



Science and
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Facilities Council



GALAHAD

CRO

USER DOCUMENTATION

GALAHAD Optimization Library version 4.1

1 SUMMARY

This package provides a **crossover** from a solution to the **convex quadratic programming problem**

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

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

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

found by an interior-point method to one in which the **matrix of defining active constraints/variables is of full rank**. Here, the n by n symmetric, positive-semi-definite matrix \mathbf{H} , the vectors \mathbf{g} , \mathbf{a}_i , \mathbf{c}^l , \mathbf{c}^u , \mathbf{x}^l , \mathbf{x}^u , the scalar f are given. In addition a solution \mathbf{x} along with optimal Lagrange multipliers \mathbf{y} for the general constraints and dual variables \mathbf{z} for the simple bounds must be provided (see Section 4). These will be adjusted as necessary. Any of the constraint bounds c_i^l , c_i^u , x_j^l and x_j^u may be infinite. Full advantage is taken of any zero coefficients in the matrix \mathbf{H} or the matrix \mathbf{A} of vectors \mathbf{a}_i .

ATTRIBUTES — Versions: GALAHAD_CRO_single, GALAHAD_CRO_double. **Uses:** GALAHAD_CLOCK, GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_SPECFILE, GALAHAD_TOOLS, GALAHAD_QPT, GALAHAD_SCU, GALAHAD_SLS, GALAHAD_—ULS, **Date:** January 2012. **Origin:** N. I. M. Gould, Rutherford Appleton Laboratory. **Language:** Fortran 95 + TR 15581 or Fortran 2003. **Parallelism:** Some options may use OpenMP and its runtime library.

2 HOW TO USE THE PACKAGE

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

Single precision version

```
USE GALAHAD_CRO_single
```

Double precision version

```
USE GALAHAD_CRO_double
```

If it is required to use both modules at the same time, the derived types `SMT_type`, `QPT_problem_type`, `NLPT_user-data_type`, `CRO_time_type`, `CRO_control_type`, `CRO_inform_type` and `CRO_data_type` (Section 2.2) and the sub-routines `CRO_initialize`, `CRO_crossover`, `CRO_terminate`, (Section 2.3) and `CRO_read_specfile` (Section 2.5) must be renamed on one of the `USE` statements.

2.1 Parallel usage

OpenMP may be used by the `GALAHAD_CRO` 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

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variant of `-lmpi`). Although the MPI process will be started automatically when required, it should be stopped by the 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.

2.2 The derived data types

Four derived data types are accessible from the package.

2.2.1 The derived data type for holding control parameters

The derived data type `CRO_control_type` is used to hold controlling data. Default values may be obtained by calling `CRO_initialize` (see Section 2.3.1), while components may also be changed by calling `CRO_read_specfile` (see Section 2.5.1). The components of `CRO_control_type` are:

`error` is a scalar variable of type default `INTEGER`, that holds the stream number for error messages. Printing of error messages in `CRO_crossover` and `CRO_terminate` is suppressed if `error` ≤ 0 . The default is `error` = 6.

`out` is a scalar variable of type default `INTEGER`, that holds the stream number for informational messages. Printing of informational messages in `CRO_crossover` is suppressed if `out` < 0 . The default is `out` = 6.

`print_level` is a scalar variable of type default `INTEGER`, that is used to control the amount of informational output which is required. No informational output will occur if `print_level` ≤ 0 . If `print_level` = 1, a single line of output will be produced for each iteration of the process. If `print_level` ≥ 2 , this output will be increased to provide significant detail of each iteration. The default is `print_level` = 0.

`max_schur_complement` is a scalar variable of type default `INTEGER`, that specifies the maximum number of columns permitted in the Schur complement when updating the solution (see Section 4) before a re-factorization is triggered. The default is `max_schur_complement` = 75.

`infinity` is a scalar variable of type default `REAL` (double precision in `GALAHAD_CRO_double`), that is used to specify which constraint bounds are infinite. Any bound larger than `infinity` in modulus will be regarded as infinite. The default is `infinity` = 10^{19} .

`feasibility_tolerance` is a scalar variables of type default `REAL` (double precision in `GALAHAD_CRO_double`), that specifies the maximum violation of the KKT conditions that is permitted. The default is `feasibility_tolerance` = u , where u is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_CRO_double`).

