





GALAHAD



USER DOCUMENTATION

GALAHAD Optimization Library version 5.0

1 SUMMARY

This package uses a crossover method, switching between interior-point and working-set approaches, to solve the **quadratic programming problem**

minimize
$$q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{H} \mathbf{x} + \mathbf{g}^T \mathbf{x} + f$$

subject to the general linear constraints

$$c_i^l \leq \mathbf{a}_i^T \mathbf{x} \leq c_i^u, \quad i = 1, \dots, m,$$

and the simple bound constraints

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

where the *n* by *n* symmetric matrix **H**, the vectors \mathbf{g} , \mathbf{a}_i , \mathbf{c}^l , \mathbf{c}^u , \mathbf{x}^l , \mathbf{x}^u and the scalar *f* are given. Full advantage is taken of any zero coefficients in the matrix **H** or the vectors \mathbf{a}_i . Any of the constraint bounds c_i^l , c_i^u , x_i^l and x_i^u may be infinite.

If the matrix **H** is positive semi-definite, a global solution is found. However, if **H** is indefinite, the procedure may find a (weak second-order) critical point that is not the global solution to the given problem.

ATTRIBUTES — Versions: GALAHAD_QPC_single, GALAHAD_QPC_double. Uses: GALAHAD_CLOCK, GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_NORMS, GALAHAD_SORT, GALAHAD_QPT, GALAHAD_QPP, GALAHAD_QPD, GALAHAD_EQP, GALAHAD_LSQP, GALAHAD_CQP, GALAHAD_QPA, GALAHAD_QPB, GALAHAD_SPECFILE, GALAHAD_FDC. Date: March 2006. Origin: N. I. M. Gould, Rutherford Appleton Laboratory, and Ph. L. Toint, University of Namur, Belgium. Language: Fortran 95 + TR 15581 or Fortran 2003. Parallelism: Some options may use OpenMP and its runtime library.

2 HOW TO USE THE PACKAGE

The package is available using both single and double precision reals, and either 32-bit or 64-bit integers. Access to the 32-bit integer, single precision version requires the USE statement

USE GALAHAD_QPC_single

with the obvious substitution GALAHAD_QPC_double, GALAHAD_QPC_single_64 and GALAHAD_QPC_double_64 for the other variants.

If it is required to use more than one of the modules at the same time, the derived types SMT_type, QPT_problem_type, QPC_time_type, QPC_time_type, QPC_inform_type and QPC_data_type (Section 2.4) and the subroutines QPC_initialize, QPC_solve, QPC_terminate, (Section 2.5) and QPC_read_specfile (Section 2.7) must be renamed on one of the USE statements.

2.1 Matrix storage formats

Both the Hessian matrix **H** and the constraint Jacobian **A**, the matrix whose rows are the vectors \mathbf{a}_i^T , $i = 1, \dots, m$, may be stored in a variety of input formats.

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2.1.1 Dense storage format

The matrix **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_{ij} for $i=1,\ldots,m,\ j=1,\ldots,n$. Since **H** is symmetric, only the lower triangular part (that is the part h_{ij} for $1 \le j \le i \le n$) need be held. In this case the lower triangle will be stored by rows, that is component i*(i-1)/2+j of the storage array H%val will hold the value h_{ij} (and, by symmetry, h_{ji}) for $1 \le j \le i \le n$.

2.1.2 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 a_{ij} are stored in the l-th components of the integer arrays A%row, A%col and real array A%val, respectively. The order is unimportant, but the total number of entries A%ne is also required. The same scheme is applicable to \mathbf{H} (thus requiring integer arrays H%row, H%col, a real array H%val and an integer value H%ne), except that only the entries in the lower triangle need be stored.

2.1.3 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 $\mathbf A$, the i-th component of a 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 a_{ij} of the entries in the i-th row are stored in components l= A%ptr $(i),\ldots$, A%ptr (i+1)-1 of the integer array A%col, and real array A%val, respectively. The same scheme is applicable to $\mathbf H$ (thus requiring integer arrays H%ptr, H%col, and a real array H%val), except that only the entries in the lower triangle need be stored.

For sparse matrices, this scheme almost always requires less storage than its predecessor.

2.1.4 Diagonal storage format

If **H** is diagonal (i.e., $h_{ij} = 0$ for all $1 \le i \ne j \le n$) only the diagonals entries h_{ii} , $1 \le i \le n$, need be stored, and the first n components of the array H%val may be used for the purpose. There is no sensible equivalent for the non-square **A**.

2.2 Real and integer kinds

We use the terms integer and real to refer to the fortran keywords REAL(rp_) and INTEGER(ip_), where rp_ and ip_ are the relevant kind values for the real and integer types employed by the particular module in use. The former are equivalent to default REAL for the single precision versions and DOUBLE PRECISION for the double precision cases, and correspond to rp_ = real32 and rp_ = real64, respectively, as supplied by the fortran iso_fortran_env module. The latter are default (32-bit) and long (64-bit) integers, and correspond to ip_ = int32 and ip_ = int64, respectively, again from the iso_fortran_env module.

2.3 Parallel usage

OpenMP may be used by the GALAHAD_QPC package to provide parallelism for some solvers in shared memory environments. See the documentation for the GALAHAD package SLS for more details. To run in parallel, OpenMP must be enabled at compilation time by using the correct compiler flag (usually some variant of -openmp). The number of threads may be controlled at runtime by setting the environment variable OMP_NUM_THREADS.

MPI may also be used by the package to provide parallelism for some solvers in a distributed memory environment. To use this form of parallelism, MPI must be enabled at runtime by using the correct compiler flag (usually some variant of <code>-lmpi</code>). Although the MPI process will be started automatically when required, it should be stopped by the

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calling program once no further use of this form of parallelism is needed. Typically, this will be via statements of the form

```
CALL MPI_INITIALIZED( flag, ierr )
IF ( flag ) CALL MPI_FINALIZE( ierr )
```

The code may be compiled and run in serial mode.

2.4 The derived data types

Ten derived data types are accessible from the package.

2.4.1 The derived data type for holding matrices

The derived data type SMT_TYPE is used to hold the matrices A and H. The components of SMT_TYPE used here are:

- m is a scalar component of type INTEGER (ip_), that holds the number of rows in the matrix.
- n is a scalar component of type INTEGER (ip_), that holds the number of columns in the matrix.
- ne is a scalar variable of type INTEGER (ip_), 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 §2.4.2).
- is a rank-one allocatable array of type REAL (rp_) and dimension at least ne, that holds the values of the entries. Each pair of off-diagonal entries $h_{ij} = h_{ji}$ of a *symmetric* matrix **H** is represented as a single entry (see §2.1.1–2.1.3). Any duplicated entries that appear in the sparse co-ordinate or row-wise schemes will be summed.
- is a rank-one allocatable array of type INTEGER (ip_), and dimension at least ne, that may hold the row indices of the entries. (see §2.1.2).
- is a rank-one allocatable array of type INTEGER (ip_), and dimension at least ne, that may the column indices of the entries (see §2.1.2–2.1.3).
- ptr is a rank-one allocatable array of type INTEGER (ip_), and dimension at least m + 1, that may hold the pointers to the first entry in each row (see §2.1.3).

2.4.2 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:

- new_problem_structure is a scalar variable of type default LOGICAL, that is .TRUE. if this is the first (or only) problem in a sequence of problems with identical "structure" to be attempted, and .FALSE. if a previous problem with the same "structure" (but different numerical data) has been solved. Here, the term "structure" refers both to the sparsity patterns of the Jacobian matrices $\bf A$ involved (but not their numerical values), to the zero/nonzero/infinity patterns (a bound is either zero, \pm infinity, or a finite but arbitrary nonzero) of each of the constraint bounds, and to the variables and constraints that are fixed (both bounds are the same) or free (the lower and upper bounds are \pm infinity, respectively).
- n is a scalar variable of type INTEGER (ip_-), that holds the number of optimization variables, n.
- m is a scalar variable of type INTEGER (ip_), that holds the number of general linear constraints, m.
- H is scalar variable of type SMT_TYPE that holds the Hessian matrix **H**. The following components are used:

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H%type is an allocatable array of rank one and type default CHARACTER, that is used to indicate the storage scheme used. If the dense storage scheme (see Section 2.1.1) is used, the first five components of H%type must contain the string DENSE. For the sparse co-ordinate scheme (see Section 2.1.2), the first ten components of H%type must contain the string COORDINATE, for the sparse row-wise storage scheme (see Section 2.1.3), the first fourteen components of H%type must contain the string SPARSE_BY_ROWS, and for the diagonal storage scheme (see Section 2.1.4), the first eight components of H%type must contain the string DIAGONAL.

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

```
CALL SMT_put( prob%H%type, 'COORDINATE' )
```

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

- H%ne is a scalar variable of type INTEGER(ip_), that holds the number of entries in the **lower triangular** part of **H** in the sparse co-ordinate storage scheme (see Section 2.1.2). It need not be set for any of the other three schemes.
- H%val is a rank-one allocatable array of type REAL (rp_), that holds the values of the entries of the **lower triangular** part of the Hessian matrix **H** in any of the storage schemes discussed in Section 2.1.
- H%row is a rank-one allocatable array of type INTEGER (ip_), that holds the row indices of the **lower triangular** part of **H** in the sparse co-ordinate storage scheme (see Section 2.1.2). It need not be allocated for any of the other three schemes.
- H%col is a rank-one allocatable array variable of type INTEGER(ip_), that holds the column indices of the **lower triangular** part of **H** in either the sparse co-ordinate (see Section 2.1.2), or the sparse row-wise (see Section 2.1.3) storage scheme. It need not be allocated when the dense or diagonal storage schemes are used.
- H%ptr is a rank-one allocatable array of dimension n+1 and type INTEGER (ip_), that holds the starting position of each row of the **lower triangular** part of **H**, as well as the total number of entries plus one, in the sparse row-wise storage scheme (see Section 2.1.3). It need not be allocated when the other schemes are used.
- is a rank-one allocatable array of dimension n and type REAL (rp_), that holds the gradient **g** of the linear term of the quadratic objective function. The *j*-th component of G, j = 1, ..., n, contains \mathbf{g}_j .
- f is a scalar variable of type REAL (rp_), that holds the constant term, f, in the objective function.
- A is scalar variable of type SMT_TYPE that holds the Jacobian matrix A. The following components are used:
 - 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 storage scheme (see Section 2.1.1) is used, the first five components of A%type must contain the string DENSE. For the sparse co-ordinate scheme (see Section 2.1.2), the first ten components of A%type must contain the string COORDINATE, while for the sparse row-wise storage scheme (see Section 2.1.3), the first fourteen components of A%type must contain the string SPARSE_BY_ROWS.

Just as for H%type above, the procedure SMT_put may be used to allocate sufficient space and insert the required keyword into A%type. Once again, if prob is of derived type QPC_problem_type and involves a Jacobian we wish to store using the sparse row-wise storage scheme, we may simply

```
CALL SMT_put( prob%A%type, 'SPARSE_BY_ROWS' )
```

- A%ne is a scalar variable of type INTEGER (ip_), that holds the number of entries in A in the sparse co-ordinate storage scheme (see Section 2.1.2). It need not be set for either of the other two schemes.
- A%val is a rank-one allocatable array of type REAL (rp_), that holds the values of the entries of the Jacobian matrix $\bf A$ in any of the storage schemes discussed in Section 2.1.

