `REAL` (double precision in `GALAHAD_BLLS_`-double), that holds the gradient of the objective $\mathbf{g}(\mathbf{x}) = \mathbf{A}^T \mathbf{c}(\mathbf{x})$, at the point \mathbf{x} . The j -th component of `G`, $j = 1, \dots, n$, contains $\mathbf{g}_j(\mathbf{x})$.
- `X_l` is a rank-one allocatable array of dimension n and type default `REAL` (double precision in `GALAHAD_BLLS_`-double), that holds the vector of lower bounds \mathbf{x}^l on the variables. The j -th component of `X_l`, $j = 1, \dots, n$, contains \mathbf{x}_j^l . Infinite bounds are allowed by setting the corresponding components of `X_l` to any value smaller than `-infinity`, where `infinity` is a component of the control array `control` (see Section 2.2.3).
- `X_u` is a rank-one allocatable array of dimension n and type default `REAL` (double precision in `GALAHAD_BLLS_`-double), that holds the vector of upper bounds \mathbf{x}^u on the variables. The j -th component of `X_u`, $j = 1, \dots, n$, contains \mathbf{x}_j^u . Infinite bounds are allowed by setting the corresponding components of `X_u` to any value larger than `infinity`, where `infinity` is a component of the control array `control` (see Section 2.2.3).
- `X` is a rank-one allocatable array of dimension n and type default `REAL` (double precision in `GALAHAD_BLLS_`-double), that holds the values \mathbf{x} of the optimization variables. The j -th component of `X`, $j = 1, \dots, n$, contains x_j .
- `Z` is a rank-one allocatable array of dimension n and type default `REAL` (double precision in `GALAHAD_BLLS_`-double), that holds the values \mathbf{z} of estimates of the dual variables corresponding to the simple bound constraints (see Section 4). The j -th component of `Z`, $j = 1, \dots, n$, contains z_j .

2.2.3 The derived data type for holding control parameters

The derived data type `BLLS_control_type` is used to hold controlling data. Default values may be obtained by calling `BLLS_initialize` (see Section 2.3.1), while components may also be changed by calling `BLLS_read_specfile` (see Section 2.7.1). The components of `BLLS_control_type` are:

- `error` is a scalar variable of type default `INTEGER`, that holds the stream number for error messages. Printing of error messages in `BLLS_solve` and `BLLS_terminate` is suppressed if `error` ≤ 0 . The default is `error` = 6.
- `out` is a scalar variable of type default `INTEGER`, that holds the stream number for informational messages. Printing of informational messages in `BLLS_solve` is suppressed if `out` < 0 . The default is `out` = 6.
- `print_level` is a scalar variable of type default `INTEGER`, that is used to control the amount of informational output which is required. No informational output will occur if `print_level` ≤ 0 . If `print_level` = 1, a single line of output will be produced for each iteration of the process. If `print_level` ≥ 2 , this output will be increased to provide significant detail of each iteration. The default is `print_level` = 0.
- `start_print` is a scalar variable of type default `INTEGER`, that specifies the first iteration for which printing will be permitted in `GALAHAD_BLLS_solve`. If `start_print` is negative, printing will be permitted from the outset. The default is `start_print` = -1.

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`stop_print` is a scalar variable of type default INTEGER, that specifies the last iteration for which printing will be permitted in `GALAHAD_BLLS_solve`. If `stop_print` is negative, printing will be permitted once it has been started by `start_print`. The default is `stop_print = -1`.

`print_gap` is a scalar variable of type default INTEGER. Once printing has been started, output will occur once every `print_gap` iterations. If `print_gap` is no larger than 1, printing will be permitted on every iteration. The default is `print_gap = 1`.

`maxit` is a scalar variable of type default INTEGER, that holds the maximum number of iterations which will be allowed in `GALAHAD_BLLS_solve`. The default is `maxit = 1000`.

`cg_maxit` is a scalar variable of type default INTEGER, that holds the maximum number of conjugate-gradient iterations which will be allowed per main iteration in `GALAHAD_BLLS_solve`. The default is `cg_maxit = 1000`.

`infinity` is a scalar variable of type default REAL (double precision in `GALAHAD_BLLS_double`), that is used to specify which constraint bounds are infinite. Any bound larger than `infinity` in modulus will be regarded as infinite. The default is `infinity = 1019`.

`stop_p` is a scalar variable of type default REAL (double precision in `GALAHAD_BLLS_double`), that holds the required accuracy for the primal infeasibility (see Section 4). The default is `stop_p = $u^{1/3}$` , where u is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_BLLS_double`).

`stop_d` is a scalar variable of type default REAL (double precision in `GALAHAD_BLLS_double`), that holds the required accuracy for the dual infeasibility (see Section 4). The default is `stop_d = $u^{1/3}$` , where u is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_BLLS_double`).