`check_io` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if the user wishes to check the input and output data and `.FALSE.` otherwise. The package may run faster if `space_critical` is `.FALSE.` but at the possible expense of errors. The default is `check_io` = `.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.`.

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`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'`, but we recommend 'ma97' if it available.

`unsymmetric_linear_solver` is a scalar variable of type default CHARACTER and length 30, that specifies the external package to be used to solve any unsymmetric linear systems that might arise. Possible choices are 'gls', 'ma28' and 'ma48', although only 'gls' is installed by default. See the documentation for the GALAHAD package ULS for further details. The default is `unsymmetric_linear_solver = 'gls'`, but we recommend 'ma48' if it available.

`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 solve any symmetric linear systems that might arise. See the documentation for the GALAHAD package SLS for further details. In particular, default values are as for SLS.

`ULS_control` is a scalar variable argument of type `ULS_control_type` that is used to pass control options to external packages used to solve any unsymmetric linear systems that might arise. See the documentation for the GALAHAD package ULS for further details. In particular, default values are as for ULS.

2.2.2 The derived data type for holding timing information

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

`total` is a scalar variable of type default REAL (double precision in `GALAHAD_CRO_double`), that gives the total CPU time spent in the package.

`analyse` is a scalar variable of type default REAL (double precision in `GALAHAD_CRO_double`), that gives the CPU time spent analysing the required matrices prior to factorization.

`factorize` is a scalar variable of type default REAL (double precision in `GALAHAD_CRO_double`), that gives the CPU time spent factorizing the required matrices.

`solve` is a scalar variable of type default REAL (double precision in `GALAHAD_CRO_double`), that gives the CPU time spent computing corrections to the current solution.

`clock_total` is a scalar variable of type default REAL (double precision in `GALAHAD_CRO_double`), that gives the total elapsed system clock time spent in the package.

`clock_analyse` is a scalar variable of type default REAL (double precision in `GALAHAD_CRO_double`), that gives the elapsed system clock time spent analysing the required matrices prior to factorization.

`clock_factorize` is a scalar variable of type default REAL (double precision in `GALAHAD_CRO_double`), that gives the elapsed system clock time spent factorizing the required matrices.

`clock_solve` is a scalar variable of type default REAL (double precision in `GALAHAD_CRO_double`), that gives the elapsed system clock time spent computing corrections to the current solution.

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2.2.3 The derived data type for holding informational parameters

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

`status` is a scalar variable of type default `INTEGER`, that gives the exit status of the algorithm. See Section 2.4 for details.

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

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

`dependent` is a scalar variable of type default `INTEGER`, that gives the number of dependent active constraints.

`time` is a scalar variable of type `CRO_time_type` whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.2.2).

`SLS_control` is a scalar variable argument of type `SLS_control_type` that is used to pass control options to external packages used to solve any symmetric linear systems that might arise. See the documentation for the GALAHAD package `SLS` for further details. In particular, default values are as for `SLS`.

`ULS_control` is a scalar variable argument of type `ULS_control_type` that is used to pass control options to external packages used to solve any unsymmetric linear systems that might arise. See the documentation for the GALAHAD package `ULS` for further details. In particular, default values are as for `ULS`.

`scu_status` is a scalar variable of type default `INTEGER`, that gives the return status from the Schur-complement updating package `GALAHAD_SCU`. See the specification sheet for `GALAHAD_SCU` for details.

`SCU_inform` is a scalar variable of type `SCU_info_type` whose components are used to provide information about Schur-complement updating applied by the package `GALAHAD_SCU`. See the specification sheet for `GALAHAD_SCU` for details.

2.2.4 The derived data type for holding problem data

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

2.3 Argument lists and calling sequences

There are three procedures for user calls (see Section 2.5 for further features):

1. The subroutine `CRO_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 `CRO_crossover` is called to solve the problem.
3. The subroutine `CRO_terminate` is provided to allow the user to automatically deallocate array components of the private data, allocated by `CRO_crossover`, at the end of the solution process.

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

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2.3.1 The initialization subroutine

Default values are provided as follows:

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

`data` is a scalar `INTENT(INOUT)` argument of type `CRO_data_type` (see Section 2.2.4). It is used to hold private data used by the crossover algorithm.

`control` is a scalar `INTENT(OUT)` argument of type `CRO_control_type` (see Section 2.2.1). On exit, `control` contains default values for the components as described in Section 2.2.1. These values should only be changed after calling `CRO_initialize`.