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- A%row is a rank-one allocatable array of type INTEGER (ip_), that holds the row indices of **A** in the sparse coordinate storage scheme (see Section 2.1.2). It need not be allocated for either of the other two schemes.
- A%col is a rank-one allocatable array variable of type INTEGER(ip_{-}), that holds the column indices of **A** in either the sparse co-ordinate (see Section 2.1.2), or the sparse row-wise (see Section 2.1.3) storage scheme. It need not be allocated when the dense storage scheme is used.
- A%ptr is a rank-one allocatable array of dimension m+1 and type INTEGER (ip_), that holds the starting position of each row of $\bf A$, as well as the total number of entries plus one, in the sparse row-wise storage scheme (see Section 2.1.3). It need not be allocated when the other schemes are used.
- c_l is a rank-one allocatable array of dimension m and type REAL (rp_), that holds the vector of lower bounds \mathbf{c}^l on the general constraints. The *i*-th component of C_l, i = 1, ..., m, contains \mathbf{c}^l_i . Infinite bounds are allowed by setting the corresponding components of C_l to any value smaller than -infinity, where infinity is a component of the control array control (see Section 2.4.7).
- C_u is a rank-one allocatable array of dimension m and type REAL (rp_), that holds the vector of upper bounds \mathbf{c}^u on the general constraints. The *i*-th component of C_u, i = 1, ..., m, contains \mathbf{c}^u_i . Infinite bounds are allowed by setting the corresponding components of C_u to any value larger than infinity, where infinity is a component of the control array control (see Section 2.4.7).
- x_1 is a rank-one allocatable array of dimension n and type REAL (rp_), that holds the vector of lower bounds \mathbf{x}^l on the the variables. The j-th component of x_1, $j = 1, \ldots, n$, contains \mathbf{x}^l_j . Infinite bounds are allowed by setting the corresponding components of x_1 to any value smaller than -infinity, where infinity is a component of the control array control (see Section 2.4.7).
- X_u is a rank-one allocatable array of dimension n and type REAL (rp_), that holds the vector of upper bounds \mathbf{x}^u on the variables. The j-th component of X_u , $j=1,\ldots,n$, contains \mathbf{x}^u_j . Infinite bounds are allowed by setting the corresponding components of X_u to any value larger than that infinity, where infinity is a component of the control array control (see Section 2.4.7).
- X is a rank-one allocatable array of dimension n and type REAL (rp_), that holds the values **x** of the optimization variables. The *j*-th component of X, j = 1, ..., n, contains x_j .
- is a rank-one allocatable array of dimension n and type default REAL (rp_), that holds the values **z** of estimates of the dual variables corresponding to the simple bound constraints (see Section 4). The *j*-th component of \mathbb{Z} , $j = 1, \ldots, n$, contains z_j .
- is a rank-one allocatable array of dimension m and type default REAL (rp_), that holds the values $\mathbf{A}\mathbf{x}$ of the constraints. The *i*-th component of \mathbb{C} , $i=1,\ldots,m$, contains $\mathbf{a}_i^T\mathbf{x} \equiv (\mathbf{A}\mathbf{x})_i$.
- is a rank-one allocatable array of dimension m and type REAL (rp_), that holds the values \mathbf{y} of estimates of the Lagrange multipliers corresponding to the general linear constraints (see Section 4). The i-th component of \mathbf{y} , $i = 1, \dots, m$, contains y_i .

2.4.3 The derived data type for holding control parameters specifically for the interior-point phase

The derived data type QPB_control_type is used to hold controlling data for the interior-point phase of the calculation, performed by the GALAHAD package GALAHAD_QPB. Components may be changed by calling QPB_read_specfile (see the documentation for GALAHAD_QPB for details). The components of QPB_control_type are:

- error is a scalar variable of type INTEGER(ip_), that holds the stream number for error messages. Printing of error messages in QPB_solve and QPB_terminate is suppressed if error ≤ 0 . The default is error = 6.
- out is a scalar variable of type INTEGER(ip_), that holds the stream number for informational messages. Printing of informational messages in QPB_solve is suppressed if out < 0. The default is out = 6.

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print_level is a scalar variable of type INTEGER(ip_), 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 INTEGER(ip_), that specifies the first iteration for which printing will occur in QPB_solve. If start_print is negative, printing will occur from the outset. The default is start_print = -1.
- stop_print is a scalar variable of type INTEGER(ip_), that specifies the last iteration for which printing will occur in QPB_solve. If stop_print is negative, printing will occur once it has been started by start_print. The default is stop_print = -1.
- maxit is a scalar variable of type INTEGER (ip_), that holds the maximum number of iterations which will be allowed in QPB_solve. The default is maxit = 1000.
- infeas_max is a scalar variable of type INTEGER(ip_), that specifies the number of iterations for which the overall infeasibility of the problem is not reduced by at least a factor reduce_infeas before the problem is flagged as infeasible (see reduce_infeas). The default is infeas_max = 200.
- cg_maxit is a scalar variable of type INTEGER(ip_), that holds the maximum number of conjugate-gradient inner iterations that may be performed during the computation of each search direction in QPB_solve. If cg_maxit is set to a negative number, it will be reset by QPB_solve to the dimension of the relevant linear system +1. The default is cg_maxit = 200.
- indicator_type is a scalar variable of type INTEGER (ip_), that specifies the type of indicator used to assess when a variable or constraint is active. Possible values are:
 - 1 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator_tol_p (see below).
 - 2 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator_tol-_pd (see below) times the magnitude of its corresponding dual variable.
 - 3 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator_tol_tapia (see below) times the distance to the same bound at the previous iteration.

The default is indicator_type = 3.

- restore_problem is a scalar variable of type INTEGER(ip_), that specifies how much of the input problem is to be retored on output. Possible values are:
 - 0 nothing is restored.
 - 1 the vector data $\mathbf{g}, \mathbf{c}^l, \mathbf{c}^u, \mathbf{x}^l$, and \mathbf{x}^u will be restored to their input values.
 - 2 the entire problem, that is the above vector data along with the Hessian matrix **H** and the Jacobian matrix **A**, will be restored.

The default is restore_problem = 2.

- extrapolate is a scalar variable of type INTEGER(ip_), that specifies whether extrapolation should be used to track the central path. Possible values are:
 - 0 no extrapolation should be used.
 - 1 extrapolation should be used after the final update of the barrier parameter.
 - 2 extrapolation should be used after each update of the barrier parameter.

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- The default is extrapolate = 2.
- path_history is a scalar variable of type INTEGER (ip_), that specifies the maximum number of previous path points used when extrapolating to track the central path. The default is path_history = 1.
- path_derivatives is a scalar variable of type INTEGER (ip_), that specifies the maximum order of derivatives to use when extrapolating to track the central path. The default is path_derivatives = 5.
- fit_order is a scalar variable of type INTEGER(ip_), that specifies the order of (Puiseux or Taylor) series to fit to the available data when building the extrapolant to track the central path. If fit_order ≤ 0 , the order will be such that all available data as specified by path_history and path_derivatives will be used. The default is fit_order = -1.
- infinity is a scalar variable of type REAL(rp_), 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 = 10^{19} .
- stop_p is a scalar variable of type REAL (rp_), 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_QPC_double).
- stop_d is a scalar variable of type default REAL(rp_), 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 GALAH-AD_QPC_double).
- stop_c is a scalar variable of type default REAL (rp_), 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_QPC_double).
- prfeas is a scalar variable of type REAL(rp_), that aims to specify the closest that any initial variable may be to infeasibility. Any variable closer to infeasibility than prfeas will be moved to prfeas from the offending bound. However, if a variable is range bounded, and its bounds are closer than prfeas apart, it will be moved to the mid-point of the two bounds. The default is prfeas = 1.0.
- dufeas is a scalar variable of type REAL (rp_), that aims to specify the closest that any initial dual variable or Lagrange multiplier may be to infeasibility. Any variable closer to infeasibility than prfeas will be moved to dufeas from the offending bound. However, if a dual variable is range bounded, and its bounds are closer than dufeas apart, it will be moved to the mid-point of the two bounds. The default is dufeas = 1.0.
- muzero is a scalar variable of type REAL(rp_), that holds the initial value of the barrier parameter. If muzero is not positive, it will be reset automatically to an appropriate value. The default is muzero = -1.0.
- reduce_infeas is a scalar variable of type default REAL(rp_), that specifies the least factor by which the overall infeasibility of the problem must be reduced, over infeas_max consecutive iterations, for it not be declared infeasible (see infeas_max). The default is reduce_infeas = 0.99.
- obj_unbounded is a scalar variable of type default REAL (rp_), that specifies smallest value of the objective function that will be tolerated before the problem is declared to be unbounded from below. The default is obj_unbounded $= -u^{-2}$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- identical_bounds_tol is a scalar variable of type REAL(rp_). Every pair of constraint bounds (c_i^l, c_i^u) or (x_j^l, x_j^u) that is closer than identical_bounds_tol will be reset to the average of their values, $\frac{1}{2}(c_i^l + c_i^u)$ or $\frac{1}{2}(x_j^l + x_j^u)$ respectively. The default is identical_bounds_tol = u, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- indicator_tol_p is a scalar variable of type REAL (rp_) that provides the indicator tolerance associated with the test indicator_type = 1. The default is indicator_tol_p = $u^{1/3}$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).

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indicator_tol_pd is a scalar variable of type REAL (rp_) that provides the indicator tolerance associated with the test indicator_type = 2. The default is indicator_tol_pd = 1.0.

- indicator_tol_tapia is a scalar variable of type REAL(rp_) that provides the indicator tolerance associated with the test indicator_type = 3. The default is indicator_tol_tapia = 0.9.
- inner_stop_relative and inner_stop_absolute are scalar variables of type REAL(rp_), that hold the relative and absolute convergence tolerances for the inner iteration (search direction) problem using the package GA-LAHAD_GLTR, and correspond to the values control%stop_relative and control%stop_absolute in that package. The defaults are inner_stop_relative = 0.01 and inner_stop_absolute = \sqrt{u} , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- initial_radius is a scalar variable of type default REAL(rp_), that specifies the initial trust-region radius. If initial_radius is not positive, it will be reset automatically to an appropriate value. The default is initial_radius = -1.0.
- inner_fraction_opt is a scalar variable of type default REAL (rp_), that specifies the fraction of the optimal value which is acceptable for the solution of the inner iteration (search direction) problem using the package GALAH—AD_GLTR, and corresponds to the value control%fraction_opt in that package. A negative value is considered to be zero, and a value of larger than one is considered to be one. Reducing fraction_opt below one will result in a reduction of the computation performed at the expense of an inferior optimal value. The default is inner_fraction_opt = 0.1.
- cpu_time_limit is a scalar variable of type REAL(rp_), 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.
- clock_time_limit is a scalar variable of type REAL(rp_), that is used to specify the maximum permitted elapsed system clock time. Any negative value indicates no limit will be imposed. The default is clock_time_limit = -1.0.
- remove_dependencies is a scalar variable of type default LOGICAL, that must be set .TRUE. if the algorithm is to attempt to remove any linearly dependent constraints before solving the problem, and .FALSE. otherwise. We recommend removing linearly dependencies. The default is remove_dependencies = .TRUE..
- treat_zero_bounds_as_general is a scalar variable of type default LOGICAL. If it is set to .FALSE., variables which are only bounded on one side, and whose bound is zero, will be recognised as non-negativities/non-positivities rather than simply as lower- or upper-bounded variables. If it is set to .TRUE., any variable bound x_j^l or x_j^u which has the value 0.0 will be treated as if it had a general value. Setting treat_zero_bounds_as_general to .TRUE. has the advantage that if a sequence of problems are reordered, then bounds which are "accidentally" zero will be considered to have the same structure as those which are nonzero. However, GALAHAD_QPC is able to take special advantage of non-negativities/non-positivities, so if a single problem, or if a sequence of problems whose bound structure is known not to change, is/are to be solved, it will pay to set the variable to .FALSE.. The default is treat_zero_bounds_as_general = .FALSE..
- center is a scalar variable of type default LOGICAL, that must be set .TRUE. if the algorithm will should use the analytic center of the feasible set as its initial feasible point, and .FALSE. otherwise. We recommend using the analytic center. The default is center = .TRUE..
- primal is a scalar variable of type default LOGICAL, that must be set .TRUE. if a primal-barrier Hessian will be used and .FALSE. if the primal-dual Hessian is preferred. We recommend using the primal-dual Hessian. The default is primal = .FALSE..
- puiseux is a scalar variable of type default LOGICAL, that must be set .TRUE. if a Puiseux series will be used when extrapolating along the central path and .FALSE. if a Taylor series is preferred. We recommend using the Puiseux series unless the solution is known to be non-degenerate. The default is puiseux = .TRUE..