`stop_c` is a scalar variable of type default REAL (double precision in `GALAHAD_BLLS_double`), that holds the required accuracy for the violation of complementarity slackness (see Section 4). The default is `stop_c = $u^{1/3}$` , where u is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_BLLS_double`).

`identical_bounds_tol` is a scalar variable of type default REAL (double precision in `GALAHAD_BLLS_double`). Each pair of variable bounds (x_j^l, x_j^u) that is closer than `identical_bounds_tol` will be reset to the average of their values, $\frac{1}{2}(x_j^l + x_j^u)$. The default is `identical_bounds_tol = u` , where u is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_BLLS_double`).

`stop_cg_relative` and `stop_cg_absolute` are scalar variables of type default REAL (double precision in `GALAHAD_BLLS_double`), that hold the relative and absolute convergence tolerances for the conjugate-gradient iteration that occurs in the face of currently-active constraints when constructing the search direction. `_stop_cg_relative = 0.01` and `stop_cg_absolute = \sqrt{u}` , where u is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_BLLS_double`).

`zero_curvature` is a scalar variable of type default REAL (double precision in `GALAHAD_BLLS_double`) that specifies the threshold below which any constraint curvature encountered is regarded as zero. The default is `zero_curvature = $10u$` , where u is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_BLLS_double`).

`cpu_time_limit` is a scalar variable of type default REAL (double precision in `GALAHAD_BLLS_double`), that is used to specify the maximum permitted CPU time. Any negative value indicates no limit will be imposed. The default is `cpu_time_limit = -1.0`.

`exact_gcp` is a scalar variable of type default LOGICAL, that should be set `.TRUE.` if the exact generalized Cauchy point, the first estimate of the minimizer of the objective in the Cauchy direction within the feasible box, is required, and `.FALSE.` if an approximation suffices. The default is `exact_gcp = .TRUE..`

`space_critical` is a scalar variable of type default LOGICAL, that must be set `.TRUE.` if space is critical when allocating arrays and `.FALSE.` otherwise. The package may run faster if `space_critical` is `.FALSE.` but at the possible expense of a larger storage requirement. The default is `space_critical = .FALSE..`

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`deallocate_error_fatal` is a scalar variable of type default LOGICAL, that must be set `.TRUE.` if the user wishes to terminate execution if a deallocation fails, and `.FALSE.` if an attempt to continue will be made. The default is `deallocate_error_fatal = .FALSE..`

`prefix` is a scalar variable of type default CHARACTER and length 30, that may be used to provide a user-selected character string to preface every line of printed output. Specifically, each line of output will be prefaced by the string `prefix(2:LEN(TRIM(prefix))-1)`, thus ignoring the first and last non-null components of the supplied string. If the user does not want to preface lines by such a string, they may use the default `prefix = ""`.

`SBLS_control` is a scalar variable of type `SBLS_control_type` whose components are used to control the factorization and/or preconditioner used, performed by the package `GALAHAD_SBLS`. See the documentation for `GALAHAD_SBLS` for further details.

2.2.4 The derived data type for holding timing information

The derived data type `BLLS_time_type` is used to hold elapsed CPU times for the various parts of the calculation. The components of `BLLS_time_type` are:

`total` is a scalar variable of type default REAL, that gives the total time spent in the package.

`analyse` is a scalar variable of type default REAL, that gives the time spent analysing the required matrices prior to factorization.

`factorize` is a scalar variable of type default REAL, that gives the time spent factorizing the required matrices.

`solve` is a scalar variable of type default REAL, that gives the time spent computing the search direction.

2.2.5 The derived data type for holding informational parameters

The derived data type `BLLS_inform_type` is used to hold parameters that give information about the progress and needs of the algorithm. The components of `BLLS_inform_type` are:

`status` is a scalar variable of type default INTEGER, that gives the exit status of the algorithm. See Section 2.6 for details.

`alloc_status` is a scalar variable of type default INTEGER, that gives the status of the last attempted array allocation or deallocation. This will be 0 if `status = 0`.

`bad_alloc` is a scalar variable of type default CHARACTER and length 80, that gives the name of the last internal array for which there were allocation or deallocation errors. This will be the null string if `status = 0`.

`factorization_status` is a scalar variable of type default INTEGER, that gives the return status from the matrix factorization.

`iter` is a scalar variable of type default INTEGER, that gives the number of iterations performed.

`obj` is a scalar variable of type default REAL (double precision in `GALAHAD_BLLS_double`), that holds the value of the objective function at the best estimate of the solution found.

`time` is a scalar variable of type `BLLS_time_type` whose components are used to hold elapsed CPU times for the various parts of the calculation (see Section 2.2.4).

`SBLS_inform` is a scalar variable of type `SBLS_inform_type` whose components provide information about the progress and needs of the factorization/preconditioner performed by the package `GALAHAD_SBLS`. See the documentation for `GALAHAD_SBLS` for further details.

