



GALAHAD

NREK

USER DOCUMENTATION

GALAHAD Optimization Library version 5.4

1 SUMMARY

Given real n by n symmetric matrices \mathbf{H} and \mathbf{S} (with \mathbf{S} diagonally dominant), a real n vector \mathbf{c} and scalars f , $p > 2$ and $\sigma > 0$, this package uses an **extended Krylov-subspace method** to find a **global minimizer of the norm-regularized quadratic objective function** $\frac{1}{2}\mathbf{x}^T\mathbf{H}\mathbf{x} + \mathbf{c}^T\mathbf{x} + f + \frac{1}{p}\sigma\|\mathbf{x}\|_{\mathbf{S}}^p$, where the \mathbf{S} -norm of \mathbf{x} is $\|\mathbf{x}\|_{\mathbf{S}} = \sqrt{\mathbf{x}^T\mathbf{S}\mathbf{x}}$. This problem commonly occurs as a regularization subproblem in nonlinear optimization calculations. The matrix \mathbf{S} need not be provided in the commonly-occurring ℓ_2 -regularization case for which $\mathbf{S} = \mathbf{I}$, the n by n identity matrix.

A factorization of the matrix \mathbf{H} (and \mathbf{S} , if it is required) will be used, so this package is most suited for the case where such a factorization may be found efficiently. If this is not the case, the package `GALAHAD_GLRT` may be preferred.

ATTRIBUTES — Versions: `GALAHAD_NREK_single`, `GALAHAD_NREK_double`. **Uses:** `GALAHAD_CLOCK`, `GALAHAD_SYMBOLS`, `GALAHAD_SPACE`, `GALAHAD_NORMS`, `GALAHAD_ROOTS`, `GALAHAD_SPECFILE`, `GALAHAD_SMT`, `GALAHAD_RAND`, `GALAHAD_RQS`, `GALAHAD_SLS`, `GALAHAD_MOP` **Date:** November 2025. **Origin:** H. Al Daas and 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