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- feasol is a scalar variable of type default LOGICAL, that should be set .TRUE. if the final solution obtained will be perturbed so that variables close to their bounds are moved onto these bounds, and .FALSE. otherwise. The default is feasol = .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 = "".
- LSQP_control is a scalar variable of type LSQP_control_type whose components are used to control the initial feasible point calculation performed by the package GALAHAD_LSQP. See the specification sheet for the package GALAHAD_LSQP for details, and appropriate default values (but note that default value for LSQP_control%feasol is changed to .FALSE..
- FDC_control is a scalar variable of type FDC_control_type whose components are used to control any detection of linear dependencies performed by the package GALAHAD_FDC. See the specification sheet for the package GALAHAD_FDC for details, and appropriate default values.
- SBLS_control is a scalar variable of type SBLS_control_type whose components are used to control preconditioning, needed to accelerate the step calculation, performed by the package GALAHAD_SBLS. See the specification sheet for the package GALAHAD_SBLS for details, and appropriate default values (but note that if SBLS_control*preconditioner = 5, the diagonal matrix used is corresponds to replacing the Hesian matrix by its barrier terms).
- GLTR_control is a scalar variable of type GLTR_control_type whose components are used to control the step calculation performed by the package GALAHAD_GLTR. See the specification sheet for the package GALAHAD_GLTR for details, and appropriate default values.

2.4.4 The derived data type for holding control parameters specifically for the interior-point phase in the convex case

The derived data type CQP_control_type is used to hold controlling data for the interior-point phase of the calculation for convex problems, performed by the GALAHAD package GALAHAD_CQP. Components may be changed by calling CQP_read_specfile (see the documentation for GALAHAD_CQP for details). The components of CQP_control_type are:

- error is a scalar variable of type INTEGER (ip_), that holds the stream number for error messages. Printing of error messages in QPC_solve and QPC_terminate is suppressed if error ≤ 0 . The default is error = 6.
- out is a scalar variable of type INTEGER(ip_), that holds the stream number for informational messages. Printing of informational messages in QPC_solve is suppressed if out < 0. The default is out = 6.
- print_level is a scalar variable of type INTEGER(ip_), 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.
- maxit is a scalar variable of type INTEGER (ip_), that holds the maximum number of iterations which will be allowed in QPC_solve. The default is maxit = 1000.
- start_print is a scalar variable of type INTEGER(ip_), that specifies the first iteration for which printing will occur in QPC_solve. If start_print is negative, printing will occur from the outset. The default is start_print = -1

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stop_print is a scalar variable of type INTEGER(ip_), that specifies the last iteration for which printing will occur in QPC_solve. If stop_print is negative, printing will occur once it has been started by start_print. The default is stop_print = -1.

- infeas_max is a scalar variable of type INTEGER (ip_), that specifies the number of iterations for which the overall infeasibility of the problem is not reduced by at least a factor reduce_infeas before the problem is flagged as infeasible (see reduce_infeas). The default is infeas_max = 200.
- muzero_fixed is a scalar variable of type INTEGER(ip_), that specifies the number of iterations before the initial barrier parameter (see muzero) may be altered. The default is muzero_fixed = 1.
- indicator_type is a scalar variable of type INTEGER(ip_), that specifies the type of indicator used to assess when a variable or constraint is active. Possible values are:
 - 1 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator—tol_p (see below).
 - 2 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator—tol_pd (see below) times the magnitude of its corresponding dual variable.
 - 3 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator_tol_tapia (see below) times the distance to the same bound at the previous iteration.

The default is indicator_type = 3.

- arc is a scalar variable of type INTEGER (ip_), that specifies the type of residual trajectory used to define the path to the solution. Possible values are:
 - 1 the residual trajectory proposed by Zhang will be used.
 - 2 the residual trajectory proposed by Zhao and Sun will be used; note this trajectory does not necessarily ensure convergence, so should be used with caution.
 - 3 a combination in which Zhang's trajectory is used until the method determines that Zhou and Sun's will be better.
 - 4 a mixed linear-quadratic variant of Zhang's proposal will be used.

The default is arc = 1.

- series_order is a scalar variable of type INTEGER(ip_), that specifies the order of (Puiseux or Taylor) series to approximate the residual trajectory. The default is series_order = 2.
- infinity is a scalar variable of type REAL(rp_), 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 = 10^{19} .
- stop_abs_p and stop_rel_p are scalar variables of type REAL(rp_), that hold the required absolute and relative accuracy for the primal infeasibility (see Section 4). The absolute value of each component of the primal infeasibility on exit is required to be smaller than the larger of stop_abs_p and stop_rel_p times a "typical value" for this component. The defaults are stop_abs_p = stop_rel_p = $u^{1/3}$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- stop_abs_d and stop_rel_d are scalar variables of type REAL (rp_), that hold the required absolute and relative accuracy for the dual infeasibility (see Section 4). The absolute value of each component of the dual infeasibility on exit is required to be smaller than the larger of stop_abs_p and stop_rel_p times a "typical value" for this component. The defaults are stop_abs_d = stop_rel_d = $u^{1/3}$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).

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- stop_abs_c and stop_rel_c are scalar variables of type REAL(rp_), that hold the required absolute and relative accuracy for the violation of complementary slackness (see Section 4). The absolute value of each component of the complementary slackness on exit is required to be smaller than the larger of stop_abs_p and stop_rel_p times a "typical value" for this component. The defaults are stop_abs_c = stop_rel_c = $u^{1/3}$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- perturb_h is a scalar variable of type REAL (rp_), that specifies any perturbation that is to be added to the diagonal of **H**. The default is perturb_h = 0.0.
- prfeas is a scalar variable of type REAL (rp_), that aims to specify the closest that any initial variable may be to infeasibility. Any variable closer to infeasibility than prfeas will be moved to prfeas from the offending bound. However, if a variable is range bounded, and its bounds are closer than prfeas apart, it will be moved to the mid-point of the two bounds. The default is prfeas = 10⁴.
- dufeas is a scalar variable of type REAL (rp_), that aims to specify the closest that any initial dual variable or Lagrange multiplier may be to infeasibility. Any variable closer to infeasibility than prfeas will be moved to dufeas from the offending bound. However, if a dual variable is range bounded, and its bounds are closer than dufeas apart, it will be moved to the mid-point of the two bounds. The default is dufeas = 10⁴.
- muzero is a scalar variable of type REAL (rp_), that holds the initial value of the barrier parameter. If muzero is not positive, it will be reset automatically to an appropriate value. The default is muzero = -1.0.
- tau is a scalar variable of type REAL(rp_), that holds the weight attached to primal-dual infeasibility compared to complementarity when assessing step acceptance. The default is tau = 1.0.
- gamma_c is a scalar variable of type REAL (rp_), that holds the smallest value that individual complementarity pairs are allowed to be relative to the average as the iteration proceeds. The default is gamma_c = 10^{-5} .
- gamma_f is a scalar variable of type REAL (rp_), that holds the smallest value the average complementarity is allowed to be relative to the primal-dual infeasibility as the iteration proceeds. The default is gamma_c = 10^{-5} .
- reduce_infeas is a scalar variable of type default REAL(rp_), that specifies the least factor by which the overall infeasibility of the problem must be reduced, over infeas_max consecutive iterations, for it not be declared infeasible (see infeas_max). The default is reduce_infeas = 0.99.
- obj_unbounded is a scalar variable of type default REAL (rp_), that specifies smallest value of the objective function that will be tolerated before the problem is declared to be unbounded from below. The default is obj_unbounded $= -u^{-2}$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- potential_unbounded is a scalar variable of type default REAL(rp_), that specifies smallest value of the potential function divided by the number of one-sided variable and constraint bounds that will be tolerated before the analytic center is declared to be unbounded. The default is potential_unbounded = -10.0.
- identical_bounds_tol is a scalar variable of type REAL(rp_). Every pair of constraint bounds (c_i^l, c_i^u) or (x_j^l, x_j^u) that is closer than identical_bounds_tol will be reset to the average of their values, $\frac{1}{2}(c_i^l + c_i^u)$ or $\frac{1}{2}(x_j^l + x_j^u)$ respectively. The default is identical_bounds_tol = u, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- mu_pounce is a scalar variable of type REAL (rp_) that specifies the value of the barrier parameter that must be attained before an extrapolating "pounce" may be attempted. The default is mu_pounce = 10^{-5} .
- indicator_tol_p is a scalar variable of type REAL (rp_) that provides the indicator tolerance associated with the test indicator_type = 1. The default is indicator_tol_p = $u^{1/3}$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).

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indicator_tol_pd is a scalar variable of type REAL(rp_) that provides the indicator tolerance associated with the test indicator_type = 2. The default is indicator_tol_pd = 1.0.

- indicator_tol_tapia is a scalar variable of type REAL (rp_) that provides the indicator tolerance associated with the test indicator_type = 3. The default is indicator_tol_tapia = 0.9.
- cpu_time_limit is a scalar variable of type REAL(rp_), 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.
- clock_time_limit is a scalar variable of type REAL(rp_), that is used to specify the maximum permitted elapsed system clock time. Any negative value indicates no limit will be imposed. The default is clock_time_limit = 1.0.
- remove_dependencies is a scalar variable of type default LOGICAL, that must be set .TRUE. if the algorithm is to attempt to remove any linearly dependent constraints before solving the problem, and .FALSE. otherwise. We recommend removing linearly dependencies. The default is remove_dependencies = .TRUE..
- treat_zero_bounds_as_general is a scalar variable of type default LOGICAL. If it is set to .FALSE., variables which are only bounded on one side, and whose bound is zero, will be recognised as non-negativities/non-positivities rather than simply as lower- or upper-bounded variables. If it is set to .TRUE., any variable bound x_j^l or x_j^u which has the value 0.0 will be treated as if it had a general value. Setting treat_zero_bounds_as_general to .TRUE. has the advantage that if a sequence of problems are reordered, then bounds which are "accidentally" zero will be considered to have the same structure as those which are nonzero. However, GALAHAD_QPC is able to take special advantage of non-negativities/non-positivities, so if a single problem, or if a sequence of problems whose bound structure is known not to change, is/are to be solved, it will pay to set the variable to .FALSE.. The default is treat_zero_bounds_as_general = .FALSE..
- just_feasible is a scalar variable of type default LOGICAL, that must be set .TRUE. if the algorithm should stop as soon as a feasible point of the constraint set is found, and .FALSE. otherwise. The default is just_feasible = .FALSE..
- getdua is a scalar variable of type default LOGICAL, that must be set .TRUE. if the user-provided estimates of the dual variables should be replaced by estimates whose aim is to try to balance the requirements of dual feasibility and complementary slackness, and .FALSE. if users estimates are to be used. The default is getdua = .FALSE..
- puiseux is a scalar variable of type default LOGICAL, that must be set .TRUE. if a Puiseux series will be used when extrapolating along the central path and .FALSE. if a Taylor series is preferred. We recommend using the Puiseux series unless the solution is known to be non-degenerate. The default is puiseux = .TRUE..
- every_order is a scalar variable of type default LOGICAL, that must be set .TRUE. if every order of approximation up to series_order will be tried and the best taken, and .FALSE. if only the exact order specified by series_order will be used. The default is every_order = .TRUE..
- feasol is a scalar variable of type default LOGICAL, that should be set .TRUE. if the final solution obtained will be perturbed so that variables close to their bounds are moved onto these bounds, and .FALSE. otherwise. The default is feasol = .FALSE..
- balance_initial_complentarity is a scalar variable of type default LOGICAL, that should be set .TRUE. if the initial complementarity is required to be balanced, and .FALSE. otherwise. The default is balance_initial_complentarity = .FALSE..
- crossover is a scalar variable of type default LOGICAL, that must be set .TRUE. if the solution is to be defined in terms of linearly-independent constraints, and .FALSE. otherwise. The default is crossover = .TRUE..