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2.2.6 The derived data type for holding problem data

The derived data type `BLLS_data_type` is used to hold all the data for a particular problem, or sequences of problems with the same structure, between calls of BLLS procedures. This data should be preserved, untouched, from the initial call to `BLLS_initialize` to the final call to `BLLS_terminate`.

2.2.7 The derived data type for holding user data

The derived data type `NLPT_userdata_type` is available to allow the user to pass data to and from user-supplied matrix-vector product and preconditioning subroutines (see Section 2.4). Components of variables of type `NLPT_userdata_type` may be allocated as necessary. The following components are available:

`integer` is a rank-one allocatable array of type default `INTEGER`.

`real` is a rank-one allocatable array of type default `REAL` (double precision in `GALAHAD_BLLS_double`)

`complex` is a rank-one allocatable array of type default `COMPLEX` (double precision complex in `GALAHAD_BLLS_double`).

`character` is a rank-one allocatable array of type default `CHARACTER`.

`logical` is a rank-one allocatable array of type default `LOGICAL`.

`integer_pointer` is a rank-one pointer array of type default `INTEGER`.

`real_pointer` is a rank-one pointer array of type default `REAL` (double precision in `GALAHAD_BLLS_double`)

`complex_pointer` is a rank-one pointer array of type default `COMPLEX` (double precision complex in `GALAHAD_BLLS_double`).

`character_pointer` is a rank-one pointer array of type default `CHARACTER`.

`logical_pointer` is a rank-one pointer array of type default `LOGICAL`.

2.2.8 The derived data type for holding reverse-communication data

The derived data type `BLLS_reverse_type` is used to hold data needed for reverse communication when this is required. The components of `BLLS_reverse_type` are:

`nz_v_start` is a scalar variable of type default `INTEGER`, that may be used to hold the starting position in `NZ_v` (see below) of the list of indices of nonzero components of `v`.

`nz_v_end` is a scalar variable of type default `INTEGER`, that may be used to hold the finishing position in `NZ_v` (see below) of the list of indices of nonzero components of `v`.

`NZ_v` is a rank-one allocatable array of dimension n and type default `INTEGER`, that may be used to hold the indices of the nonzero components of `v`. If used, components `NZ_v(nz_v_start:nz_v_end)` of `V` (see below) will be nonzero.

`V` is a rank-one allocatable array of dimension n and type default `REAL` (double precision in `GALAHAD_BLLS_double`), that is used to hold the components of the output vector `v`.

`P` is a rank-one allocatable array of dimension m and type default `REAL` (double precision in `GALAHAD_BLLS_double`), that is used to record the components of the resulting vector `Av`.

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`nz_p_end` is a scalar variable of type default `INTEGER`, that is used to record the finishing position in `NZ_p` (see below) of the list of indices of nonzero components of $\mathbf{A}\mathbf{v}$ if required.

`NZ_p` is a rank-one allocatable array of dimension n and type default `INTEGER`, that is used to record the list of indices of nonzero components of $\mathbf{A}\mathbf{v}$ if required. Components `NZ_p(1:nz_prod_end)` of `P` should then be nonzero.

2.3 Argument lists and calling sequences

There are three procedures for user calls (see Section 2.7 for further features):

1. The subroutine `BLLS_initialize` is used to set default values, and initialize private data, before solving one or more problems with the same sparsity and bound structure.
2. The subroutine `BLLS_solve` is called to solve the problem.
3. The subroutine `BLLS_terminate` is provided to allow the user to automatically deallocate array components of the private data, allocated by `BLLS_solve`, at the end of the solution process.

We use square brackets `[]` to indicate `OPTIONAL` arguments.

2.3.1 The initialization subroutine

Default values are provided as follows:

```
CALL BLLS_initialize( data, control )
```

`data` is a scalar `INTENT(INOUT)` argument of type `BLLS_data_type` (see Section 2.2.6). It is used to hold data about the problem being solved.

`control` is a scalar `INTENT(OUT)` argument of type `BLLS_control_type` (see Section 2.2.3). On exit, `control` contains default values for the components as described in Section 2.2.3. These values should only be changed after calling `BLLS_initialize`.

2.3.2 The bound-constrained linear least-squares subroutine

The bound-constrained linear least-squares solution algorithm is called as follows:

```
CALL BLLS_solve( prob, X_stat, data, control, inform, userdata[, reverse, &
                 eval_APROD, eval_ASPROD] )
```

`prob` is a scalar `INTENT(INOUT)` argument of type `QPT_problem_type` (see Section 2.2.2). It is used to hold data about the problem being solved. The user must allocate and set values for the array components, and set values for the components `prob%B`, `prob%X_l`, `prob%X_u` and `prob%X`. Additionally, the user can provide \mathbf{A} by allocating the relevant array components and setting values for `prob%A` using whichever of the matrix formats described in Section 2.1 is appropriate for the user's application; if the effect of \mathbf{A} and its transpose are only available to form products via reverse communication (see `reverse` below) or with a pair of user-supplied subroutines (see `eval_APROD` and `eval_ASPROD` below), `prob%A` is not needed.