`inform` is a scalar `INTENT(OUT)` argument of type `CRO_inform_type` (see Section 2.2.3). A successful call to `CRO_initialize` is indicated when the component status has the value 0. For other return values of status, see Section 2.4.

2.3.2 The crossover subroutine

The crossover algorithm is called as follows:

```
CALL CRO_crossover( n, m, m_equal, H_val, H_col, H_ptr, A_val, &
                  A_col, A_ptr, G, C_l, C_u, X_l, X_u, C, X, Y, &
                  Z, C_stat, X_stat, data, control, inform )
```

`n` is a scalar `INTENT(IN)` argument of type default `INTEGER`, that must be set to the number of optimization variables, n . **Restriction:** $n > 0$.

`m` is a scalar `INTENT(IN)` argument of type default `INTEGER`, that must be set to the number of general linear constraints, m . **Restriction:** $m \geq 0$.

`m_equal` is a scalar `INTENT(IN)` argument of type default `INTEGER`, that must be set to the number of general linear constraints that are equalities, i.e., whose lower and upper bounds coincide. **Restriction:** $m \geq m_equal > 0$.

`H_val` is an `INTENT(IN)` rank-one array argument of dimension `H_ptr(n+1)-1` and type default `REAL` (double precision in `GALAHAD_CRO_double`), that must be set to hold the values of the nonzero entries of the **lower triangular** part of the Hessian matrix **H**. The entries must be ordered so that those in row i appear directly before those in row $i + 1$ with no gaps; the order within each row is unimportant.

`H_col` is an `INTENT(IN)` rank-one array argument of dimension `H_ptr(n+1)-1` and type default `INTEGER`, that must be set to hold the column indices of the **lower triangular** part of **H**. These must be ordered so that they correspond to the values stored in `H_val`.

`H_ptr` is an `INTENT(IN)` rank-one array argument of dimension $n+1$ and type default `INTEGER`, whose j -th component, $j = 1, \dots, n$, holds the starting position of row j of the **lower triangular** part of **H** as stored in `H_val` and `H_col`. The $n + 1$ -st component must be set to the total number of entries in the lower triangular part of **H** plus one.

`A_val` is an `INTENT(IN)` rank-one array argument of dimension `A_ptr(m+1)-1` and type default `REAL` (double precision in `GALAHAD_CRO_double`), that must be set to hold the values of the nonzero entries of the Jacobian matrix **A**. The entries must be ordered so that those in row i appear directly before those in row $i + 1$ with no gaps; the order within each row is unimportant. **Restriction:** the rows of **A** must be ordered so that the first `m_equal` are equality constraints.

`A_col` is an `INTENT(IN)` rank-one array argument of dimension `A_ptr(m+1)-1` and type default `INTEGER`, that must be set to hold the column indices of **A**. These must be ordered so that they correspond to the values stored in `A_val`.