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- 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..
- 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 = "".
- FDC_control is a scalar variable of type FDC_control_type whose components are used to control any detection of linear dependencies performed by the package GALAHAD_FDC. See the specification sheet for the package GALAHAD_FDC for details, and appropriate default values.
- SBLS_control is a scalar variable of type SBLS_control_type whose components are used to control factorizations performed by the package GALAHAD_SBLS. See the specification sheet for the package GALAHAD_SBLS for details, and appropriate default values.
- FIT_control is a scalar variable of type FIT_control_type whose components are used to control fitting of data to polynomials performed by the package GALAHAD_FIT. See the specification sheet for the package GALAHAD_FIT for details, and appropriate default values.
- ROOTS_control is a scalar variable of type ROOTS_control_type whose components are used to control the polynomial root finding performed by the package GALAHAD_ROOTS. See the specification sheet for the package GALAHAD_ROOTS for details, and appropriate default values.
- CRO_control is a scalar variable of type CRO_control_type whose components are used to control crossover performed by the package GALAHAD_CRO. See the specification sheet for the package GALAHAD_CRO for details, and appropriate default values.

2.4.5 The derived data type for holding control parameters specifically for the working-set phase

The derived data type <code>QPA_control_type</code> is used to hold controlling data for the working-set phase of the calculation performed by the GALAHAD package <code>GALAHAD_QPA</code>. Components may be changed by calling <code>QPA_read_specfile</code> (see the documentation for <code>GALAHAD_QPA</code> for details). The components of <code>QPA_control_type</code> are:

- error is a scalar variable of type INTEGER (ip_), that holds the stream number for error messages. Printing of error messages in QPA_solve and QPA_terminate is suppressed if error ≤ 0 . The default is error = 6.
- out is a scalar variable of type INTEGER(ip_), that holds the stream number for informational messages. Printing of informational messages in QPA_solve is suppressed if out < 0. The default is out = 6.
- print_level is a scalar variable of type INTEGER(ip_), 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.
- maxit is a scalar variable of type INTEGER (ip_), that holds the maximum number of iterations which will be allowed in QPA_solve. The default is maxit = 1000.
- start_print is a scalar variable of type INTEGER(ip_), that specifies the first iteration for which printing will occur in QPA_solve. If start_print is negative, printing will occur from the outset. The default is start_print = -1.

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stop_print is a scalar variable of type INTEGER(ip_), that specifies the last iteration for which printing will occur in QPA_solve. If stop_print is negative, printing will occur once it has been started by start_print. The default is stop_print = -1.

- factor is a scalar variable of type INTEGER(ip_), that indicates the type of factorization of the preconditioner to be used. Possible values are:
 - 0 the type is chosen automatically on the basis of which option looks likely to be the most efficient.
 - 1 a Schur-complement factorization will be used.
 - 2 an augmented-system factorization will be used.

The default is factor = 0.

- max_col is a scalar variable of type INTEGER(ip_), that specifies the maximum number of nonzeros in a column of **A** which is permitted by the Schur-complement factorization. The default is max_col = 35.
- max_sc is a scalar variable of type INTEGER(ip_), that specifies the maximum number of columns permitted in the Schur complement of the reference matrix (see Section 4) before a refactorization is triggered. The default is max_sc = 75.
- itref_max is a scalar variable of type INTEGER(ip_), that specifies the maximum number of iterative refinements allowed with each application of the preconditioner. The default is itref_max = 1.
- cg_maxit is a scalar variable of type INTEGER(ip_), that holds the maximum number of conjugate-gradient inner iterations that may be performed during the computation of each search direction in QPA_solve. If cg_itmax is set to a negative number, it will be reset by QPA_solve to the dimension of the relevant linear system +1. The default is cq_itmax = -1.
- precon is a scalar variable of type INTEGER (ip_), that specifies which preconditioner to be used to accelerate the conjugate-gradient inner iteration. Possible values are:
 - 0 the type is chosen automatically on the basis of which option looks likely to be the most efficient at any given stage of the solution process. Different preconditioners may be used at different stages.
 - 1 a full factorization using the Hessian, which is equivalent to replacing the conjugate gradient inner iteration by a direct method. The Hessian may be perturbed to ensure that the resultant matrix is a preconditioner.
 - 2 the Hessian matrix is replaced by the identity matrix.
 - 3 the Hessian matrix is replaced by a band of given semi-bandwidth (see nsemib below).
 - 4 the Hessian matrix terms in the current reference matrix (see Section 4) are replaced by the identity matrix.
 - 5 the Hessian matrix terms outside a band of given semi-bandwidth in the current reference matrix are replaced by zeros (see nsemib below).

The default is precon = 0.

- nsemib is a scalar variable of type INTEGER (ip_), that specifies the semi-bandwidth of the band preconditioner when precon = 3, if appropriate. The default is nsemib = 5.
- full_max_fill is a scalar variable of type INTEGER(ip_). If the ratio of the number of nonzeros in the factors of the reference matrix (see Section 4) to the number of nonzeros in the matrix itself exceeds full_max_fil, and the preconditioner is being selected automatically (precon = 0), a banded approximation (see precon = 3) will be used instead. The default is full_max_fill = 10.

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- deletion_strategy is a scalar variable of type INTEGER(ip_), that specifies the rules used to determine which constraint to remove from the working set (see Section 4) when necessary to ensure further progress towards the solution. Possible values are:
 - 0 the constraint whose Lagrange multiplier most violates its required optimality bound will be removed.
 - 1 the most-recently added constraint whose Lagrange multiplier violates its required optimality bound will be removed.
 - k > 1 among the k most-recently added constraints whose Lagrange multipliers violates their required optimality bounds, the one which most violates its bound will be removed.

The default is deletion_strategy = 0.

- restore_problem is a scalar variable of type INTEGER(ip_), that specifies how much of the input problem is to be retored on output. Possible values are:
 - 0 nothing is restored.
 - 1 the vector data \mathbf{g} , \mathbf{c}^l , \mathbf{c}^u , \mathbf{x}^l , and \mathbf{x}^u will be restored to their input values.
 - 2 the entire problem, that is the above vector data along with the Hessian matrix **H** and the Jacobian matrix **A**, will be restored.

The default is restore_problem = 2.

- monitor_residuals is a scalar variable of type INTEGER(ip_), that specifies the frequency at which working constraint residuals will be monitored to ensure feasibility. The residuals will be monitored every monitor_residual iterations. The default is monitor_residuals = 1.
- cold_start is a scalar variable of type INTEGER (ip_), that controls the initial working set (see Section 4)). Possible values are:
 - 0 a "warm start" will be performed. The values set in C_stat and B_stat indicate which constraints will be included in the initial working set. (see C_stat and B_stat in Section 2.5.2).
 - 1 the constraints "active" at p%X (see Section 2.5.2) will determine the initial working set.
 - 2 the initial working set will be empty.
 - 3 the initial working set will only contain equality constraints.
 - 4 the initial working set will contain as many active constraints as possible, chosen (in order) from equality constraints, simple bounds, and finally general linear constraints.

The default is cold_start = 3.

- infeas_check_interval is a scalar variable of type INTEGER(ip_), that gives the number of iterations that are permitted before the infeasibility is checked for improvement. The default is infeas_check_interval = 100.
- infinity is a scalar variable of type REAL(rp_), 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 = 10^{19} .
- feas_tol is a scalar variable of type REAL(rp_), that specifies the maximum amount by which a constraint may be violated and yet still be considered to be satisfied. The default is feas_tol = $u^{3/4}$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- obj_unbounded is a scalar variable of type default REAL (rp_), that specifies smallest value of the objective function that will be tolerated before the problem is declared to be unbounded from below. The default is potential_unbounded = $-u^{-2}$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).

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increase_rho_g_factor is a scalar variable of type REAL(rp_), that gives the factor by which the current penalty parameter ρ_g for the general constraints may be increased when solving quadratic programs. The default is increase_rho_g_factor = 2.

- increase_rho_b_factor is a scalar variable of type REAL (rp_), that gives the factor by which the current penalty parameter ρ_b for the simple bound constraints may be increased when solving quadratic programs. The default is increase_rho_b_factor = 2.
- infeas_g_improved_by_factor is a scalar variable of type default REAL (rp_), that specifies the relative improvement in the infeasibility that must be achieved when solving quadratic programs if the current value of ρ_g is to be maintained. Specifically if the infeasibility of the general constraints has not fallen by at least a factor infeas_g_improved_by_factor during the previous infeas_check_interval iterations, the penalty parameter will be increased by a factor increase_rho_g_factor. The default is infeas_improved_g_by_factor = 0.75
- infeas_b_improved_by_factor is a scalar variable of type default REAL (rp_), that specifies the relative improvement in the infeasibility that must be achieved when solving quadratic programs if the current value of ρ_b is to be maintained. Specifically if the infeasibility of the simple bound constraints has not fallen by at least a factor infeas_b_improved_by_factor during the previous infeas_check_interval iterations, the penalty parameter will be increased by a factor increase_rho_b_factor. The default is infeas_improved_b_by_factor = 0.75.
- pivot_tol_for_dependencies is a scalar variable of type default REAL(rp_), that holds the relative threshold pivot tolerance used by the matrix factorization when attempting to detect linearly dependent constraints. A value larger than pivot_tol is appropriate. See the documentation for the package SLS for details. The default is pivot_tol_for_dependencies = 0.5.
- multiplier_tol is a scalar variable of type REAL (rp_). Any dual variable or Lagrange multiplier which is less than multiplier_tol outside its optimal interval will be regarded as being acceptable when checking for optimality. The default is zero_pivot = \sqrt{u} , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- inner_stop_relative and inner_stop_absolute are scalar variables of type REAL(rp_), that hold the relative and absolute convergence tolerances for the inner iteration (search direction) problem. and correspond to the values control%stop_relative and control%stop_absolute in the GALAHAD package GALAHAD_GLTR. The defaults are inner_stop_relative = 0.0 and inner_stop_absolute = \sqrt{u} , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- cpu_time_limit is a scalar variable of type REAL(rp_), 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.
- clock_time_limit is a scalar variable of type REAL(rp_), that is used to specify the maximum permitted elapsed system clock time. Any negative value indicates no limit will be imposed. The default is clock_time_limit = 1.0.
- treat_zero_bounds_as_general is a scalar variable of type default LOGICAL. If it is set to .FALSE., variables which are only bounded on one side, and whose bound is zero, will be recognised as non-negativities/non-positivities rather than simply as lower- or upper-bounded variables. If it is set to .TRUE., any variable bound x_j^l or x_j^u which has the value 0.0 will be treated as if it had a general value. Setting treat_zero_bounds_as_general to .TRUE. has the advantage that if a sequence of problems are reordered, then bounds which are "accidentally" zero will be considered to have the same structure as those which are nonzero. However, GALAHAD_QPC is able to take special advantage of non-negativities/non-positivities, so if a single problem, or if a sequence of problems whose bound structure is known not to change, is/are to be solved, it will pay to set the variable to .FALSE.. The default is treat_zero_bounds_as_general = .FALSE..