The components `prob%X` must be set to initial estimates of the primal variables, \mathbf{x} . Inappropriate initial values will be altered, so the user should not be overly concerned if suitable values are not apparent, and may be content with merely setting `prob%X=0.0`. The components `prob%C` and `prob%G` need not be set or allocated on entry.

On exit, the components `prob%X` and `prob%Z` will contain the best estimates of the primal variables \mathbf{x} , and dual variables for the bound constraints \mathbf{z} , respectively. The components `prob%C` and `prob%G` will contain the residuals $\mathbf{c}(\mathbf{x})$ and gradients $\mathbf{g}(\mathbf{x})$ at \mathbf{x} , respectively. **Restrictions:** `prob%n` > 0 , `prob%m` > 0 and (if \mathbf{A} is provided) `prob%A`'s ≥ -2 . `prob%A_type` $\in \{ \text{'DENSE'}, \text{'COORDINATE'}, \text{'SPARSE-BY-ROWS'} \}$.

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`X_stat` is a rank-one `INTENT(INOUT)` array argument of dimension `prob%n` and type default `INTEGER`, that indicates which of the simple bound constraints are in the current working set. Possible values for `X_stat(j)`, $j = 1, \dots, \text{prob}\%n$, and their meanings are

- <0 the j -th simple bound constraint is in the working set, on its lower bound,
- >0 the j -th simple bound constraint is in the working set, on its upper bound, and
- 0 the j -th simple bound constraint is not in the working set.

Suitable values must be supplied if `control%blls_control%cold_start = 0` on entry, but need not be provided for other input values of `control%cold_start`. Inappropriate values will be ignored. On exit, `X_stat` will contain values appropriate for the ultimate working set.

`data` is a scalar `INTENT(INOUT)` argument of type `BLLS_data_type` (see Section 2.2.6). It is used to hold data about the problem being solved. It must not have been altered **by the user** since the last call to `BLLS_initialize`.

`control` is a scalar `INTENT(IN)` argument of type `BLLS_control_type` (see Section 2.2.3). Default values may be assigned by calling `BLLS_initialize` prior to the first call to `BLLS_solve`.

`inform` is a scalar `INTENT(INOUT)` argument of type `BLLS_inform_type` (see Section 2.2.5). On initial entry, the component `status` must be set to 1, while other components need not be set. A successful call to `BLLS_solve` is indicated when the component `status` has the value 0. For other return values of `status`, see Sections 2.5 and 2.6.

`userdata` is a scalar `INTENT(INOUT)` argument of type `NLPT_userdata_type` whose components may be used to communicate user-supplied data (see Section 2.2.7) to and from the OPTIONAL subroutines `eval_APROD` and `eval_ASPROD` (see below).

`reverse` is an OPTIONAL scalar `INTENT(INOUT)` argument of type `BLLS_reverse_type` (see Section 2.2.8). It is used to communicate reverse-communication data between the subroutine and calling program. If `reverse` is PRESENT and `eval%APROD` or `eval%ASPROD` (see below) are absent, the user should monitor `inform%status` on exit (see Section 2.5).

`eval_APROD` is an OPTIONAL user-supplied subroutine whose purpose is to evaluate the value of the product $\mathbf{p} + \mathbf{A}\mathbf{v}$ or $\mathbf{p} + \mathbf{A}^T\mathbf{v}$ involving the Jacobian (and its transpose) and given vectors \mathbf{v} and \mathbf{p} . See Section 2.4.1 for details. If `eval_APROD` is present, it must be declared EXTERNAL in the calling program. If `eval_APROD` is absent, `GALAHAD_BLLS_solve` will use reverse communication (see Section 2.5) to obtain Jacobian-vector products if `reverse` is PRESENT or otherwise require that the user has provided all relevant components of `prob%A`.

`eval_ASPROD` is an OPTIONAL user-supplied subroutine whose purpose is to evaluate the value of the product $\mathbf{A}\mathbf{v}$ involving the Jacobian and a given *sparse* vector \mathbf{v} . See Section 2.4.2 for details. If `eval_APROD` is present, it must be declared EXTERNAL in the calling program. If `eval_APROD` is absent, `GALAHAD_BLLS_solve` will use reverse communication (see Section 2.5) to obtain Jacobian-sparse-vector products if `reverse` is PRESENT or otherwise require that the user has provided all relevant components of `prob%A`.