The package is available with single, double and (if available) quadruple 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_NREK_single
```

with the obvious substitution `GALAHAD_NREK_double`, `GALAHAD_NREK_quadruple`, `GALAHAD_NREK_single_64`, `GALAHAD_NREK_double_64` and `GALAHAD_NREK_quadruple_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`, `NREK_control_type`, `NREK_inform_type`, `NREK_data_type`, (Section 2.4) and the subroutines `NREK_initialize`, `NREK_solve`, `NREK_terminate` (Section 2.5) and `NREK_read_specfile` (Section 2.7) must be renamed on one of the `USE` statements.

2.1 Matrix storage formats

The matrices \mathbf{H} and (if required) \mathbf{S} may be stored in a variety of input formats.

2.1.1 Dense storage format

The matrix \mathbf{H} is stored as a compact dense matrix by rows, that is, the values of the entries of each row in turn are stored in order within an appropriate real one-dimensional array. Since \mathbf{H} is symmetric, only the lower triangular part (that is the part h_{ij} for $1 \leq j \leq i \leq n$) need be held. In this case the lower triangle should 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 $1 \leq j \leq i \leq n$. The same is true for \mathbf{S} if it is used.

2.1.2 Sparse co-ordinate storage format

Only the nonzero entries of the matrices are stored. For the l -th entry of \mathbf{H} , $1 \leq j \leq i \leq n$, its row index i , column index j and value h_{ij} are stored in the l -th components of the integer arrays `H%row`, `H%col` and real array `H%val`, respectively. Note that only the entries in the lower triangle should be stored. The same scheme may be used for \mathbf{S} if it is required.

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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{H} , the i -th component of the integer array $\mathbb{H}^{\%}\text{ptr}$ holds the position of the first entry in this row, while $\mathbb{H}^{\%}\text{ptr}(m + 1)$ holds the total number of entries plus one. The column indices j , $1 \leq j \leq i$, and values h_{ij} of the entries in the i -th row are stored in components $l = \mathbb{H}^{\%}\text{ptr}(i), \dots, \mathbb{H}^{\%}\text{ptr}(i + 1) - 1$ of the integer array $\mathbb{H}^{\%}\text{col}$, and real array $\mathbb{H}^{\%}\text{val}$, respectively. Note that as before only the entries in the lower triangle should be stored. For sparse matrices, this scheme almost always requires less storage than its predecessor. This scheme may also be used for \mathbf{S} if it is required.

2.1.4 Diagonal storage format

If \mathbf{H} is diagonal (i.e., $h_{ij} = 0$ for all $1 \leq i \neq j \leq n$) only the diagonals entries h_{ii} , $1 \leq i \leq n$, need be stored, and the first n components of the array $\mathbb{H}^{\%}\text{val}$ may be used for the purpose. The same applies to \mathbf{S} if it is required.

2.1.5 Scaled-identity-matrix storage format

If \mathbf{H} is a scalar multiple of the identity matrix (i.e., $h_{ii} = h_{11}$ and $h_{ij} = 0$ for all $1 \leq i \neq j \leq n$) only the first diagonal entry h_{11} needs be stored, and the first component of the array $\mathbb{H}^{\%}\text{val}$ may be used for the purpose. The same applies to \mathbf{S} if it is required.

2.1.6 Identity-matrix storage format

If \mathbf{H} is the identity matrix (i.e., $h_{ii} = 1$ and $h_{ij} = 0$ for all $1 \leq i \neq j \leq n$), no explicit entries needs be stored. The same would be true for \mathbf{S} , but \mathbf{S} need not be provided if $\mathbf{S} = \mathbf{I}$.

2.1.7 Zero-matrix storage format

If $\mathbf{H} = \mathbf{0}$ (i.e., $h_{ij} = 0$ for all $1 \leq i, j \leq n$), no explicit entries needs be stored. This is not relevant for \mathbf{S} , as \mathbf{S} is required to be non-singular.

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, `DOUBLE PRECISION` for the double precision cases and quadruple-precision if 128-bit reals are available, and correspond to `rp_ = real32`, `rp_ = real64` and `rp_ = real128` respectively as defined 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_NREK` 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 `-lmpi`). 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

Six 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 **H** and perhaps **S**. 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.
- val 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 the *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.
- row 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).
- col is a rank-one allocatable array of type INTEGER(ip_), and dimension at least ne, that may hold 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 n + 1, that may holds the pointers to the first entry in each row (see §2.1.3).

2.4.2 The derived data type for holding control parameters

The derived data type NREK_control_type is used to hold controlling data. Default values may be obtained by calling NREK_initialize (see Section 2.5.1). The components of NREK_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 NREK_solve and NREK_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 NREK_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.

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`eks_max` is a scalar variable of type `INTEGER(ip_)`, that specifies the maximum dimension of the extended Krylov space employed. If a negative value is given, this will be replaced by 100. The default is `eks_max = - 1`.

`it_max` is a scalar variable of type `INTEGER(ip_)`, that is used to specify the maximum number of iterations allowed. If a negative value is given, this will be replaced by 100. The default is `it_max = - 1`.

`f` is a scalar variable of type `default REAL(rp_)`, that gives the value of the constant term f in the quadratic objective function. This value has no effect on the computed minimizer \mathbf{x} . The default is `f = 0.0`.

`increase` is a scalar variable of type `REAL(rp_)`, that holds the value of the increase factor for suggested subsequent regularization weights (see `control%next_weight`). The suggested weight will be reduction times the current weight. The default is `increase = 2.0`.

`stop_residual` is a scalar variable of type `REAL(rp_)`, that holds the value of the stopping tolerance used by the algorithm. The iteration stops as soon as \mathbf{x} and λ are found to satisfy $\|(\mathbf{H} + \lambda \mathbf{S})\mathbf{x} + \mathbf{c}\| < \text{stop_residual} \times \max(1, \|\mathbf{c}\|)$. The default is `stop_residual = 10\sqrt{u}`, where u is `EPSILON(1.0_rp_)`

`reorthogonalize` is a scalar variable of type `default LOGICAL`, that may be set `.TRUE.` if the user wishes the package to reorthogonalise the generated basis of the extended Krylov space at every iteration. This can be very expensive, and is generally not warranted. The default is `reorthogonalize = .FALSE.` which is our recommendation.

`s_version_52` is a scalar variable of type `default LOGICAL`, that may be set `.TRUE.` if the user wishes to use Algorithm 5.2 in the paper to generate the extended Krylov space recurrences when a non-unit S is given, and `.FALSE.` if those from Algorithm B.3 should be used instead. In practice, there is very little difference in performance and accuracy. The default is `s_version_52 = .TRUE..`

`perturb_c` is a scalar variable of type `default LOGICAL`, that may be set `.TRUE.` if the user wishes the package make a tiny pseudo-random perturbations to the components of the term \mathbf{c} to try to protect from the so-called (probability zero) “hard case”. Perturbations are generally not needed, and should only be used in very exceptional cases. The default is `perturb_c = .FALSE..`

`stop_check_all_orders` is a scalar variable of type `default LOGICAL`, that may be set `.TRUE.` if the user wishes the package to check for termination for each new member of the extended Krylov space. Such checks incur some extra cost, and experience shows that testing every second member is sufficient, using `stop_check_all_orders = .FALSE..` The default is `stop_check_all_orders = .FALSE..`

`new_weight` is a scalar variable of type `default LOGICAL`, that if `.TRUE.` will resolve the problem with the previous \mathbf{H} , \mathbf{c} and (if provided) \mathbf{S} , but with the larger radius, `radius`, provided to `NREK_solve`. The default is `new_radius = .FALSE..`