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- ramdomize is a scalar variable of type default LOGICAL, that must be set .TRUE. if the user wishes to perturb the constraint bounds by small random quantities during the first stage of the solution process, and .FALSE. otherwise. Any randomization will ultimately be removed. Randomization helps when solving degenerate problems and is usually to be recommended. The default is randomize = .TRUE..
- symmetric_linear_solver is a scalar variable of type default CHARACTER and length 30, that specifies the external package to be used to solve any symmetric linear system that might arise. Current possible choices are 'sils', 'ma27', 'ma57', 'ma77', 'ma86', 'ma97', ssids, 'pardiso' and 'wsmp', although only 'sils' and, for OMP 4.0-compliant compilers, 'ssids' are installed by default. See the documentation for the GALAHAD package SLS for further details. The default is symmetric_linear_solver = 'sils'.
- definite_linear_solver is a scalar variable of type default CHARACTER and length 30, that specifies the external package to be used to solve any symmetric positive-definite linear system that might arise. Current possible choices are 'sils', 'ma27', 'ma57', 'ma77', 'ma86', 'ma87', 'ma97', ssids, 'pardiso' and 'wsmp', although only 'sils' and, for OMP 4.0-compliant compilers, 'ssids' are installed by default. See the documentation for the GALAHAD package SLS for further details. The default is definite_linear_solver = 'sils'.
- 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 = "".
- SLS_control is a scalar variable argument of type SLS_control_type that is used to pass control options to external packages used to factorize relevant symmetric matrices that arise. See the documentation for the GALAHAD package SLS for further details. In particular, default values are as for SLS, except that SLS_control%relative_pivot_tolerance is reset to pivot_tol.

2.4.6 The derived data type for holding control parameters specifically for the equality-constrained phase

The derived data type EQP_control_type is used to hold controlling data for the equality-constrained QP phase of the calculation (if any), performed by the GALAHAD package GALAHAD_EQP. Components may be changed by calling EQP_read_specfile (see the documentation for GALAHAD_EQP for details). The components of EQP_control_type are:

- error is a scalar variable of type INTEGER (ip_), that holds the stream number for error messages. Printing of error messages in QPC_solve and QPC_terminate is suppressed if error ≤ 0 . The default is error = 6.
- out is a scalar variable of type INTEGER(ip_), that holds the stream number for informational messages. Printing of informational messages in QPC_solve is suppressed if out < 0. The default is out = 6.
- print_level is a scalar variable of type INTEGER(ip_), 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.
- new_h is a scalar variable of type INTEGER(ip_), that is used to indicate how H has changed (if at all) since the previous call to QPC_solve. Possible values are:
 - 0 **H** is unchanged
 - 1 the values in **H** have changed, but its nonzero structure is as before.
 - 2 both the values and structure of **H** have changed.

The default is $new_h = 2$.

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new_a is a scalar variable of type INTEGER(ip_), that is used to indicate how A has changed (if at all) since the previous call to QPC_solve. Possible values are:

- 0 A is unchanged
- 1 the values in **A** have changed, but its nonzero structure is as before.
- 2 both the values and structure of **A** have changed.

The default is new_a = 2.

- cg_maxit is a scalar variable of type INTEGER (ip_), that is used to limit the number of conjugate-gradient iterations performed in the optimality phase. If cg_maxit is negative, no limit will be impossed. The default is cg_maxit = 200.
- radius is a scalar variable of type default REAL (rp_), that may be used to specify an upper bound on the norm of the allowed solution (a "trust-region" constraint) during the iterative solution of the optimality phase of the problem. This is particularly useful if the problem is unbounded from below. If radius is set too small, there is a possibility that this will preclude the package from finding the actual solution. If initial_radius is not positive, it will be reset to the default value, initial_radius = SQRT(0.1*HUGE(1.0)) (SQRT(0.1*HUGE(1.0D0)) in GALAHAD_QPC_double).
- inner_stop_relative and inner_stop_absolute are scalar variables of type REAL(rp_), that hold the relative and absolute convergence tolerances for the iterative solution of the optimality phase of the problem using the package GALAHAD_GLTR, and correspond to the values control%stop_relative and control%stop_absolute in that package. The defaults are inner_stop_relative = 0.01 and inner_stop_absolute = \sqrt{u} , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- max_infeasibility_relative and max_infeasibility_absolute are scalar variables of type REAL(rp_), that hold the relative and absolute tolerances for assessing infeasibility in the feasibility phase. If the constraints are believed to be rank defficient and the norm of the residual $\mathbf{A}\mathbf{x}_T + \mathbf{c}$ at a "typical" feasiblke point is larger than $\max(\max_i \text{nfeasibility}_relative*||A||, \max_i \text{nfeasibility}_absolute)$, the problem will be marked as infeasible, The defaults are $\max_i \text{nfeasibility}_relative = \max_i \text{nfeasibility}_absolute = u^{0.75}$ where u is EPSILON(1.0) (EPSILON(1.000) in $\text{GALAHAD}_QPC_double$).
- remove_dependencies is a scalar variable of type default LOGICAL, that must be set .TRUE. if linear dependent constraints Ax + c = 0 should be removed and .FALSE. otherwise. The default is remove_dependencies = 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..
- 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..
- FDC_control is a scalar variable of type FDC_control_type whose components are used to control any detection of linear dependencies performed by the package GALAHAD_FDC. See the specification sheet for the package GALAHAD_FDC for details, and appropriate default values.
- GLTR_control is a scalar variable argument of type GLTR_control_type that is used to pass control options to the conjugate-gradient solver used to solve linear systems that arise. See the documentation for the GALAHAD package GLTR for further details. In particular, default values are as for GLTR.

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- SBLS_control is a scalar variable argument of type SBLS_control_type that is used to pass control options to the symmetric block linear equation preconditioner used to help solve linear systems that arise. See the documentation for the GALAHAD package SBLS for further details. In particular, default values are as for SBLS.
- 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 ignoreing 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 = ""

2.4.7 The derived data type for holding control parameters

The derived data type QPC_control_type is used to hold controlling data. Default values may be obtained by calling QPC_initialize (see Section 2.5.1), while components may also be changed by calling QPC_read_specfile (see Section 2.7.1). The components of QPC_control_type are:

- error is a scalar variable of type INTEGER (ip_), that holds the stream number for error messages. Printing of error messages in QPC_solve and QPC_terminate is suppressed if error ≤ 0 . The default is error = 6.
- out is a scalar variable of type INTEGER(ip_), that holds the stream number for informational messages. Printing of informational messages in QPC_solve is suppressed if out < 0. The default is out = 6.
- print_level is a scalar variable of type INTEGER(ip_), 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.
- restore_problem is a scalar variable of type INTEGER(ip_), that specifies how much of the input problem is to be retored on output. Possible values are:
 - 0 nothing is restored.
 - 1 the vector data \mathbf{g} , \mathbf{c}^l , \mathbf{c}^u , \mathbf{x}^l , and \mathbf{x}^u will be restored to their input values.
 - 2 the entire problem, that is the above vector data along with the Hessian matrix **H** and the Jacobian matrix **A**, will be restored.

The default is restore_problem = 2.

- infinity is a scalar variable of type REAL(rp_), 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 = 10^{19} .
- identical_bounds_tol is a scalar variable of type REAL(rp_). Every pair of constraint bounds (c_i^l, c_i^u) or (x_j^l, x_j^u) that is closer than identical_bounds_tol will be reset to the average of their values, $\frac{1}{2}(c_i^l + c_i^u)$ or $\frac{1}{2}(x_j^l + x_j^u)$ respectively. The default is identical_bounds_tol = u, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).
- rho_g is a scalar variable of type REAL(rp_), that holds the initial values of the parameter, ρ_g , used to weight the infeasibility term $\nu_g(\mathbf{x})$ for the working-set phase (see Section 4).
- rho_b is a scalar variable of type REAL (rp_), that holds the initial values of the parameter, ρ_b , used to weight the infeasibility term $v_b(\mathbf{x})$ for the working-set phase (see Section 4).
- on_bound_tol is a scalar variable of type REAL (rp_) that specifies the furthest a variable or constraint may be from one of its bounds to be regarded as active. The default is on_bound_tol = u, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_QPC_double).

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cpu_time_limit is a scalar variable of type REAL(rp_), 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.

- clock_time_limit is a scalar variable of type REAL(rp_), that is used to specify the maximum permitted elapsed system clock time. Any negative value indicates no limit will be imposed. The default is clock_time_limit = 1.0.
- convex is a scalar variable of type default LOGICAL, that must be set .TRUE. if the problem is convex (i.e., if the matrix **H** is positive semi-definite) and the user wishes to take advantage of the fact, and .FALSE. otherwise. The package will usually run faster for convex problems if convex is .TRUE., but convex must be set .FALSE. if the user is uncertain as otherwise the package may fail. The default is convex = .FALSE.
- treat_zero_bounds_as_general is a scalar variable of type default LOGICAL. If it is set to .FALSE., variables which are only bounded on one side, and whose bound is zero, will be recognised as non-negativities/non-positivities rather than simply as lower- or upper-bounded variables. If it is set to .TRUE., any variable bound x_j^l or x_j^u which has the value 0.0 will be treated as if it had a general value. Setting treat_zero_bounds_as_general to .TRUE. has the advantage that if a sequence of problems are reordered, then bounds which are "accidentally" zero will be considered to have the same structure as those which are nonzero. However, GALAHAD_QPC is able to take special advantage of non-negativities/non-positivities, so if a single problem, or if a sequence of problems whose bound structure is known not to change, is/are to be solved, it will pay to set the variable to .FALSE.. The default is treat_zero_bounds_as_general = .FALSE..
- 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..
- 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..
- no_qpa is a scalar variable of type default LOGICAL, that must be set .TRUE. if the user wishes to skip the working-set phase of the computation, and .FALSE. if this phase is required. The default is no_qpa = .FALSE..
- no_qpb is a scalar variable of type default LOGICAL, that must be set .TRUE. if the user wishes to skip the interior-point phase of the computation, and .FALSE. if this phase is required. The default is no_qpa = .FALSE..
- qpb_or_qpa is a scalar variable of type default LOGICAL, that must be set .TRUE. if the user wishes to use the interiorpoint phase of the computation, but only to follow this with the working-set phase if the former is unsuccessful,
 and to .FALSE. if both phases are to be used (subject to the requests made in no_qpa and no_qpb). The default
 is qpb_or_qpa = .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 = "".
- QPA_control is a scalar variable of type QPA_control_type (see Section 2.4.5 whose components are used to control the working-set phase of the calculation, performed by the package GALAHAD_QPA.
- QPB_control is a scalar variable of type QPB_control_type (see Section 2.4.3 whose components are used to control the interior-point phase of the calculation, performed by the package GALAHAD_QPB.
- CQP_control is a scalar variable of type CQP_control_type (see Section 2.4.4 whose components are used to control the convex primal-dual phase of the calculation, performed by the package GALAHAD_CQP.

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- EQP_control is a scalar variable of type EQP_control_type (see Section 2.4.6 whose components are used to control the equality-constrained phase of the calculation (if any), performed by the package GALAHAD_EQP.
- FDC_control is a scalar variable of type FDC_control_type whose components are used to control any detection of linear dependencies performed by the package GALAHAD_FDC. See the specification sheet for the package GALAHAD_FDC for details, and appropriate default values.