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- `A_ptr` is an `INTENT (IN)` rank-one array argument of dimension $m+1$ and type default `INTEGER`, whose i -th component, $i = 1, \dots, m$, holds the starting position of row i of \mathbf{A} as stored in `A_val` and `A_col`. The $m+1$ -st component must be set to the total number of entries in \mathbf{A} plus one.
- `G` is an `INTENT (IN)` rank-one array argument of dimension n and type default `REAL` (double precision in `GALAHAD_CRO_double`), that holds the gradient \mathbf{g} of the linear term of the quadratic objective function. The j -th component of `G`, $j = 1, \dots, n$, must be set to \mathbf{g}_j .
- `C_l` is an `INTENT (IN)` rank-one array argument of dimension m and type default `REAL` (double precision in `GALAHAD_CRO_double`), that holds the vector of lower bounds \mathbf{c}^l on the general constraints. The i -th component of `C_l`, $i = 1, \dots, m$, must be set to \mathbf{c}_i^l . 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 2.2.1).
- `C_u` is an `INTENT (IN)` rank-one array argument of dimension m and type default `REAL` (double precision in `GALAHAD_CRO_double`), that holds the vector of upper bounds \mathbf{c}^u on the general constraints. The i -th component of `C_u`, $i = 1, \dots, m$, must be set to \mathbf{c}_i^u . 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 2.2.1).
- `X_l` is an `INTENT (IN)` rank-one array argument of dimension n and type default `REAL` (double precision in `GALAHAD_CRO_double`), that holds the vector of lower bounds \mathbf{x}^l on the variables. The j -th component of `X_l`, $j = 1, \dots, n$, must be set to \mathbf{x}_j^l . Infinite bounds are allowed by setting the corresponding components of `X_l` to any value smaller than `-infinity`, where `infinity` is a component of the control array `control` (see Section 2.2.1).
- `X_u` is an `INTENT (IN)` rank-one array argument of dimension n and type default `REAL` (double precision in `GALAHAD_CRO_double`), that holds the vector of upper bounds \mathbf{x}^u on the variables. The j -th component of `X_u`, $j = 1, \dots, n$, must be set to \mathbf{x}_j^u . 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 2.2.1).
- `X` is an `INTENT (INOUT)` rank-one array argument of dimension n and type default `REAL` (double precision in `GALAHAD_CRO_double`), that holds the values \mathbf{x} of the optimization variables. The j -th component of `X`, $j = 1, \dots, n$, must be set to x_j on input, and may have been adjusted to provide another solution on output.
- `C` is an `INTENT (INOUT)` rank-one array argument of dimension m and type default `REAL` (double precision in `GALAHAD_CRO_double`), that holds the values \mathbf{Ax} of the constraints. The i -th component of `C`, $i = 1, \dots, m$, must be set to $\mathbf{a}_i^T \mathbf{x} \equiv (\mathbf{Ax})_i$ on input, and may have been adjusted to provide another solution on output.
- `Y` is an `INTENT (INOUT)` rank-one array argument of dimension m and type default `REAL` (double precision in `GALAHAD_CRO_double`), 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 `Y`, $i = 1, \dots, m$, must be set to y_i on input, and may have been adjusted to provide another solution on output.
- `Z` is an `INTENT (INOUT)` rank-one array argument of dimension n and type default `REAL` (double precision in `GALAHAD_CRO_double`), that holds the values \mathbf{z} of estimates of the dual variables corresponding to the simple bound constraints (see Section 4). The j -th component of `Z`, $j = 1, \dots, n$, must be set to z_j on input, and may have been adjusted to provide another solution on output.
- `C_stat` is an `INTENT (IN)` rank-one `INTENT (INOUT)` array argument of dimension m and type default `INTEGER`, that indicates which of the general linear constraints are in the current active set. Possible input values for `C_stat(i)`, $i = 1, \dots, m$, and their meanings are
- < 0 the i -th general constraint is in the active set on its lower bound, i.e., $\mathbf{a}_i^T \mathbf{x} = \mathbf{c}_i^l$,

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- >0 the i -th general constraint is in the active set on its upper bound, i.e., $\mathbf{a}_i^T \mathbf{x} = \mathbf{c}_i^u$, and
- 0 the i -th general constraint is not in the active set, i.e., $\mathbf{c}_i^l < \mathbf{a}_i^T \mathbf{x} < \mathbf{c}_i^u$.

On output, the value of `C_stat(i)` may have changed to mean

- 1 the i -th general constraint is both independent and active on its lower bound,
- 2 the i -th general constraint is on its lower bound but linearly dependent on others,
- 1 the i -th general constraint is both independent and active on its upper bound,
- 2 the i -th general constraint is on its upper bound but linearly dependent on others, and
- 0 the i -th general constraint is not in the active set.

`X_stat` is an `INTENT(IN)` rank-one `INTENT(INOUT)` array argument of dimension n and type default `INTEGER`, that indicates which of the simple bound constraints are in the current active set. Possible input values for `X_stat(j)`, $j = 1, \dots, n$, and their meanings are

- <0 the j -th simple bound constraint is in the active set on its lower bound, i.e., $\mathbf{x}_j = \mathbf{x}_j^l$,
- >0 the j -th simple bound constraint is in the active set on its upper bound, i.e., $\mathbf{x}_j = \mathbf{x}_j^u$, and
- 0 the j -th simple bound constraint is not in the active set, i.e., $\mathbf{x}_j^l < \mathbf{x}_j < \mathbf{x}_j^u$.

On output, the value of `X_stat(j)` may have changed to mean

- 1 the j -th simple bound constraint is both independent and active on its lower bound,
- 2 the j -th simple bound constraint is on its lower bound but linearly dependent on others,
- 1 the j -th simple bound constraint is both independent and active on its upper bound,
- 2 the j -th simple bound constraint is on its upper bound but linearly dependent on others, and
- 0 the j -th simple bound constraint is not in the active set.