`new_values` is a scalar variable of type `default LOGICAL`, that if `PRESENT` and `.TRUE.` will resolve the problem with the data structures set for the previous \mathbf{H} and (if provided) \mathbf{S} , but with new values `H%val`, `C` and/or `S%val` provided to `NREK_solve`. The default is `new_values = .FALSE..`

`space_critical` is a scalar variable of type `default LOGICAL`, that may be set `.TRUE.` if the user wishes the package to allocate as little internal storage as possible, and `.FALSE.` otherwise. The package may be more efficient if `space_critical` is set `.FALSE..` The default is `space_critical = .FALSE..`

`deallocate_error_fatal` is a scalar variable of type `default LOGICAL`, that may be set `.TRUE.` if the user wishes the package to return to the user in the unlikely event that an internal array deallocation fails, and `.FALSE.` if the package should be allowed to try to continue. The default is `deallocate_error_fatal = .FALSE..`

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`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 involving **H** that might arise. Current possible choices are '`sils'`, '`ma27'`, '`ma57'`, '`ma77'`, '`ma86'`, '`ma87'`, '`ma97'`, '`ssids`', '`pardiso`', '`wsmp`', '`sytr`', '`potr`' and '`pbtr`' although only '`sytr`', '`potr`', '`pbtr`' 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 `linear_solver = 'ssids'`, but we recommend '`pbtr`' instead if **H** is banded with a small bandwidth.

`linear_solver_for_S` 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 involving the optional **S** that might arise. Current possible choices are '`sils'`, '`ma27'`, '`ma57'`, '`ma77'`, '`ma86'`, '`ma87'`, '`ma97'`, '`ssids`', '`pardiso`', '`wsmp`', '`sytr`', '`potr`' and '`pbtr`' although only '`sytr`', '`potr`', '`pbtr`' 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 `linear_solver = 'ssids'`, but we recommend '`pbtr`' instead if **S** is banded with a small bandwidth.

`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 of type `SLS_control_type` that is used to control various aspects of the factorization package SLS. See the documentation for GALAHAD_SLS for more details.

`SLS_S_control` is a scalar variable of type `SLS_control_type` that is used to control various aspects of the factorization package SLS when applied to **S**. See the documentation for GALAHAD_SLS for more details.

`RQS_control` is a scalar variable of type `RQS_control_type` that is used to control various aspects of the diagonal norm-regularization solver from the package RQS. See the documentation for GALAHAD_RQS for more details.

2.4.3 The derived data type for holding timing information

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

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

`assemble` is a scalar variable of type `REAL(rp_)`, that gives the CPU time spent assembling the matrices **H** and (if provided) **S** from their constituent parts.

`analyse` is a scalar variable of type `REAL(rp_)`, that gives the CPU time spent analysing the matrices **H** and (if provided) **S** prior to factorization.

`factorize` is a scalar variable of type `REAL(rp_)`, that gives the CPU time spent factorizing the matrices **H** and (if provided) **S**.

`solve` is a scalar variable of type `REAL(rp_)`, that gives the CPU time spent using the factors to solve relevant linear equations.

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

`clock_assemble` is a scalar variable of type `REAL(rp_)`, that gives the elapsed system clock time spent assembling the matrices **H** and (if provided) **S** from their constituent parts.

`clock_analyse` is a scalar variable of type `REAL(rp_)`, that gives the elapsed system clock time spent analysing the matrices **H** and (if provided) **S** prior to factorization.

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`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 using the factors to solve relevant linear equations.

2.4.4 The derived data type for holding informational parameters

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

`status` is a scalar variable of type `INTEGER(ip_)`, that gives the current 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 internal 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.

`iter` is a scalar variable of type `INTEGER(ip_)`, that gives the total number of iterations required.

`n_vec` is a scalar variable of type `INTEGER(ip_)`, that gives the number of orthogonal vectors required (the dimension of the extended-Krylov subspace).

`obj` is a scalar variable of type `REAL(rp_)`, that holds the value of the objective function $\frac{1}{2}\mathbf{x}^T \mathbf{H} \mathbf{x} + \mathbf{c}^T \mathbf{x} + f$.

`obj_regularized` is a scalar variable of type `REAL(rp_)`, that holds the value of the regularized objective function $\frac{1}{2}\mathbf{x}^T \mathbf{H} \mathbf{x} + \mathbf{c}^T \mathbf{x} + \frac{1}{p}\sigma \|\mathbf{x}\|^p$.

`x_norm` is a scalar variable of type `REAL(rp_)`, that holds the value of $\|\mathbf{x}\|_S$.

`multiplier` is a scalar variable of type `REAL(rp_)`, that holds the value of the Lagrange multiplier $\lambda = \sigma \|\mathbf{x}\|^{p-2}$ associated with the regularization.

`weight` is a scalar variable of type `REAL(rp_)`, that holds the value of the current regularization weight.

`next_weight` is a scalar variable of type `REAL(rp_)`, that holds the value of the proposed next weight to be used if the current weight proves to be too small (see `inform%increase`).

`error` is a scalar variable of type `REAL(rp_)`, that holds the value of the norm of the maximum relative residual error, $\|(\mathbf{H} + \lambda \mathbf{S})\mathbf{x} + \mathbf{c}\| / \max(1, \|\mathbf{c}\|)$.

`time` is a scalar variable of type `NREK_time_type` whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.3).

`SLS_inform` is a scalar variable of type `SLS_inform_type`, that holds informational parameters concerning the analysis, factorization and solution phases for `H` performed by the GALAHAD sparse matrix factorization package `SLS`. See the documentation for the package `SLS` for details of the derived type `SLS_inform_type`.

`SLS_S_inform` is a scalar variable of type `SLS_inform_type`, that holds informational parameters concerning the analysis, factorization and solution phases for `S`, if present, performed by the GALAHAD sparse matrix factorization package `SLS`. See the documentation for the package `SLS` for details of the derived type `SLS_inform_type`.

`RQS_inform` is a scalar variable of type `RQS_inform_type`, that holds informational parameters concerning the diagonal norm-regularization subroutine contained in the GALAHAD refinement package `RQS`. See the documentation for the package `RQS` for details of the derived type `RQS_inform_type`.

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2.4.5 The derived data type for holding problem data

The derived data type `NREK_data_type` is used to hold all the data for a particular problem between calls of `NREK` procedures. This data should be preserved, untouched, from the initial call to `NREK_initialize` to the final call to `NREK_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 `NREK_initialize` is used to set default values and initialize private data.
2. The subroutine `NREK_solve` is called to solve the problem.
3. The subroutine `NREK_terminate` is provided to allow the user to automatically deallocate array components of the private data, allocated by `NREK_solve`, at the end of the solution process.

We use square brackets [] to indicate OPTIONAL arguments.

2.5.1 The initialization subroutine

Default values are provided as follows:

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

`data` is a scalar `INTENT(INOUT)` argument of type `NREK_data_type` (see Section 2.4.5). It is used to hold data about the problem being solved.

`control` is a scalar `INTENT(OUT)` argument of type `NREK_control_type` (see Section 2.4.2). On exit, `control` contains default values for the components as described in Section 2.4.2. These values should only be changed after calling `NREK_initialize`.

`inform` is a scalar `INTENT(OUT)` argument of type `NREK_inform_type` (see Section 2.4.4). A successful call to `NREK_initialize` is indicated when the component `status` has the value 0. For other return values of `status`, see Section 2.6.

2.5.2 The optimization problem solution subroutine

The norm-regularization solution algorithm is called as follows:

```
CALL NREK_solve( n, H, C, power, weight, X, data, control, inform[, S])
```

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

`H` is scalar `INTENT(IN)` argument of type `SMT_TYPE` that holds the Hessian matrix `H`. The following components are used here:

`H` 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` must contain the string `DENSE`. For the sparse co-ordinate scheme (see Section 2.1.2), the first ten components of `H` must contain the string `COORDINATE`, for the sparse row-wise storage scheme (see Section 2.1.3), the first fourteen components of `H` must contain the string `SPARSE_BY_ROWS`, and for the diagonal storage scheme (see Section 2.1.4), the first eight components of `H` must contain the

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string `DIAGONAL`, for the scaled-identity matrix storage scheme (see Section 2.1.5), the first fifteen components of `H%type` must contain the string `SCALED_IDENTITY`, for the identity matrix storage scheme (see Section 2.1.6), the first eight components of `H%type` must contain the string `IDENTITY`, and for the zero matrix storage scheme (see Section 2.1.7), the first four components of `H%type` must contain the string `ZERO`.

For convenience, the procedure `SMT_put` may be used to allocate sufficient space and insert the required keyword into `H%type`. For example, if we wish to store \mathbf{S} using the co-ordinate scheme, we may simply

```
CALL SMT_put( 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 \mathbf{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 \mathbf{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 \mathbf{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 \mathbf{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 \mathbf{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.