2.4.8 The derived data type for holding timing information

The derived data type QPC_time_type is used to hold elapsed CPU and system clock times for the various parts of the calculation. The components of QPC_time_type are:

- total is a scalar variable of type REAL (rp_), that gives the total CPU time spent in the package.
- preprocess is a scalar variable of type REAL (rp_), that gives the CPU time spent reordering the problem to standard form prior to solution.
- find_dependent is a scalar variable of type REAL(rp_), that gives the CPU time spent detecting and removing linearly-dependent equality constraints
- analyse is a scalar variable of type REAL (rp_), that gives the CPU time spent analysing the required matrices prior to factorization.
- factorize is a scalar variable of type REAL (rp_), that gives the CPU time spent factorizing the required matrices.
- solve is a scalar variable of type REAL (rp_), that gives the CPU time spent computing the search direction.
- clock_total is a scalar variable of type REAL(rp_), that gives the total elapsed system clock time spent in the package.
- clock_preprocess is a scalar variable of type REAL (rp_), that gives the elapsed system clock time spent reordering the problem to standard form prior to solution.
- clock_find_dependent is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent detecting and removing linearly-dependent equality constraints
- clock_analyse is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent analysing the required matrices prior to factorization.
- clock_factorize is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent factorizing the required matrices.
- clock_solve is a scalar variable of type REAL (rp_), that gives the elapsed system clock time spent computing the search direction.

2.4.9 The derived data type for holding informational parameters specifically for the interior-point phase

The derived data type <code>QPB_inform_type</code> is used to hold parameters that give information about the progress of the working-set phase of the algorithm performed by the GALAHAD package <code>GALAHAD_QPB</code>. The components of <code>QPB_inform_type</code> are:

- status is a scalar variable of type INTEGER(ip_), that gives the exit status of the algorithm. See Section 2.6 for details.
- alloc_status is a scalar variable of type INTEGER(ip_), that gives the status of the last attempted array allocation or deallocation. This will be 0 if status = 0.

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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.

- iter is a scalar variable of type INTEGER (ip_), that gives the total number of iterations required.
- factorization_status is a scalar variable of type INTEGER(ip_), that gives the return status from the matrix factorization.
- factorization_integer is a scalar variable of type long INTEGER (ip_), that gives the amount of integer storage used for the matrix factorization.
- factorization_real is a scalar variable of type INTEGER (int 64), that gives the amount of real storage used for the matrix factorization.
- nfacts is a scalar variable of type INTEGER (ip_), that gives the total number of factorizations performed.
- nbacts is a scalar variable of type INTEGER(ip_), that gives the total number of backtracks performed during the sequence of linesearches.
- nmods is a scalar variable of type INTEGER (ip_), that gives the total number of factorizations which were modified to ensure that the matrix is an appropriate preconditioner.
- obj is a scalar variable of type REAL (rp_), that holds the value of the objective function at the best estimate of the solution found.
- non_negligible_pivot is a scalar variable of type REAL (rp_), that holds the value of the smallest pivot larger than control%zero_pivot when searching for dependent linear constraints. If non_negligible_pivot is close to control%zero_pivot, this may indicate that there are further dependent constraints, and it may be worth increasing control%zero_pivot above non_negligible_pivot and solving again.
- feasible is a scalar variable of type default LOGICAL, that has the value .TRUE. if the output value of \boldsymbol{x} satisfies the constraints, and the value .FALSE. otherwise.
- time is a scalar variable of type QPC_time_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).
- LSQP_inform is a scalar variable of type LSQP_inform_type whose components are used to provide information about the initial feasible point calculation performed by the package GALAHAD_LSQP. See the specification sheet for the package GALAHAD_LSQP for details, and appropriate default values.
- FDC_inform is a scalar variable of type FDC_inform_type whose components are used to provide information about any detection of linear dependencies performed by the package GALAHAD_FDC. See the specification sheet for the package GALAHAD_FDC for details.
- SBLS_inform is a scalar variable of type SBLS_inform_type whose components are used to provide information about factorizations performed by the package GALAHAD_SBLS. See the specification sheet for the package GALAHAD_SBLS for details.
- GLTR_inform is a scalar variable of type GLTR_inform_type whose components are used to provide information about the step calculation performed by the package GALAHAD_GLTR. See the specification sheet for the package GALAHAD_GLTR for details.

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2.4.10 The derived data type for holding informational parameters specifically for the interior-point phase in the convex case

The derived data type CQP_inform_type is used to hold parameters that give information about the progress of the working-set phase of the algorithm performed by the GALAHAD package GALAHAD_CQP. The components of CQP_inform_type are:

- status is a scalar variable of type INTEGER(ip_), that gives the exit status of the algorithm. See Section 2.6 for details.
- alloc_status is a scalar variable of type INTEGER(ip_-), 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 INTEGER(ip_), that gives the return status from the matrix factorization.
- factorization_integer is a scalar variable of type long INTEGER (ip_), that gives the amount of integer storage used for the matrix factorization.
- factorization_real is a scalar variable of type INTEGER (int 64), that gives the amount of real storage used for the matrix factorization.
- nfacts is a scalar variable of type INTEGER (ip_), that gives the total number of factorizations performed.
- nbacts is a scalar variable of type INTEGER(ip_), that gives the total number of backtracks performed during the sequence of linesearches.
- threads is a scalar variable of type INTEGER (ip_), that gives the total number of threads used for parallel execution.
- iter is a scalar variable of type INTEGER (ip_), that gives the number of iterations performed.
- obj is a scalar variable of type REAL (rp_), that holds the value of the objective function at the best estimate of the solution found.
- primal_infeasibility is a scalar variable of type REAL(rp_), that holds the norm of the violation of primal optimality (see Section 2.4.8) at the best estimate of the solution found.
- dual_infeasibility is a scalar variable of type REAL (rp_{-}) , that holds the norm of the violation of dual optimality (see Section 2.4.8) at the best estimate of the solution found.
- complementary_slackness is a scalar variable of type REAL(rp_), that holds the norm of the violation of complementary slackness (see Section 2.4.8) at the best estimate of the solution found.
- potential is a scalar variable of type REAL (rp_), that holds the value of the logarithmic potential function sum -log(distance to constraint boundary).
- non_negligible_pivot is a scalar variable of type REAL (rp_), that holds the value of the smallest pivot which was not judged to be zero when detecting linearly dependent constraints.
- feasible is a scalar variable of type default LOGICAL, that has the value . TRUE. if the output value of x satisfies the constraints, and the value . FALSE. otherwise.
- time is a scalar variable of type QPC_time_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).

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FDC_inform is a scalar variable of type FDC_inform_type whose components are used to provide information about any detection of linear dependencies performed by the package GALAHAD_FDC. See the specification sheet for the package GALAHAD_FDC for details.

- SBLS_inform is a scalar variable of type SBLS_inform_type whose components are used to provide information about factorizations performed by the package GALAHAD_SBLS. See the specification sheet for the package GALAHAD_SBLS for details.
- FIT_inform is a scalar variable of type FIT_inform_type whose components are used to provide information about the fitting of data to polynomials performed by the package GALAHAD_FIT. See the specification sheet for the package GALAHAD_FIT for details.
- ROOTS_inform is a scalar variable of type ROOTS_inform_type whose components are used to provide information about the polynomial root finding performed by the package GALAHAD_ROOTS. See the specification sheet for the package GALAHAD_ROOTS for details.
- CRO_inform is a scalar variable of type CRO_inform_type whose components are used to provide information about the crossover performed by the package GALAHAD_CRO. See the specification sheet for the package GALAHAD_CRO for details.

2.4.11 The derived data type for holding informational parameters specifically from the working-set phase

The derived data type QPA_inform_type is used to hold parameters that give information about the progress of the working-set phase of the algorithm performed by the GALAHAD package GALAHAD_QPA. The components of QPA_inform_type are:

- status is a scalar variable of type INTEGER (ip_), that gives the exit status of the algorithm. See Section 2.6 for details.
- alloc_status is a scalar variable of type INTEGER(ip_{-}), 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.
- major_iter is a scalar variable of type INTEGER(ip_), that gives the total number of major iterations required.
- iter is a scalar variable of type INTEGER (ip_), that gives the total number of iterations required.
- cg_iter is a scalar variable of type INTEGER(ip_), that gives the total number of conjugate-gradient inner iterations required.
- factorization_status is a scalar variable of type INTEGER(ip_), that gives the return status from the matrix factorization.
- factorization_integer is a scalar variable of type long INTEGER (ip_), that gives the amount of integer storage used for the matrix factorization.
- factorization_real is a scalar variable of type INTEGER (int 64), that gives the amount of real storage used for the matrix factorization.
- nfacts is a scalar variable of type INTEGER (ip_), that gives the total number of factorizations performed.
- nmods is a scalar variable of type INTEGER (ip_), that gives the total number of factorizations which were modified to ensure that the matrix is an appropriate preconditioner.

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- num_g_infeas is a scalar variable of type INTEGER(ip_), that gives the total number of general constraints that are violated.
- num_b_infeas is a scalar variable of type INTEGER (ip_), that gives the total number of simple bound constraints that are violated.
- obj is a scalar variable of type REAL (rp_), that holds the value of the objective function at the best estimate of the solution found.
- infeas_g is a scalar variable of type REAL (rp_), that holds the value of the infeasibility $v_g(\mathbf{x})$.
- infeas_b is a scalar variable of type REAL (rp_), that holds the value of the infeasibility $v_b(\mathbf{x})$.
- merit is a scalar variable of type REAL (rp_), that holds the value of the merit function $q(\mathbf{x}) + \rho_g v_g(\mathbf{x}) + \rho_b v_b(\mathbf{x})$ at the best estimate of the solution found.
- time is a scalar variable of type QPC_time_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).
- SLS_inform is a scalar variable argument of type SLS_inform_type that is used to pass information concerning the progress of the external packages used to factorize relevant symmetric matrices that arise. See the documentation for the GALAHAD package SLS for further details.

2.4.12 The derived data type for holding informational parameters specifically for the equality-constrained phase

The derived data type EQP_inform_type is used to hold parameters that give information about the progress of the equality-constrained phase of the algorith (if any) performed by the GALAHAD package GALAHAD_EQP. The components of EQP_inform_type are:

- status is a scalar variable of type INTEGER(ip_), that gives the exit status of the algorithm. See Section 2.6 for details.
- alloc_status is a scalar variable of type INTEGER(ip_-), 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.
- cg_iter is a scalar variable of type INTEGER(ip_), that gives the total number of conjugate-gradient iterations required.
- factorization_integer is a scalar variable of type long INTEGER(ip_), that gives the amount of integer storage used for the matrix factorization.
- factorization_real is a scalar variable of type INTEGER (int64), that gives the amount of real storage used for the matrix factorization.
- obj is a scalar variable of type REAL (rp_), that holds the value of the objective function at the best estimate of the solution found.
- time is a scalar variable of type QPC_time_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).
- FDC_inform is a scalar variable of type FDC_inform_type whose components are used to provide information about any detection of linear dependencies performed by the package GALAHAD_FDC. See the specification sheet for the package GALAHAD_FDC for details.

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SBLS_inform is a scalar variable of type SBLS_inform_type whose components are used to hold information relating to the formation and factorization of the preconditioner. See the documentation for the GALAHAD package SBLS for further details.

GLTR_inform is a scalar variable of type GLTR_inform_type whose components are used to hold information relating to the computation of the solution via the conjugate-gradient method. See the documentation for the GALAHAD package GLTR for further details.