`data` is a scalar `INTENT(INOUT)` argument of type `CRO_data_type` (see Section 2.2.4). It is used to hold private data used by the crossover algorithm and must not have been altered **by the user** since the last call to `CRO_initialize`.

`control` is a scalar `INTENT(IN)` argument of type `CRO_control_type` (see Section 2.2.1). Default values may be assigned by calling `CRO_initialize` prior to the first call to `CRO_crossover`.

`inform` is a scalar `INTENT(INOUT)` argument of type `CRO_inform_type` (see Section 2.2.3). A successful call to `CRO_crossover` is indicated when the component status has the value 0. For other return values of `status`, see Section 2.4.

2.3.3 The termination subroutine

All previously allocated arrays are deallocated as follows:

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

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

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

`inform` is a scalar `INTENT(OUT)` argument of type `CRO_inform_type` exactly as for `CRO_crossover`. Only the component status will be set on exit, and a successful call to `CRO_terminate` is indicated when this component status has the value 0. For other return values of `status`, see Section 2.4.

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2.4 Warning and error messages

A negative value of `inform%status` on exit from `CRO_crossover` or `CRO_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 the requirement that `prob%H_type` contain its relevant string 'DENSE', 'COORDINATE', 'SPARSE_BY_ROWS' or 'DIAGONAL' when **H** is available, has been violated.
- 4. The bound constraints are inconsistent.
- 7. The objective function appears to be unbounded from below on the feasible set.
- 9. An error was reported by `SLS_analyse`. The return status from `SLS_analyse` is given in `inform%SLS_inform_status`. See the documentation for the GALAHAD package SLS for further details.
- 10. An error was reported by `SLS_factorize` or `SCU_append`. The return status from `SLS_factorize` is given in `inform%SLS_inform_status` and that from `SCU_append` in `inform%scu_status`. See the documentation for the GALAHAD packages SLS and SCU for further details.
- 11. An error was reported by `SLS_solve` or `SCU_solve`. The return status from `SLS_solve` is given in `inform%SLS_inform_status` and that from `SCU_solve` in `inform%scu_status`. See the documentation for the GALAHAD packages SLS and SCU for further details.
- 13. An error was reported by `ULS_factorize`. The return status from `ULS_factorize` is given in `inform%uls_factorize_status`. See the documentation for the GALAHAD package ULS for further details.
- 14. An error was reported by `ULS_solve`. The return status from `ULS_solve` is given in `inform%uls_solve_status`. See the documentation for the GALAHAD package ULS for further details.

2.5 Further features

In this section, we describe an alternative means of setting control parameters, that is components of the variable `control` of type `CRO_control_type` (see Section 2.2.1), by reading an appropriate data specification file using the subroutine `CRO_read_specfile`. This facility is useful as it allows a user to change CRO control parameters without editing and recompiling programs that call CRO.

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

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

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```
( .. lines ignored by CRO_read_specfile .. )
BEGIN CRO
  keyword      value
  .....      .....
  keyword      value
END
( .. lines ignored by CRO_read_specfile .. )
```

where keyword and value are two strings separated by (at least) one blank. The “BEGIN CRO” 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 CRO SPECIFICATION
```

and

```
END CRO SPECIFICATION
```

are acceptable. Furthermore, between the “BEGIN CRO” 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 CRO_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 CRO_read_specfile.