2.3.3 The termination subroutine

All previously allocated arrays are deallocated as follows:

```
CALL BLLS_terminate( data, control, inform )
```

`data` is a scalar `INTENT(INOUT)` argument of type `BLLS_data_type` exactly as for `BLLS_solve`, which must not have been altered **by the user** since the last call to `BLLS_initialize`. On exit, array components will have been deallocated.

`control` is a scalar `INTENT(IN)` argument of type `BLLS_control_type` exactly as for `BLLS_solve`.

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`inform` is a scalar `INTENT(OUT)` argument of type `BLLS_inform_type` exactly as for `BLLS_solve`. Only the component status will be set on exit, and a successful call to `BLLS_terminate` is indicated when this component status has the value 0. For other return values of status, see Section 2.6.

2.4 Matrix-vector operations

2.4.1 Jacobian-vector products via internal evaluation

If the argument `eval_APROD` is present when calling `GALAHAD_BLLS_solve`, the user is expected to provide a subroutine of that name to evaluate the sum $\mathbf{p} + \mathbf{A}\mathbf{v}$ or $\mathbf{p} + \mathbf{A}^T\mathbf{v}$ involving the product of the residual Jacobian \mathbf{A} or its transpose \mathbf{A}^T and a given vector \mathbf{v} . The routine must be specified as

```
SUBROUTINE eval_APROD( status, userdata, transpose, V, P )
```

whose arguments are as follows:

`status` is a scalar `INTENT(OUT)` argument of type default `INTEGER`, that should be set to 0 if the routine has been able to evaluate the sum $\mathbf{p} + \mathbf{A}\mathbf{v}$ or $\mathbf{p} + \mathbf{A}^T\mathbf{v}$ and to a non-zero value if the evaluation has not been possible.

`userdata` is a scalar `INTENT(INOUT)` argument of type `NLPT_userdata_type` whose components may be used to communicate user-supplied data to and from the subroutines `eval_APROD` (see Section 2.2.7).

`transpose` is a scalar `INTENT(IN)` array argument of type default that will be set `.TRUE.` if the product involves the transpose of the Jacobian \mathbf{A}^T and `.FALSE.` if the product involves the Jacobian \mathbf{A} itself.

`V` is a rank-one `INTENT(IN)` array argument of type default `REAL` (double precision in `GALAHAD_BLLS_double`) whose components contain the vector \mathbf{v} .

`P` is a rank-one `INTENT(INOUT)` array argument of type default `REAL` (double precision in `GALAHAD_BLLS_double`) whose components on input contain the vector \mathbf{p} and on output the sum $\mathbf{p} + \mathbf{A}\mathbf{v}$ when `%transpose` is `.FALSE.` or $\mathbf{p} + \mathbf{A}^T\mathbf{v}$ when `%transpose` is `.TRUE.`.

2.4.2 Jacobian-sparse-vector products via internal evaluation

If the argument `eval_ASPROD` is present when calling `GALAHAD_BLLS_solve`, the user is expected to provide a subroutine of that name to evaluate the product of the Jacobian \mathbf{A} with a given vector \mathbf{v} . The routine must be specified as

```
SUBROUTINE eval_ASPROD( status, userdata, V, P[, NZ_in, nz_in_start, nz_in_end,      &
                        NZ_out, nz_out_end] )
```

whose arguments are as follows:

`status` is a scalar `INTENT(OUT)` argument of type default `INTEGER`, that should be set to 0 if the routine has been able to evaluate the product $\mathbf{A}\mathbf{v}$ and to a non-zero value if the evaluation has not been possible.

`userdata` is a scalar `INTENT(INOUT)` argument of type `NLPT_userdata_type` whose components may be used to communicate user-supplied data to and from the subroutine (see Section 2.2.7).

`V` is a rank-one `INTENT(IN)` array argument of type default `REAL` (double precision in `GALAHAD_BLLS_double`) whose components contain the vector \mathbf{v} . If components `nz_in_start`, `nz_in_end` and `NZ_in` (see below) are PRESENT, only components `NZ_in(nz_in_start:nz_in_end)` of \mathbf{V} will be nonzero and the remaining components of \mathbf{V} should be ignored. Otherwise, all components of \mathbf{V} should be presumed to be nonzero.

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`P` is a rank-one `INTENT (OUT)` array argument of type default `REAL` (double precision in `GALAHAD_BLLS_double`) whose components on output contain the required components of \mathbf{Av} . If components `nz_out_end` and `NZ_out` (see below) are `PRESENT`, only the nonzero components `NZ_out(1:nz_out_end)` of `P` need be assigned. Otherwise, all components of `P` must be set.

`nz_in_start` is an `OPTIONAL` scalar variable of type default `INTEGER`, that, if `PRESENT`, holds the starting position in `NZ_in` of the list of indices of nonzero components of \mathbf{v} .

`nz_in_end` is an `OPTIONAL` scalar variable of type default `INTEGER`, that, if `PRESENT`, holds the finishing position in `NZ_in` of the list of indices of nonzero components of \mathbf{v} .