2.4.13 The derived data type for holding informational parameters

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

- status is a scalar variable of type INTEGER(ip_), that gives the exit status of the algorithm. See Section 2.6 for details.
- alloc_status is a scalar variable of type INTEGER(ip_-), 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 INTEGER(ip_), that gives the return status from the matrix factorization.
- factorization_integer is a scalar variable of type long INTEGER(ip_), that gives the amount of integer storage used for the matrix factorization.
- factorization_real is a scalar variable of type INTEGER (int 64), that gives the amount of real storage used for the matrix factorization.
- nfacts is a scalar variable of type INTEGER (ip_), that gives the total number of factorizations performed.
- nmods is a scalar variable of type INTEGER (ip_), that gives the total number of factorizations which were modified to ensure that the matrix is an appropriate preconditioner.
- obj is a scalar variable of type REAL (rp_), that holds the value of the objective function at the best estimate of the solution found.
- non_negligible_pivot is a scalar variable of type REAL (rp_), that holds the value of the smallest pivot larger than control%zero_pivot when searching for dependent linear constraints. If non_negligible_pivot is close to control%zero_pivot, this may indicate that there are further dependent constraints, and it may be worth increasing control%zero_pivot above non_negligible_pivot and solving again.
- p_found is a scalar variable of type default LOGICAL, that has the value .TRUE. if the active-set predictions have been computed, and the value .FALSE. otherwise.
- time is a scalar variable of type QPC_time_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).
- QPA_inform is a scalar variable of type QPA_inform_type (see Section 2.4.11 whose components provide information about the progress and needs of the working-set phase of the calculation performed by the package GALAH—AD_QPA.

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- QPB_inform is a scalar variable of type QPB_inform_type (see Section 2.4.9 whose components provide information about the progress and needs of the interior-point phase of the calculation performed by the package GALAH-AD_QPB.
- CQP_inform is a scalar variable of type CQP_inform_type (see Section 2.4.10 whose components provide information about the progress and needs of the primal-dual phase of the calculation performed by the package GALAHAD_CQP.
- EQP_inform is a scalar variable of type EQP_inform_type (see Section 2.4.12 whose components provide information about the progress and needs of the equality-constrained phase of the calculation (if any) performed by the package GALAHAD_EQP.
- FDC_inform is a scalar variable of type FDC_inform_type whose components are used to provide information about any detection of linear dependencies performed by the package GALAHAD_FDC. See the specification sheet for the package GALAHAD_FDC for details.

2.4.14 The derived data type for holding problem data

The derived data type QPC_data_type is used to hold all the data for a particular problem, or sequences of problems with the same structure, between calls of QPC procedures. This data should be preserved, untouched, from the initial call to QPC_initialize to the final call to QPC_terminate.

2.5 Argument lists and calling sequences

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

- 1. The subroutine QPC_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 QPC_solve is called to solve the problem.
- 3. The subroutine QPC_terminate is provided to allow the user to automatically deallocate array components of the private data, allocated by QPC_solve, at the end of the solution process. It is important to do this if the data object is re-used for another problem with a different structure since QPC_initialize cannot test for this situation, and any existing associated targets will subsequently become unreachable.

We use square brackets [] to indicate OPTIONAL arguments.

2.5.1 The initialization subroutine

Default values are provided as follows:

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

- data is a scalar INTENT (INOUT) argument of type QPC_data_type (see Section 2.4.14). It is used to hold data about the problem being solved.
- control is a scalar INTENT (OUT) argument of type QPC_control_type (see Section 2.4.7). On exit, control contains default values for the components as described in Section 2.4.7. These values should only be changed after calling QPC_initialize.
- inform is a scalar INTENT (OUT) argument of type QPC_inform_type (see Section 2.4.13). A successful call to QPC_initialize is indicated when the component status has the value 0. For other return values of status, see Section 2.6.

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2.5.2 The quadratic programming subroutine

The quadratic programming solution algorithm is called as follows:

```
CALL QPC_solve(p, C_stat, B_stat, data, control, inform)
```

p is a scalar INTENT (INOUT) argument of type QPT_problem_type (see Section 2.4.2). It is used to hold data about the problem being solved. For a new problem, the user must allocate all the array components, and set values for all components except p%C. p%new_problem_structure must be set .TRUE., but will have been reset to .FALSE. on exit from QPC_solve. Users are free to choose whichever of the matrix formats described in Section 2.1 is appropriate for A and H for their application—different formats may be used for the two matrices.

For a problem with the same structure as one that has just been solved, the user may set p%new_problem_structure to .FALSE., so long as QPC_terminate has not been called in the interim. The INTEGER(ip_) components must be unaltered since the previous call to QPC_solve, but the REAL(rp_) may be altered to reflect the new problem.

The components p % X, p % Y and p % Z must be set to initial estimates, \mathbf{x}^0 , of the primal variables, \mathbf{x} , Lagrange multipliers for the general constraints, \mathbf{y} , and dual variables for the bound constraints, \mathbf{z} , respectively. 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 p % X = 0.0, p % Y = 0.0 and p % Z = 0.0. The component p % C need not be set on entry.

On exit, the components p%X, p%Y, p%Z and p%C will contain the best estimates of the primal variables x, Lagrange multipliers for the general constraints y, dual variables for the bound constraints z, and values of the constraints Ax respectively. What of the remaining problem data has been restored depends upon the input value of the control parameter control%restore_problem. The return format for a restored array component will be the same as its input format. **Restrictions:** p%n > 0, p%m ≥ 0 , p%A%ne ≥ -2 and p%H%ne ≥ -2 .

- C_stat is a rank-one INTENT (INOUT) array argument of dimension p%m and type INTEGER (ip_), that indicates which of the general linear constraints are in the current working set. Possible values for C_stat (i), $i=1,\ldots,p$ %m, and their meanings are
 - <0 the *i*-th general constraint is in the working set, on its lower bound,
 - >0 the *i*-th general constraint is in the working set, on its upper bound, and
 - 0 the *i*-th general constraint is not in the working set.

Suitable values must be supplied if control%qpa_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, C_stat will contain values appropriate for the ultimate working set.

- B_stat is a rank-one INTENT (INOUT) array argument of dimension p%n and type INTEGER (ip_), that indicates which of the simple bound constraints are in the current working set. Possible values for B_stat(j), $j=1,\ldots,p$ %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%qpa_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, B_stat will contain values appropriate for the ultimate working set.

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data is a scalar INTENT (INOUT) argument of type QPC_data_type (see Section 2.4.14). 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 QPC_initialize.

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- control is a scalar INTENT(IN) argument of type QPC_control_type (see Section 2.4.7). Default values may be assigned by calling QPC_initialize prior to the first call to QPC_solve.
- inform is a scalar INTENT (INOUT) argument of type QPC_inform_type (see Section 2.4.13). A successful call to QPC_solve is indicated when the component status has the value 0. For other return values of status, see Section 2.6.

2.5.3 The termination subroutine

All previously allocated arrays are deallocated as follows:

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

- data is a scalar INTENT (INOUT) argument of type QPC_data_type exactly as for QPC_solve, which must not have been altered by the user since the last call to QPC_initialize. On exit, array components will have been deallocated.
- control is a scalar INTENT (IN) argument of type QPC_control_type exactly as for QPC_solve.
- inform is a scalar INTENT (OUT) argument of type QPC_inform_type exactly as for QPC_solve. Only the component status will be set on exit, and a successful call to QPC_terminate is indicated when this component status has the value 0. For other return values of status, see Section 2.6.

2.6 Warning and error messages

A negative value of inform%status on exit from QPC_solve or QPC_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.
- -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 or prob%m ≥ 0 or requirements that prob%A_type and prob%H_type contain its relevant string 'DENSE', 'COORDINATE', 'SPARSE_BY_ROWS' or 'DIAGONAL' has been violated.
- -4. The bound constraints are inconsistent.
- -5. The constraints appear to have no feasible point.
- -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.

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-19. The elapsed CPU or system clock time limit has been reached. This may happen if either control%cpu_time_limit or control%clock_time_limit is too small, but may also be symptomatic of a badly scaled problem.

-23. An entry from the strict upper triangle of **H** has been specified.

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 QPC_control_type (see Section 2.4.7), by reading an appropriate data specification file using the subroutine QPC_read_specifie. This facility is useful as it allows a user to change QPC control parameters without editing and recompiling programs that call QPC.

A specification file, or specifie, 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 specifie is limited to 80 characters, including the blanks separating keyword and value.

The portion of the specification file used by QPC_read_specfile must start with a "BEGIN QPC" command and end with an "END" command. The syntax of the specifile is thus defined as follows:

where keyword and value are two strings separated by (at least) one blank. The "BEGIN QPC" 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

```
BEGIN QPC SPECIFICATION

and

END QPC SPECIFICATION
```

are acceptable. Furthermore, between the "BEGIN QPC" 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 QPC_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 QPC_read_specfile.

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Control parameters corresponding to the components CQP_control, QPA_control and QPB_control may be changed by including additional sections enclosed by "BEGIN CQP" and "END CQP", "BEGIN QPA" and "END QPA", and "BEGIN QPB" and "END QPB", respectively. See the specification sheets for the packages GALAHAD_CQP, GALAHAD_QPA and GALAHAD_QPB for further details.