2.5.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
CALL CRO_read_specfile( control, device )
```

`control` is a scalar `INTENT(INOUT)` argument of type `CRO_control_type` (see Section 2.2.1). Default values should have already been set, perhaps by calling `CRO_initialize`. On exit, individual components of `control` may have been changed according to the commands found in the specfile. Specfile commands and the component (see Section 2.2.1) of `control` that each affects are given in Table 2.1.

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

2.6 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 indicating how many dependent constraints will be removed. If `control%print_level ≥ 2`, this output will be increased to provide details of the dependent constraints, while if `control%print_level ≥ 5`, full debugging details (probably only of interest to the code developer) are provided.

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command	component of control	value type
error-printout-device	%error	integer
printout-device	%out	integer
print-level	%print_level	integer
maximum-dimension-of-schur-complement	%max_schur_complement	integer
infinity-value	%infinity	real
feasibility-tolerance	%feasibility_tol	real
check-input-output	%check_io	logical
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
output-line-prefix	%prefix	character
symmetric-linear-equation-solver	%symmetric_linear_solver	character
unsymmetric-linear-equation-solver	%unsymmetric_linear_solver	character

Table 2.1: Specfile commands and associated components of control.

3 GENERAL INFORMATION

Use of common: None.

Workspace: Provided automatically by the module.

Other routines called directly: None.

Other modules used directly: CRO_crossover calls the GALAHAD packages GALAHAD_CLOCK, GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_SPECFILE, GALAHAD_TOOLS, GALAHAD_QPT, GALAHAD_SCU, GALAHAD_SLS and GALAHAD_ULS.

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

Restrictions: $n > 0$, $m \geq m_equal$, $m_equal \geq 0$, prob%A_type and prob%H_type $\in \{ 'DENSE', 'COORDINATE', 'SPARSE_BY_ROWS', 'DIAGONAL' \}$. (if **H** and **A** are explicit).

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

4 METHOD

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

$$\mathbf{Ax} = \mathbf{c} \quad (4.1)$$

and

$$\mathbf{c}^l \leq \mathbf{c} \leq \mathbf{c}^u, \quad \mathbf{x}^l \leq \mathbf{x} \leq \mathbf{x}^u, \quad (4.2)$$

the dual optimality conditions

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

and

$$\mathbf{y}^l \geq 0, \quad \mathbf{y}^u \leq 0, \quad \mathbf{z}^l \geq 0 \quad \text{and} \quad \mathbf{z}^u \leq 0, \quad (4.4)$$

and the complementary slackness conditions

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

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where the vectors \mathbf{y} and \mathbf{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 componentwise.

Denote the active constraints by $\mathbf{A}_A \mathbf{x} = \mathbf{c}_A$ and the active bounds by $\mathbf{I}_A \mathbf{x} = \mathbf{x}_A$. Then any optimal solution satisfies the linear system

$$\begin{pmatrix} \mathbf{H} & -\mathbf{A}_A^T & -\mathbf{I}_A^T \\ \mathbf{A}_A & 0 & 0 \\ \mathbf{I}_A & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{y}_A \\ \mathbf{z}_A \end{pmatrix} = \begin{pmatrix} -\mathbf{g} \\ \mathbf{c}_A \\ \mathbf{x}_A \end{pmatrix},$$

where \mathbf{y}_A and \mathbf{z}_A are the corresponding active Lagrange multipliers and dual variables respectively. Consequently the difference between any two solutions $(\Delta \mathbf{x}, \Delta \mathbf{y}, \Delta \mathbf{z})$ must satisfy