`c` is an array `INTENT(IN)` argument of dimension `n` and type `REAL(rp_)`, whose i -th entry holds the component c_i of the vector \mathbf{c} for the objective function.

`power` is a scalar `INTENT(IN)` variable of type `REAL(rp_)`, that must be set on initial entry to the power of the regularization, p . **Restriction:** $p > 2$.

`weight` is a scalar `INTENT(IN)` variable of type `REAL(rp_)`, that must be set on initial entry to the value of the regularization weight, σ . **Restriction:** $\sigma > 0$.

`x` is an array `INTENT(OUT)` argument of dimension `n` and type `REAL(rp_)`, that holds an estimate of the solution \mathbf{x} of the problem on exit.

`data` is a scalar `INTENT(INOUT)` argument of type `NREK_data_type` (see Section 2.4.5). 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 `NREK_initialize`.

`control` is a scalar `INTENT(IN)` argument of type `NREK_control_type`. (see Section 2.4.2). Default values may be assigned by calling `NREK_initialize` prior to the first call to `NREK_solve`.

`inform` is a scalar `INTENT(INOUT)` argument of type `NREK_inform_type` (see Section 2.4.4) whose components need not be set on entry. A successful call to `NREK_solve` is indicated when the component `status` has the value 0. For other return values of `status`, see Section 2.6.

`s` is an OPTIONAL scalar `INTENT(IN)` argument of type `SMT_TYPE` that holds the diagonally dominant scaling matrix \mathbf{S} . It need only be set if $\mathbf{S} \neq \mathbf{I}$ and in this case the following components are used:

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`S%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 `S%type` must contain the string DENSE. For the sparse co-ordinate scheme (see Section 2.1.2), the first ten components of `S%type` must contain the string COORDINATE, for the sparse row-wise storage scheme (see Section 2.1.3), the first fourteen components of `S%type` must contain the string SPARSE_BY_ROWS, and for the diagonal storage scheme (see Section 2.1.4), the first eight components of `S%type` must contain the string DIAGONAL, for the scaled-identity matrix storage scheme (see Section 2.1.5), the first fifteen components of `S%type` must contain the string SCALED_IDENTITY, for the identity matrix storage scheme (see Section 2.1.6), the first eight components of `S%type` must contain the string IDENTITY, and for the zero matrix storage scheme (see Section 2.1.7), the first four components of `S%type` must contain the string ZERO.