`NZ_in` is an `OPTIONAL` rank-one allocatable array of dimension n and type default `INTEGER` that, if `PRESENT`, holds the indices of the nonzero components of \mathbf{v} . If any of `nz_in_start`, `nz_in_end` and `NZ_in` are absent, all components of \mathbf{v} are assumed to be nonzero.

`nz_out_end` is an `OPTIONAL` scalar variable of type default `INTEGER` that, if `PRESENT`, must be set to record the number of non-zeros in \mathbf{Av} .

`NZ_out` is an `OPTIONAL` rank-one allocatable array of dimension m and type default `INTEGER` that, if `PRESENT` must be set to record the list of indices of nonzero components of \mathbf{Av} . If either of `nz_out_end` and `NZ_out` are absent, all components of `P` should be set even if they are zero.

2.5 Reverse Communication Information

A positive value of `inform%status` on exit from `BLLS_solve` indicates that `GALAHAD_BLLS_solve` is seeking further information—this will happen if the user has chosen to evaluate matrix-vector products by reverse communication. The user should compute the required information and re-enter `GALAHAD_BLLS_solve` with `inform%status` and all other arguments (except those specifically mentioned below) unchanged.

Possible values of `inform%status` and the information required are

1. The user should compute ones of the sums $\mathbf{p} + \mathbf{Av}$ or $\mathbf{p} + \mathbf{A}^T \mathbf{v}$ involving the product of the residual Jacobian \mathbf{A} or its transpose with a given vector \mathbf{v} . The vectors \mathbf{p} and \mathbf{v} are given in `data%P` and `data%V` respectively. If `data%transpose` is `.FALSE.`, the resulting vector $\mathbf{p} + \mathbf{Av}$ should overwrite `data%P` and `data%eval_status` should be set to 0. Conversely if `data%transpose` is `.TRUE.`, the resulting vector $\mathbf{p} + \mathbf{A}^T \mathbf{v}$ should overwrite `data%P` and `data%eval_status` set to 0. If the user is unable to evaluate the sum, the user need not set `data%P`, but should then set `data%eval_status` to a non-zero value.
2. The user should compute the nonzero components of the matrix-vector product \mathbf{Av} using the vector \mathbf{v} whose nonzero components are stored in positions `reverse%NZ_in(reverse%nz_in_start:reverse%nz_in_end)` of `reverse%V`. The remaining components of `reverse%V` should be ignored. The nonzero components must occupy positions `reverse%NZ_out(1:reverse%nz_out_end)` of `reverse%P`, and the components `reverse%NZ_out` and `reverse%nz_out_end` must be set. This return can only happen if `control%exact_gcp` is `.TRUE.`.

2.6 Warning and error messages

A negative value of `inform%status` on exit from `BLLS_solve` or `BLLS_terminate` indicates that an error has occurred. No further calls should be made until the error has been corrected. Possible values are:

- 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.

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- 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. One of the restrictions `prob%n > 0`, `prob%m > 0` or the requirement that `prob%A_type` contain its relevant string 'DENSE', 'COORDINATE' or 'SPARSE_BY_ROWS' when **A** is available, has been violated.
- 4. The bound constraints are inconsistent.
- 7. The objective function appears to be unbounded from below on the feasible set.
- 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`.
- 16. The problem is so ill-conditioned that further progress is impossible.
- 17. The step is too small to make further impact.
- 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.

2.7 Further features

In this section, we describe an alternative means of setting control parameters, that is components of the variable `control` of type `BLLS_control_type` (see Section 2.2.3), by reading an appropriate data specification file using the subroutine `BLLS_read_specfile`. This facility is useful as it allows a user to change BLLS control parameters without editing and recompiling programs that call BLLS.

A specification file, or *specfile*, is a data file containing a number of "specification commands". Each command occurs on a separate line, and comprises a "keyword", which is a string (in a close-to-natural language) used to identify a control parameter, and an (optional) "value", which defines the value to be assigned to the given control parameter. All keywords and values are case insensitive, keywords may be preceded by one or more blanks but values must not contain blanks, and each value must be separated from its keyword by at least one blank. Values must not contain more than 30 characters, and each line of the specfile is limited to 80 characters, including the blanks separating keyword and value.