$$\begin{pmatrix} \mathbf{H} & -\mathbf{A}_A^T & -\mathbf{I}_A^T \\ \mathbf{A}_A & 0 & 0 \\ \mathbf{I}_A & 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta \mathbf{x} \\ \Delta \mathbf{y}_A \\ \Delta \mathbf{z}_A \end{pmatrix} = 0. \quad (4.6)$$

Thus there can only be multiple solution if the coefficient matrix \mathbf{K} of (4.6) is singular. The algorithm used in GALAHAD_CRO exploits this. The matrix \mathbf{K} is checked for singularity using the GALAHAD package GALAHAD_ULS. If \mathbf{K} is non singular, the solution is unique and the solution input by the user provides a linearly independent active set. Otherwise \mathbf{K} is singular, and partitions $\mathbf{A}_A^T = (\mathbf{A}_{AB}^T \ \mathbf{A}_{AN}^T)$ and $\mathbf{I}_A^T = (\mathbf{I}_{AB}^T \ \mathbf{I}_{AN}^T)$ are found so that

$$\begin{pmatrix} \mathbf{H} & -\mathbf{A}_{AB}^T & -\mathbf{I}_{AB}^T \\ \mathbf{A}_{AB} & 0 & 0 \\ \mathbf{I}_{AB} & 0 & 0 \end{pmatrix}$$

is non-singular and the “non-basic” constraints \mathbf{A}_{AN}^T and \mathbf{I}_{AN}^T are linearly dependent on the “basic” ones $(\mathbf{A}_{AB}^T \ \mathbf{I}_{AB}^T)$. In this case (4.6) is equivalent to

$$\begin{pmatrix} \mathbf{H} & -\mathbf{A}_{AB}^T & -\mathbf{I}_{AB}^T \\ \mathbf{A}_{AB} & 0 & 0 \\ \mathbf{I}_{AB} & 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta \mathbf{x} \\ \Delta \mathbf{y}_{AB} \\ \Delta \mathbf{z}_{AB} \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{AN}^T \\ 0 \\ 0 \end{pmatrix} \Delta \mathbf{y}_{AN} + \begin{pmatrix} \mathbf{I}_{AN}^T \\ 0 \\ 0 \end{pmatrix} \Delta \mathbf{z}_{AN}. \quad (4.7)$$

Thus, starting from the user’s $(\mathbf{x}, \mathbf{y}, \mathbf{z})$ and with a factorization of the coefficient matrix of (4.7) found by the GALAHAD package GALAHAD_SLS, the alternative solution $(\mathbf{x} + \alpha \mathbf{x}, \mathbf{y} + \alpha \mathbf{y}, \mathbf{z} + \alpha \mathbf{z})$, featuring $(\Delta \mathbf{x}, \Delta \mathbf{y}_{AB}, \Delta \mathbf{z}_{AB})$ from (4.7) in which successively one of the components of $\Delta \mathbf{y}_{AN}$ and $\Delta \mathbf{z}_{AN}$ in turn is non zero, is taken. The scalar α at each stage is chosen to be the largest possible that guarantees (4.4); this may happen when a non-basic multiplier/dual variable reaches zero, in which case the corresponding constraint is disregarded, or when this happens for a basic multiplier/dual variable, in which case this constraint is exchanged with the non-basic one under consideration and disregarded. The latter corresponds to changing the basic-non-basic partition in (4.7), and subsequent solutions may be found by updating the factorization of the coefficient matrix in (4.7) following the basic-non-basic swap using the GALAHAD package GALAHAD_SCU.

5 EXAMPLE OF USE

Suppose we have solved the quadratic program

$$\begin{aligned} & \underset{\mathbf{x}}{\text{minimize}} && \frac{1}{2} \sum_{i=1}^{11} x_i^2 + \frac{1}{2} \sum_{i=1}^{10} x_i x_{i+1} + \frac{1}{2} x_1 - \frac{1}{2} x_2 - \sum_{i=1}^{10} x_i - \frac{1}{2} x_{11} \\ & \text{subject to} && \sum_{i=1}^{11} x_i = 10, \quad \sum_{i=3}^{11} x_i \geq 9, \quad \sum_{i=2}^{11} x_i \leq 10 \\ & && \text{and } x_1 \geq 0, \quad x_i \geq 1 \text{ for } i = 2, \dots, 11 \end{aligned}$$

(using, for example, GALAHAD’s CQP package), and have found the primal-dual solution $\mathbf{x} = (0, 1, 1, \dots, 1)$, $\mathbf{y} = (-1, \frac{3}{2}, -2)$ and $\mathbf{z} = (2, 4, \frac{5}{2}, \frac{5}{2}, \dots, \frac{5}{2})$ for which all variables and constraints are active; clearly such a solution has

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dependent active constraints. Then we may find a crossover solution in which the defining active set is linearly independent using the following code:

```
! THIS VERSION: GALAHAD 2.5 - 06/01/2012 AT 08:30 GMT.
PROGRAM GALAHAD_CRO_EXAMPLE
USE GALAHAD_CRO_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 ( CRO_data_type ) :: data
TYPE ( CRO_control_type ) :: control
TYPE ( CRO_inform_type ) :: inform
INTEGER :: i
INTEGER, PARAMETER :: n = 11, m = 3, m_equal = 1, a_ne = 30, h_ne = 21
INTEGER, DIMENSION( h_ne ) :: H_col
INTEGER, DIMENSION( n + 1 ) :: H_ptr
REAL ( KIND = wp ), DIMENSION( h_ne ) :: H_val
INTEGER, DIMENSION( a_ne ) :: A_col
INTEGER, DIMENSION( m + 1 ) :: A_ptr
REAL ( KIND = wp ), DIMENSION( a_ne ) :: A_val
REAL ( KIND = wp ), DIMENSION( n ) :: G, X_l, X_u, X, Z
REAL ( KIND = wp ), DIMENSION( m ) :: C_l, C_u, C, Y
INTEGER, DIMENSION( m ) :: C_stat
INTEGER, DIMENSION( n ) :: X_stat
! start problem data
H_val = (/ 1.0D+0, 5.0D-1, 1.0D+0, 5.0D-1, 1.0D+0, 5.0D-1, 1.0D+0, 5.0D-1, &
          1.0D+0, 5.0D-1, 1.0D+0, 5.0D-1, 1.0D+0, 5.0D-1, 1.0D+0, 5.0D-1, &
          1.0D+0, 5.0D-1, 1.0D+0, 5.0D-1, 1.0D+0 /) ! H values
H_col = (/ 1, 1, 2, 2, 3, 3, 4, 4, 5, 5, 6, 6, 7, 7, 8, 8, 9, 9, 10, 10, &
          11 /) ! H columns
H_ptr = (/ 1, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22 /) ! pointers to H col
A_val = (/ 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, &
          1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, &
          1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, &
          1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0 /) ! A values
A_col = (/ 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 3, 4, 5, 6, 7, 8, 9, 10, 11, &
          2, 3, 4, 5, 6, 7, 8, 9, 10, 11 /) ! A columns
A_ptr = (/ 1, 12, 21, 31 /) ! pointers to A columns
G = (/ 5.0D-1, -5.0D-1, -1.0D+0, -1.0D+0, -1.0D+0, -1.0D+0, -1.0D+0, &
      -1.0D+0, -1.0D+0, -1.0D+0, -5.0D-1 /) ! objective gradient
C_l = (/ 1.0D+1, 9.0D+0, -infinity /) ! constraint lower bound
C_u = (/ 1.0D+1, infinity, 1.0D+1 /) ! constraint upper bound
X_l = (/ 0.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, &
      1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0 /) ! variable lower bound
X_u = (/ infinity, infinity, infinity, infinity, infinity, infinity, &
      infinity, infinity, infinity, infinity, infinity /) ! upper bound
C = (/ 1.0D+1, 9.0D+0, 1.0D+1 /) ! optimal constraint value
X = (/ 0.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, &
      1.0D+0, 1.0D+0, 1.0D+0 /) ! optimal variables
Y = (/ -1.0D+0, 1.5D+0, -2.0D+0 /) ! optimal Lagrange multipliers
Z = (/ 2.0D+0, 4.0D+0, 2.5D+0, 2.5D+0, 2.5D+0, 2.5D+0, &
      2.5D+0, 2.5D+0, 2.5D+0, 2.5D+0, 2.5D+0 /) ! optimal dual variables
C_stat = (/ -1, -1, 1 /) ! constraint status
X_stat = (/ -1, -1, -1, -1, -1, -1, -1, -1, -1, -1, -1 /) ! variable status
! problem data complete
CALL CRO_initialize( data, control, inform ) ! Initialize control parameters
```

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```

CALL CRO_crossover( n, m, m_equal, H_val, H_col, H_ptr, A_val, A_col,      &
                   A_ptr, G, C_l, C_u, X_l, X_u, C, X, Y, Z, C_stat,      &
                   X_stat, data, control, inform ) ! crossover
IF ( inform%status == 0 ) THEN                                           ! successful return
  WRITE( 6, "( '      x_l      x      x_u      z      stat', /, &
&      ( 4ES12.4, I5 ) )" )                                           &
  ( X_l( i ), X( i ), X_u( i ), Z( i ), X_stat( i ), i = 1, n )
  WRITE( 6, "( '      c_l      c      c_u      y      stat', /, &
&      ( 4ES12.4, I5 ) )" )                                           &
  ( C_l( i ), C( i ), C_u( i ), Y( i ), C_stat( i ), i = 1, m )
  WRITE( 6, "( ' CRO_solve exit status = ', I0 ) " ) inform%status
ELSE                                                                    ! error returns
  WRITE( 6, "( ' CRO_solve exit status = ', I0 ) " ) inform%status
END IF
CALL CRO_terminate( data, control, inform ) ! delete internal workspace
END PROGRAM GALAHAD_CRO_EXAMPLE

```

This produces the following output:

```

      x_l      x      x_u      z      stat
0.0000E+00 0.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
1.0000E+00 1.0000E+00 1.0000E+20 1.0000E+00 -1
      c_l      c      c_u      y      stat
1.0000E+01 1.0000E+01 1.0000E+01 0.0000E+00 -2
9.0000E+00 9.0000E+00 1.0000E+20 0.0000E+00 -2
-1.0000E+20 1.0000E+01 1.0000E+01 0.0000E+00 2
CRO_solve exit status = 0

```

Notice that active variable 1 and constraints 2 and 3 are found to be active but linearly dependent.