For convenience, the procedure `SMT_put` may be used to allocate sufficient space and insert the required keyword into `S%type`. For example, if we wish to store **S** using the co-ordinate scheme, we may simply

```
CALL SMT_put( M%type, 'COORDINATE' )
```

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

`S%ne` is a scalar variable of type INTEGER(ip_), that holds the number of entries in the **lower triangular** part of **S** in the sparse co-ordinate storage scheme (see Section 2.1.2). It need not be set for any of the other three schemes.

`S%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 scaling matrix **S** in any of the storage schemes discussed in Section 2.1.

`S%row` is a rank-one allocatable array of type INTEGER(ip_), that holds the row indices of the **lower triangular** part of **S** in the sparse co-ordinate storage scheme (see Section 2.1.2). It need not be allocated for any of the other three schemes.

`S%col` is a rank-one allocatable array variable of type INTEGER(ip_), that holds the column indices of the **lower triangular** part of **S** 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.

`S%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 **S**, 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.

If **S** is absent, the ℓ_2 -norm, $\|\mathbf{x}\|_2 = \sqrt{\mathbf{x}^T \mathbf{x}}$, will be employed.

2.5.3 The termination subroutine

All previously allocated arrays are deallocated as follows:

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

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

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

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

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2.6 Warning and error messages

A negative value of `inform%status` on exit from `NREK_solve` or `NREK_terminate` indicates that an error might have 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. (NREK_solve only) One of the restrictions $n > 0$, $\text{radius} > 0$, $H\%n \neq n$, $S\%n \neq n$ or the radius has not decreased when `resolve = /true/` has been violated.
- 9. (NREK_solve only) The analysis phase of the factorization of one of the matrices **H** and (if provided) **S** failed.
- 10. (NREK_solve only) The factorization of one of the matrices **H** and (if provided) **S** failed.
- 11. (NREK_solve only) The solve phase involving one of the matrices **H** and (if provided) **S** failed.
- 15. (NREK_solve only) The matrix **S** appears not to be diagonally dominant.
- 16. (NREK_solve only) The problem is so ill-conditioned that further progress is impossible.
- 18. (NREK_solve only) Too many iterations have been required. This may happen if `control%eks_max` is too small, but may also be symptomatic of a badly scaled problem.
- 31. (NREK_solve only) A resolve call has been made before an initial call (see `control%new_radius` and `control%new_values`).
- 38. (NREK_solve only) An error occurred in a call to an LAPACK subroutine.

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 `NREK_control_type` (see Section 2.4.2), by reading an appropriate data specification file using the subroutine `NREK_read_specfile`. This facility is useful as it allows a user to change NREK control parameters without editing and recompiling programs that call NREK.

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 `NREK_read_specfile` must start with a "BEGIN NREK" command and end with an "END" command. The syntax of the specfile is thus defined as follows:

```
( .. lines ignored by NREK_read_specfile .. )
BEGIN NREK
    keyword    value
    .....
    keyword    value
END
( .. lines ignored by NREK_read_specfile .. )
```

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

and

```
END NREK SPECIFICATION
```

are acceptable. Furthermore, between the “BEGIN NREK” 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 `NREK_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 `NREK_read_specfile`.

Control parameters corresponding to the components `RQS_control`, `SLS_control` and `IR_control` may be changed by including additional sections enclosed by “BEGIN RQS” and “END RQS”, and “BEGIN SLS” and “END SLS”, respectively. See the specification sheets for the packages `GALAHAD_RQS` and `GALAHAD_SLS`