The portion of the specification file used by `BLLS_read_specfile` must start with a "BEGIN BLLS" command and end with an "END" command. The syntax of the specfile is thus defined as follows:

```
( .. lines ignored by BLLS_read_specfile .. )
BEGIN BLLS
  keyword      value
  .....      .....
  keyword      value
END
( .. lines ignored by BLLS_read_specfile .. )
```

where keyword and value are two strings separated by (at least) one blank. The "BEGIN BLLS" and "END" delimiter command lines may contain additional (trailing) strings so long as such strings are separated by one or more blanks, so that lines such as

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```
BEGIN BLLS SPECIFICATION
```

and

```
END BLLS SPECIFICATION
```

are acceptable. Furthermore, between the “BEGIN BLLS” and “END” delimiters, specification commands may occur in any order. Blank lines and lines whose first non-blank character is ! or * are ignored. The content of a line after a ! or * character is also ignored (as is the ! or * character itself). This provides an easy manner to “comment out” some specification commands, or to comment specific values of certain control parameters.

The value of a control parameters may be of three different types, namely integer, logical or real. Integer and real values may be expressed in any relevant Fortran integer and floating-point formats (respectively). Permitted values for logical parameters are “ON”, “TRUE”, “.TRUE.”, “T”, “YES”, “Y”, or “OFF”, “NO”, “N”, “FALSE”, “.FALSE.” and “F”. Empty values are also allowed for logical control parameters, and are interpreted as “TRUE”.

The specification file must be open for input when `BLLS_read_specfile` is called, and the associated device number passed to the routine in `device` (see below). Note that the corresponding file is `REWINDED`, which makes it possible to combine the specifications for more than one program/routine. For the same reason, the file is not closed by `BLLS_read_specfile`.

2.7.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
CALL BLLS_read_specfile( control, device )
```

`control` is a scalar `INTENT(INOUT)` argument of type `BLLS_control_type` (see Section 2.2.3). Default values should have already been set, perhaps by calling `BLLS_initialize`. On exit, individual components of `control` may have been changed according to the commands found in the specfile. Specfile commands and the component (see Section 2.2.3) of `control` that each affects are given in Table 2.1.

`device` is a scalar `INTENT(IN)` argument of type `default_INTEGER`, that must be set to the unit number on which the specfile has been opened. If `device` is not open, `control` will not be altered and execution will continue, but an error message will be printed on unit `control%error`.

2.8 Information printed

If `control%print_level` is positive, information about the progress of the algorithm will be printed on unit `control%out`. If `control%print_level = 1`, a single line of output will be produced for each iteration of the process. For the initial-feasible-point phase, this will include values of the current primal and dual infeasibility, and violation of complementary slackness, the feasibility-phase objective value, the current steplength, the value of the barrier parameter, the number of backtracks in the linesearch and the elapsed CPU time in seconds. Once a suitable feasible point has been found, the iteration is divided into major iterations, at which the barrier parameter is reduced, and minor iterations, and which the barrier function is approximately minimized for the current value of the barrier parameter. For the major iterations, the value of the barrier parameter, the required values of dual feasibility and violation of complementary slackness, and the current constraint infeasibility are reported. Each minor iteration of the optimality phase results in a line giving the current dual feasibility and violation of complementary slackness, the objective function value, the ratio of predicted to achieved reduction of the objective function, the trust-region radius, the number of backtracks in the linesearch, the number of conjugate-gradient iterations taken, and the elapsed CPU time in seconds.

If `control%print_level ≥ 2` this output will be increased to provide significant detail of each iteration. This extra output includes residuals of the linear systems solved, and, for larger values of `control%print_level`, values of the primal and dual variables and Lagrange multipliers.

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command	component of control	value type
error-printout-device	%error	integer
printout-device	%out	integer
print-level	%print_level	integer
start-print	%start_print	integer
stop-print	%stop_print	integer
iterations-between-printing	%print_gap	integer
maximum-number-of-iterations	%maxit	integer
maximum-number-of-cg-iterations-per-iteration	%cg_maxit	integer
infinity-value	%infinity	real
primal-accuracy-required	%stop_p	real
dual-accuracy-required	%stop_d	real
complementary-slackness-accuracy-required	%stop_c	real
identical-bounds-tolerance	%identical_bounds_tol	real
cg-relative-accuracy-required	%stop_cg_relative	real
cg-absolute-accuracy-required	%stop_cg_absolute	real
zero-curvature-threshold	%zero_curvature	real
maximum-cpu-time-limit	%cpu_time_limit	real
exact-GCP-used	%exact_gcp	logical
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
output-line-prefix	%prefix	character

Table 2.1: Specfile commands and associated components of control.

3 GENERAL INFORMATION

Use of common: None.

Workspace: Provided automatically by the module.

Other routines called directly: None.

Other modules used directly: BLLS_solve calls the GALAHAD packages GALAHAD_CPU_time, GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_SBLs, GALAHAD_QPT and GALAHAD_SPECFILE.

Input/output: Output is under control of the arguments control%error, control%out and control%print_level.

Restrictions: prob%n > 0, prob%m > 0, prob%A_type ∈ { 'DENSE', 'COORDINATE', 'SPARSE_BY_ROWS' } (if **A** is explicit).

Portability: ISO Fortran 95 + TR 15581 or Fortran 2003. The package is thread-safe.