2.7.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
CALL QPC_read_specfile( control, device )
```

control is a scalar INTENT (INOUT) argument of type QPC_control_type (see Section 2.4.7). Default values should have already been set, perhaps by calling QPC_initialize. On exit, individual components of control may have been changed according to the commands found in the specifile. Specifile commands and the component (see Section 2.4.7) of control that each affects are given in Table 2.1.

command	component of control	value type
error-printout-device	%error	integer
printout-device	%out	integer
print-level	%print_level	integer
restore-problem-on-output	%restore_problem	integer
infinity-value	%infinity	real
identical-bounds-tolerance	%identical_bounds_tol	real
initial-rho-g	%rho_g	real
initial-rho-b	%rho_b	real
on-bound-tolerance	%on_bound_tol	real
maximum-cpu-time-limit	%cpu_time_limit	real
maximum-clock-time-limit	%clock_time_limit	real
convex	%convex	logical
treat-zero-bounds-as-general	%treat_zero_bounds_as_general	logical
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
no-qpa-phase	%no_qpa	logical
no-qpb-phase	%no_qpb	logical

Table 2.1: Specfile commands and associated components of control.

device is a scalar INTENT (IN) argument of type INTEGER (ip_), that must be set to the unit number on which the specifile 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.

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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.

GENERAL INFORMATION 3

Use of common: None.

Workspace: Provided automatically by the module.

Other routines called directly: None.

Other modules used directly: QPC_solve calls the GALAHAD packages GALAHAD_CLOCK, GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_NORMS, GALAHAD_SORT, GALAHAD_QPT, GALAHAD_QPP, GALAHAD_QPD, GALAHAD_EQP, GALAHAD_LSQP, GALAHAD_QPA, GALAHAD_QPA, GALAHAD_QPB, GALAHAD_SPECFILE and GALAHAD_FDC.

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

Restrictions: prob%n > 0, $prob%m \ge 0$, $prob%A_type$ and $prob%H_type \in \{'DENSE', 'COORDINATE', 'SPARSE_BY_-$ ROWS', 'DIAGONAL' }.

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

METHOD

The required solution \mathbf{x} necessarily satisfies the primal optimality conditions

$$\mathbf{A}\mathbf{x} = \mathbf{c} \tag{4.1}$$

and

$$\mathbf{c}^l \le \mathbf{c} \le \mathbf{c}^u, \ \mathbf{x}^l \le \mathbf{x} \le \mathbf{x}^u, \tag{4.2}$$

the dual optimality conditions

$$\mathbf{H}\mathbf{x} + \mathbf{g} = \mathbf{A}^T \mathbf{y} + \mathbf{z}, \ \mathbf{y} = \mathbf{y}^l + \mathbf{y}^u \text{ and } \mathbf{z} = \mathbf{z}^l + \mathbf{z}^u,$$
 (4.3)

and

$$\mathbf{y}^l \ge 0, \ \mathbf{y}^u \le 0, \ \mathbf{z}^l \ge 0 \text{ and } \mathbf{z}^u \le 0,$$
 (4.4)

and the complementary slackness conditions

$$(\mathbf{A}\mathbf{x} - \mathbf{c}^l)^T \mathbf{y}^l = 0, \ (\mathbf{A}\mathbf{x} - \mathbf{c}^u)^T \mathbf{y}^u = 0, \ (\mathbf{x} - \mathbf{x}^l)^T \mathbf{z}^l = 0 \ \text{and} \ (\mathbf{x} - \mathbf{x}^u)^T \mathbf{z}^u = 0,$$
(4.5)

where the vectors y and z are known as the Lagrange multipliers for the general linear constraints, and the dual variables for the bounds, respectively, and where the vector inequalities hold component-wise. Primal-dual interior point methods iterate towards a point that satisfies these conditions by ultimately aiming to satisfy (4.1), (4.3) and (4.5), while ensuring that (4.2) and (4.4) are satisfied as strict inequalities at each stage. Appropriate norms of the amounts by which (4.1), (4.3) and (4.5) fail to be satisfied are known as the primal and dual infeasibility, and the

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violation of complementary slackness, respectively. The fact that (4.2) and (4.4) are satisfied as strict inequalities gives such methods their other title, namely interior-point methods.

The problem is solved in three phases. The goal of the first "initial feasible point" phase is to find a strictly interior point which is primal feasible, that is that (4.1) is satisfied. The GALAHAD package GALAHAD_LSQP is used for this purpose, and offers the options of either accepting the first strictly feasible point found, or preferably of aiming for the so-called "analytic center" of the feasible region. Having found such a suitable initial feasible point, the second "optimality" phase ensures that (4.1) remains satisfied while iterating to satisfy accurately (but not exactly) the dual feasibility (4.3) and complementary slackness (4.5) using the GALAHAD package GALAHAD_QPB. This optimality phase proceeds by approximately minimizing a sequence of barrier functions

$$q(\mathbf{x}) - \mu \left[\sum_{i=1}^{m} \log(c_i - c_i^l) + \sum_{i=1}^{m} \log(c_i^u - c_i) + \sum_{j=1}^{n} \log(x_j - x_j^l) + \sum_{j=1}^{n} \log(x_j^u - x_j) \right],$$

for an approriate sequence of positive barrier parameters μ converging to zero while ensuring that (4.1) remain satisfied and that \mathbf{x} and \mathbf{c} are strictly interior points for (4.2). Note that terms in the above sumations corresponding to infinite bounds are ignored, and that equality constraints are treated specially. See the documentation of GALAHAD_QPB.for more details.

Since GALAHAD_QPB may not give a fully accurate solution, the last phase uses the GALAHAD package GALAHAD_QPA to refine this solution. This package uses a active/working-set method to solve the related ℓ_1 quadratic programming problem

$$\underset{\mathbf{x} \in \mathbb{R}^n}{\text{minimize}} \quad q(\mathbf{x}) + \rho_g v_g(\mathbf{x}) + \rho_b v_b(\mathbf{x}),$$

where the he infeasibilities

$$v_g(\mathbf{x}) = \sum_{i=1}^m \max(c_i^l - \mathbf{a}_i^T \mathbf{x}, 0) + \sum_{i=1}^m \max(\mathbf{a}_i^T \mathbf{x} - c_i^u, 0)$$

and

$$v_b(\mathbf{x}) = \sum_{i=1}^n \max(x_j^l - x_j, 0) + \sum_{i=1}^n \max(x_j - x_j^u, 0),$$

and ρ_g and ρ_b are appropriately chosen positive weights. See the documentation of GALAHAD_QPA.for more details.

In order to make the solution as efficient as possible, the variables and constraints are reordered internally by the GALAHAD package GALAHAD_QPP prior to solution. In particular, fixed variables, and free (unbounded on both sides) constraints are temporarily removed.

If at any stage only equality constraints remain, a much simpler equality-constrained phase is performed, by GALAHAD package GALAHAD_EQP, in place of the three inequality-based phases described above.

References:

The interior-point and working-set methods are described in detail in

A. R. Conn, N. I. M. Gould, D. Orban and Ph. L. Toint (1999). "A primal-dual trust-region algorithm for minimizing a non-convex function subject to general inequality and linear equality constraints". Mathematical Programming 87 215–249.

N. I. M. Gould and Ph. L. Toint (2002). "An iterative working-set method for large-scale non-convex quadratic programming". Applied Numerical Mathematics **43** (1–2) 109–128.

5 EXAMPLE OF USE

Suppose we wish to minimize $\frac{1}{2}x_1^2 + x_2^2 + \frac{3}{2}x_3^2 + 4x_1x_3 + 2x_2 + 1$ subject to the general linear constraints $1 \le 2x_1 + x_2 \le 2$ and $x_2 + x_3 = 2$, and simple bounds $-1 \le x_1 \le 1$ and $x_3 \le 2$. Then, on writing the data for this problem

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as

$$\mathbf{H} = \begin{pmatrix} 1 & 4 \\ 2 & \\ 4 & 3 \end{pmatrix}, \ \mathbf{g} = \begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix}, \ \mathbf{x}^l = \begin{pmatrix} -1 \\ -\infty \\ -\infty \end{pmatrix} \text{ and } \mathbf{x}^u = \begin{pmatrix} 1 \\ \infty \\ 2 \end{pmatrix},$$

and

$$\mathbf{A} = \begin{pmatrix} 2 & 1 \\ & 1 & 1 \end{pmatrix}, \ \mathbf{c}^l = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \ \text{and} \ \mathbf{c}^u = \begin{pmatrix} 2 \\ 2 \end{pmatrix}$$

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

```
! THIS VERSION: GALAHAD 2.2 - 23/04/2008 AT 16:30 GMT.
  PROGRAM GALAHAD QPC EXAMPLE
  USE GALAHAD_QPC_double
                                ! double precision version
  IMPLICIT NONE
  INTEGER, PARAMETER :: wp = KIND( 1.0D+0 ) ! set precision
  REAL ( KIND = wp ), PARAMETER :: infinity = 10.0_wp ** 20
  TYPE ( QPT_problem_type ) :: p
  TYPE ( QPC_data_type ) :: data
  TYPE ( QPC_control_type ) :: control
  TYPE ( QPC_inform_type ) :: inform
  INTEGER :: s
  INTEGER, PARAMETER :: n = 3, m = 2, h_ne = 4, a_ne = 4
  INTEGER, ALLOCATABLE, DIMENSION(:):: C_stat, B_stat
! start problem data
  ALLOCATE ( p%G( n ), p%X_l( n ), p%X_u( n ) )
  ALLOCATE ( p%C ( m ), p%C_l ( m ), p%C_u ( m ) )
  ALLOCATE( p%X( n ), p%Y( m ), p%Z( n ) )
  ALLOCATE( B_stat( n ), C_stat( m ) )
  p%new_problem_structure = .TRUE.
                                           ! new structure
  p%n = n ; p%m = m ; p%f = 1.0_wp
                                           ! dimensions & objective constant
  p%G = (/ 0.0_wp, 2.0_wp, 0.0_wp /)
                                           ! objective gradient
  p\C_1 = (/ 1.0_wp, 2.0_wp /)
                                           ! constraint lower bound
  p\C_u = (/ 2.0 \text{wp}, 2.0 \text{wp} /)
                                           ! constraint upper bound
  p%X_1 = (/ - 1.0_wp, - infinity, - infinity /) ! variable lower bound
  pX_u = (/1.0_wp, infinity, 2.0_wp /)! variable upper bound
  p%X = 0.0_{wp}; p%Y = 0.0_{wp}; p%Z = 0.0_{wp}! start from zero
! sparse co-ordinate storage format
  CALL SMT_put( p%H%type, 'COORDINATE', s )
                                             ! Specify co-ordinate
! storage for H and A
  CALL SMT_put( p%A%type, 'COORDINATE', s)
  ALLOCATE( p%H%val( h_ne ), p%H%row( h_ne ), p%H%col( h_ne ) )
  ALLOCATE( p%A%val( a_ne ), p%A%row( a_ne ), p%A%col( a_ne ) )
  p%H%val = (/ 1.0_wp, 2.0_wp, 3.0_wp, 4.0_wp /) ! Hessian H
  p%H%row = (/ 1, 2, 3, 3 /)
                                                ! NB lower triangle
  p%H%col = (/ 1, 2, 3, 1 /) ; p%H%ne = h_ne
  p%A%val = (/ 2.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /) ! Jacobian A
  p%A%row = (/ 1, 1, 2, 2 /)
  p%A%col = (/ 1, 2, 2, 3 /); p%A%ne = a_ne
! problem data complete
  CALL QPC_initialize( data, control, inform ) ! Initialize control parameters
  control%infinity = infinity
                                               ! Set infinity
! control%print_level = 1
! control%QPA_control%print_level = 1
! control%QPB_control%print_level = 1
  CALL QPC_solve(p, C_stat, B_stat, data, control, inform) ! Solve problem
  WRITE(6, "('QPC:', IO, 'QPA and', IO, 'QPB iterations', /,
```

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```
% ' Optimal objective value =',
% ES12.4, /, ' Optimal solution = ', ( 5ES12.4 ) )" )
inform%QPA_inform%iter, inform%QPB_inform%iter, inform%obj, p%X
ELSE ! Error returns
WRITE( 6, "( ' QPC_solve exit status = ', I6 ) " ) inform%status
END IF
CALL QPC_terminate( data, control, inform ) ! delete internal workspace
END PROGRAM GALAHAD_QPC_EXAMPLE
```

This produces the following output:

```
QPC: -1 QPA and 7 QPB iterations Optimal objective value = 5.4459E+00 Optimal solution = -5.4054E-02 1.1081E+00 8.9189E-01
```

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
  CALL SMT_put( p%A%type, 'SPARSE_BY_ROWS', s ) ! storage for H and A
  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, 3.0_wp, 4.0_wp /) ! Hessian H
  p%H%col = (/ 1, 2, 3, 1 /)
                                                ! NB lower triangular
  p%H%ptr = (/ 1, 2, 3, 5 /)
                                                 ! Set row pointers
  p%A%val = (/ 2.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /) ! Jacobian A
  p%A%col = (/ 1, 2, 2, 3 /)
  p%A%ptr = (/ 1, 3, 5 /)
                                                 ! Set row pointers
! problem data complete
```

or using a dense storage format with the replacement lines

```
! dense storage format
    CALL SMT_put( p%H%type, 'DENSE', s ) ! Specify dense
    CALL SMT_put( p%A%type, 'DENSE', s ) ! storage for H and A
    ALLOCATE( p%H%val( n * ( n + 1 ) / 2 ) )
    ALLOCATE( p%A%val( n * m ) )
    p%H%val = (/ 1.0_wp, 0.0_wp, 2.0_wp, 4.0_wp, 0.0_wp, 3.0_wp /) ! Hessian
    p%A%val = (/ 2.0_wp, 1.0_wp, 0.0_wp, 0.0_wp, 1.0_wp, 1.0_wp /) ! Jacobian
! problem data complete
```

respectively.

If instead **H** had been the diagonal matrix

$$\mathbf{H} = \left(\begin{array}{cc} 1 & & \\ & 0 & \\ & & 3 \end{array} \right)$$

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

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See http://galahad.rl.ac.uk/galahad-www/cou.html for full details.

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```
CALL SMT_put( prob%H%type, 'DIAGONAL', s ) ! Specify dense storage for H ALLOCATE( p%H%val( n ) ) p%H%val = (/ 1.0_{\rm wp}, 0.0_{\rm wp}, 3.0_{\rm wp} /) ! Hessian values
```

Notice here that zero diagonal entries are stored.