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 NREK_read_specfile( control, device )
```

`control` is a scalar `INTENT (INOUT)` argument of type `NREK_control_type` (see Section 2.4.2). Default values should have already been set, perhaps by calling `NREK_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 2.4.2) of `control` that each affects are given in Table 2.1.

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

2.8 Information printed

If `control%print_level` is positive, information about the progress of the algorithm will be printed on unit `control%out`. If `control%print_level` = 1, a single line of output will be produced for each iteration of the process. This will include the size of the subspace, the norm of the current estimate of \mathbf{x} and the radius, the current estimate of the shift λ , the error $\|(\mathbf{H} + \lambda\mathbf{S})\mathbf{x} + \mathbf{c}\|/\max(1, \|\mathbf{c}\|)$, and the current value of the objective function. If `control%print_level` ≥ 2 , this output will be increased to provide significant detail of each iteration. This extra output includes times for various phases.

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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-subspace-dimension	%eks_max	integer
maximum-number-of-iterations	%it_max	integer
constant-term-in-objective	%f	real
weight-increase-factor	%increase	real
residual-accuracy	%stop_residual	real
reorthogonalize-vectors	%reorthogonalize	logical
s-version-52	%s_version_52	logical
perturb-c	%perturb-c	logical
stop-check-all-orders	%stop-check-all-orders	logical
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
linear-equation-solver	%linear_solver	character
linear-equation-solver-for-S	%linear_solver_for_S	character
output-line-prefix	%prefix	character

Table 2.1: Specfile commands and associated components of control.

3 GENERAL INFORMATION

Use of common: None.

Workspace: Provided automatically by the module.

Other routines called directly: None.

Other modules used directly: NREK_solve calls the GALAHAD packages GALAHAD_CLOCK, GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_NORMS, GALAHAD_ROOTS, GALAHAD_SPECFILE, GALAHAD_SMT, GALAHAD_RAND, GALAHAD_RQS, GALAHAD_SLS, and GALAHAD_MOP.

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

Restrictions: $n > 0$, $p > 2$, $\sigma > 0$.

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

4 METHOD

The required solution \mathbf{x}_* necessarily satisfies the optimality condition $\mathbf{H}\mathbf{x}_* + \lambda_*\mathbf{S}\mathbf{x}_* + \mathbf{c} = \mathbf{0}$, where $\lambda_* = \sigma\|\mathbf{x}_*\|^{p-2}$ is a Lagrange multiplier corresponding to the regularization. In addition in all cases, the matrix $\mathbf{H} + \lambda_*\mathbf{S}$ will be positive semi-definite; in most instances it will actually be positive definite, but in special “hard” cases singularity is a possibility.

The method is iterative, and is based upon building a solution approximation from an orthogonal basis of the evolving extended Krylov subspaces $\mathcal{K}_{2m+1}(\mathbf{H}, \mathbf{c}) = \text{span}\{\mathbf{c}, \mathbf{H}^{-1}\mathbf{c}, \mathbf{H}\mathbf{c}, \mathbf{H}^{-2}\mathbf{c}, \dots, \mathbf{H}^{-m}\mathbf{c}, \mathbf{H}^m\mathbf{c}\}$ as m increases. The key observations are (i) the manifold of solutions to the optimality system

$$(\mathbf{H} + \lambda\mathbf{I})\mathbf{x}(\lambda) = -\mathbf{c}$$

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as a function of σ is of approximately very low rank, (ii) the subspace $\mathcal{K}_{2m+1}(\mathbf{H}, \mathbf{c})$ rapidly gives a very good approximation to this manifold, (iii) it is straightforward to build an orthogonal basis of $\mathcal{K}_{2m+1}(\mathbf{H}, \mathbf{c})$ using short-term recurrences and a single factorization of \mathbf{H} , and (iv) solutions to the regularization subproblem restricted to elements of the orthogonal subspace may be found very efficiently using effective high-order root-finding methods. Coping with general scalings \mathbf{S} is a straightforward extension so long as factorization of \mathbf{S} is also possible.

Reference: The method is described in detail in

H. Al Daas and N. I. M. Gould. Extended-Krylov-subspace methods for trust-region and norm-regularization subproblems. Preprint STFC-P-2025-002, Rutherford Appleton Laboratory, Oxfordshire, England.

5 EXAMPLE OF USE

Suppose we wish to solve a problem in 10,000 unknowns, whose data is

$$\mathbf{H} = \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & . & \\ & . & . & . \\ & . & -2 & 1 \\ & & 1 & -2 \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} 2 & & & \\ & 2 & & \\ & & . & \\ & & & 2 \\ & & & 2 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} 1 \\ 1 \\ . \\ 1 \\ 1 \end{pmatrix} \text{ and } f = 0,$$

starting with a regularization weight $\sigma = 10$ and order $p = 3$, but then gradually doubling the weight at every subsequent stage. Then we may use the following code:

```

! THIS VERSION: GALAHAD 5.4 - 2025-11-22 AT 09:10 GMT.
PROGRAM GALAHAD_NREK_EXAMPLE
! double precision version
USE GALAHAD_NREK_double, ONLY: SMT_type, SMT_put, NREK_control_type,
     & NREK_inform_type, NREK_data_type, NREK_initialize, NREK_solve,
     & NREK_terminate
USE GALAHAD_NORMS_double, ONLY: TWO_NORM
IMPLICIT NONE
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 ) ! set precision
INTEGER, PARAMETER :: n = 10000, m = 4, h_ne = 2 * n - 1
TYPE ( SMT_type ) :: H
REAL ( KIND = wp ), DIMENSION( n ) :: C
REAL ( KIND = wp ) :: power, weight
REAL ( KIND = wp ), DIMENSION( n ) :: X
TYPE ( NREK_control_type ) :: control
TYPE ( NREK_inform_type ) :: inform
TYPE ( NREK_data_type ) :: data
INTEGER :: stat, i
H%n = n ; H%ne = h_ne
CALL SMT_put( H%type, 'COORDINATE', stat ) ! Specify co-ordinate for H
ALLOCATE( H%val( H%ne ), H%row( H%ne ), H%col( H%ne ) )
DO i = 1, n
    H%row( i ) = i ; H%col( i ) = i ; H%val( i ) = - 2.0_wp
END DO
DO i = 1, n - 1
    H%row( n + i ) = i + 1 ; H%col( n + i ) = i ; H%val( n + i ) = 1.0_wp
END DO
C = 1.0_wp ! c is a vector of ones
power = 3.0_wp ! power (cubic regularization)
weight = 10.0_wp ! initial weight

```

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```

CALL NREK_initialize( data, control, inform )
control%linear_solver = 'pbtr'
DO i = 1, m ! loop over a sequence of decreasing radii
  control%new_weight = i > 1
  inform%time%clock_total = 0.0 ! reset time
  CALL NREK_solve( n, H, C, power, weight, X, data, control, inform )
  IF ( inform%status == 0 ) THEN
    WRITE( 6, "( 1X, I0, ' vectors required, error = ', ES11.4 )" )      &
      inform%n_vec, inform%error
    WRITE( 6, "( ' weight, ||x||, f, multiplier =', 2ES11.4, 2ES12.4 )" )  &
      weight, TWO_NORM( X ), inform%obj_regularized, inform%multiplier
    IF ( i < m ) weight = inform%next_weight ! pick the next (larger) weight
  ELSE
    WRITE( 6, "( ' error exit, status = ', I0 )" ) inform%status
    STOP
  END IF
  WRITE( 6, "( ' total time NREK = ', F0.2 )" ) inform%time%clock_total
END DO
CALL NREK_terminate( data, control, inform )
DEALLOCATE( H%type, H%row, H%col, H%val )
END PROGRAM GALAHAD_NREK_EXAMPLE

```

This produces the following output:

```

8 vectors required, error = 1.7175E-08
weight, ||x||, f, multiplier = 1.0000E+01 3.1623E+00 -2.1082E+02 3.1623E+01
total time NREK = .01
8 vectors required, error = 4.0443E-09
weight, ||x||, f, multiplier = 2.0000E+01 2.2361E+00 -1.4907E+02 4.4721E+01
total time NREK = .00
8 vectors required, error = 9.7010E-10
weight, ||x||, f, multiplier = 4.0000E+01 1.5811E+00 -1.0541E+02 6.3246E+01
total time NREK = .00
8 vectors required, error = 2.3564E-10
weight, ||x||, f, multiplier = 8.0000E+01 1.1180E+00 -7.4536E+01 8.9443E+01
total time NREK = .00

```