4 METHOD

The required solution **x** necessarily satisfies the primal optimality conditions

$$\mathbf{x}^l \leq \mathbf{x} \leq \mathbf{x}^u, \quad (4.1)$$

the dual optimality conditions

$$\mathbf{A}^T(\mathbf{Ax} - \mathbf{b}) = \mathbf{z} \text{ and } \mathbf{z} = \mathbf{z}^l + \mathbf{z}^u, \quad (4.2)$$

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and

$$\mathbf{z}^l \geq 0 \text{ and } \mathbf{z}^u \leq 0, \quad (4.3)$$

and the complementary slackness conditions

$$(\mathbf{x} - \mathbf{x}^l)^T \mathbf{z}^l = 0 \text{ and } (\mathbf{x} - \mathbf{x}^u)^T \mathbf{z}^u = 0, \quad (4.4)$$

where the components of the vector \mathbf{z} are known as the dual variables for the bounds, and where the vector inequalities hold componentwise. Projected-gradient methods iterate towards a point that satisfies these conditions by ultimately aiming to satisfy (4.2), while ensuring that (4.1), and (4.3) and (4.4) are satisfied at each stage. Appropriate norms of the amounts by which (4.1), (4.2) and (4.4) fail to be satisfied are known as the primal and dual infeasibility, and the violation of complementary slackness, respectively.

The method is iterative. Each iteration proceeds in two stages. Firstly, the so-called generalized Cauchy point for the least-squares objective is found. (The purpose of this point is to ensure that the algorithm converges and that the set of bounds which are satisfied as equations at the solution is rapidly identified.) Thereafter an improvement to the objective is sought using either a direct-matrix or truncated conjugate-gradient algorithm.

References:

This is a specialised version of the method presented in

A. R. Conn, N. I. M. Gould and Ph. L. Toint (1988). Global convergence of a class of trust region algorithms for optimization with simple bounds. *SIAM Journal on Numerical Analysis* **25** 433-460,

5 EXAMPLE OF USE

Suppose we wish to minimize $\frac{1}{2}x_1^2 + x_2^2 + x_2x_3 + \frac{3}{2}x_3^2 + 2x_2 + 1$ subject to the simple bounds $-1 \leq x_1 \leq 1$ and $x_3 \leq 2$. Then, on writing the data for this problem as

$$\mathbf{H} = \begin{pmatrix} 1 & & \\ & 2 & 1 \\ & 1 & 3 \end{pmatrix}, \quad \mathbf{g} = \begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix}, \quad \mathbf{x}^l = \begin{pmatrix} -1 \\ -\infty \\ -\infty \end{pmatrix} \text{ and } \mathbf{x}^u = \begin{pmatrix} 1 \\ \infty \\ 2 \end{pmatrix}$$

in sparse co-ordinate format, we may use the following code:

This produces the following output:

The same problem may be solved holding the data in a sparse row-wise storage format by replacing the lines

```
! sparse co-ordinate storage format
...
! problem data complete
```

by

```
! sparse row-wise storage format
CALL SMT_put( p%H%type, 'SPARSE_BY_ROWS', s ) ! Specify sparse-by-row
ALLOCATE( p%H%val( h_ne ), p%H%col( h_ne ), p%H%ptr( n + 1 ) )
ALLOCATE( p%A%val( a_ne ), p%A%col( a_ne ), p%A%ptr( m + 1 ) )
p%H%val = (/ 1.0_wp, 2.0_wp, 1.0_wp, 3.0_wp /) ! Hessian H
p%H%col = (/ 1, 2, 3, 3 /) ! NB lower triangular
p%H%ptr = (/ 1, 2, 3, 5 /) ! Set row pointers
! problem data complete
```

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or using a dense storage format with the replacement lines

```
! dense storage format
CALL SMT_put( p%H$type, 'DENSE', s ) ! Specify dense
ALLOCATE( p%H$val( n * ( n + 1 ) / 2 ) )
p%H$val = (/ 1.0_wp, 0.0_wp, 2.0_wp, 0.0_wp, 1.0_wp, 3.0_wp /) ! Hessian
! problem data complete
```

respectively.

If instead \mathbf{H} had been the diagonal matrix

$$\mathbf{H} = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 3 \end{pmatrix}$$

but the other data is as before, the diagonal storage scheme might be used for \mathbf{H} , and in this case we would instead

```
CALL SMT_put( prob%H$type, 'DIAGONAL', s ) ! Specify dense storage for H
ALLOCATE( p%H$val( n ) )
p%H$val = (/ 1.0_wp, 2.0_wp, 3.0_wp /) ! Hessian values
```

The same problem may be solved using reverse communication with the following code:

Notice that storage for the Hessian is now not needed. This produces the same output.

The same problem may also be solved by user-provided matrix-vector products as follows:

Now notice how the matrix \mathbf{H} is passed to the matrix-vector product evaluation routine via the integer and real components of the derived type `userdata`.