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GALAHAD

SHA

USER DOCUMENTATION

GALAHAD Optimization Library version 5.0

1 SUMMARY

This package **computes a component-wise secant approximation to the Hessian matrix $\mathbf{H}(\mathbf{x})$** , for which $(\mathbf{H}(\mathbf{x}))_{i,j} = \partial^2 f(\mathbf{x}) / \partial x_i \partial x_j$, $1 \leq i, j \leq n$, using values of the gradient $\mathbf{g}(\mathbf{x}) = \nabla_x f(\mathbf{x})$ of the function $f(\mathbf{x})$ of n unknowns $\mathbf{x} = (x_1, \dots, x_n)^T$ at a sequence of given distinct $\{\mathbf{x}^{(k)}\}$, $k \geq 0$. More specifically, given **differences**

$$\mathbf{s}^{(k)} = \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)} \quad \text{and} \quad \mathbf{y}^{(k)} = \mathbf{g}(\mathbf{x}^{(k+1)}) - \mathbf{g}(\mathbf{x}^{(k)})$$

the package aims to find an approximation \mathbf{B} to $\mathbf{H}(\mathbf{x})$ for which the secant conditions $\mathbf{B}\mathbf{s}^{(k)} \approx \mathbf{y}^{(k)}$ hold for a chosen set of values k . The methods provided take advantage of the entries in the Hessian that are known to be zero.

The package is particularly intended to allow gradient-based optimization methods, that generate iterates $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{s}^{(k)}$ based upon the values $\mathbf{g}(\mathbf{x}^{(k)})$ for $k \geq 0$, to build a suitable approximation to the Hessian $\mathbf{H}(\mathbf{x}^{(k+1)})$. This then gives the method an opportunity to accelerate the iteration using the Hessian approximation.

ATTRIBUTES — Versions: GALAHAD_SHA_single, GALAHAD_SHA_double. **Uses:** GALAHAD_SYMBOLS, GALAHAD_SPECFILE and GALAHAD_SPACE. **Date:** August 2023. **Origin:** J. Fowkes and N. I. M. Gould, STFC-Rutherford Appleton Laboratory, **Language:** Fortran 2003.

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_SHA_single
```

with the obvious substitution `GALAHAD_SHA_double`, `GALAHAD_SHA_single_64` and `GALAHAD_SHA_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 `SHA_control_type`, `SHA_inform_type`, `SHA_data_type` and `NLPT_userdata_type`, (Section 2.3) and the subroutines `SHA_initialize`, `SHA_analyse`, `SHA_estimate`, `SHA_terminate`, (Section 2.4) and `SHA_read_specfile` (Section 2.6) must be renamed on one of the `USE` statements.

2.1 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.

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2.2 Parallel usage

OpenMP may be used by the `GALAHAD_SHA` package to provide parallelism for some solvers in shared memory environments. 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`.

The code may be compiled and run in serial mode.

2.3 The derived data types

Four derived data types are accessible from the package.

2.3.1 The derived data type for holding control parameters

The derived data type `SHA_control_type` is used to hold controlling data. Default values may be obtained by calling `SHA_initialize` (see Section 2.4.1), while components may also be changed by calling `GALAHAD_SHA_read_spec` (see Section 2.6.1). The components of `SHA_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 `SHA_analyse`, `SHA_estimate` and `SHA_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 `SHA_analyse` and `SHA_estimate` 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` > 0 , details of any data errors encountered will be reported. The default is `print_level = 0`.

`approximation_algorithm` is a scalar variable of type `INTEGER(ip_)`, that is used to select which approximation algorithm employed. This may be

1. 1. unsymmetric, parallel (Algorithm 2.1 in paper)
2. 2. symmetric (Algorithm 2.2 in paper)
3. 3. composite, parallel (Algorithm 2.3 in paper)
4. 4. composite, block parallel (Algorithm 2.4 in paper)

Any value outside this range will be reset to the default; the default is `approximation_algorithm = 4`.

`dense_linear_solver` is a scalar variable of type `INTEGER(ip_)`, that specifies which (LAPACK) dense linear equation solver to use when finding the values of entries in each row of **B**. This may be

1. 1. Gaussian elimination
2. 2. QR factorization
3. 3. singular-value decomposition
4. 4. singular-value decomposition with divide-and-conquer

Any value outside this range will be reset to the default; the default is `dense_linear_solver = 3`.

`extra_differences` is a scalar variable of type `INTEGER(ip_)`, that is used to specify how many additional gradients (in addition to the number output in `inform%differences_needed` from `SHA_analyse`) are available when calling `SHA_estimate`. The default is `extra_differences = 1`.

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`sparse_row` is a scalar variable of type `INTEGER(ip_)`, that is used to specify the maximum sparse degree if a composite parallel algorithm (`%approximation_algorithm = 3` is employed. The default is `sparse_row = 100`.

`recursion_max` is a scalar variable of type `INTEGER(ip_)`, that puts a limit on the number of levels of recursion that will be allowed if the composite block-parallel algorithm (`%approximation_algorithm = 4` is used. The default is `recursion_max = 25`.

`recursion_entries_required` is a scalar variable of type `INTEGER(ip_)`, that imposes the minimum number of entries in a reduced row that are required if a further level of recursion is allowed in the composite block-parallel algorithm (`%approximation_algorithm = 4`. The default is `recursion_entries_required = 10`.

`average_off_diagonals` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if pairs of off-diagonal Hessian estimates are to be averaged on return, and `.FALSE.` if the value from the upper triangle suffices. Averaging incurs small extra storage and calculation expenses, and rarely offers much advantage. The default is `average_off_diagonals = .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..`

`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 = ""`.

2.3.2 The derived data type for holding informational parameters

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

`status` is a scalar variable of type `INTEGER(ip_)`, that gives the exit status of the algorithm. See Section 2.5 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`.

`max_degree` is a scalar variable of type `INTEGER(ip_)`, that holds the maximum degree in the adjacency graph.

`differences_needed` is a scalar variable of type `INTEGER(ip_)`, that holds the number of differences that will be needed (more may be helpful) by `SHA_estimate`. This value is computed by `SHA_analyse`.

`max_reduced_degree` is a scalar variable of type `INTEGER(ip_)`, that holds the maximum reduced degree in the adjacency graph.

`approximation_algorithm_used` is a scalar variable of type `INTEGER(ip_)`, that specifies the actual approximation algorithm used (see `control%approximation_algorithm`).

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`bad_row` is a scalar variable of type `INTEGER(ip_)`, that holds the index of the first row for which a failure occurred when forming its Hessian values (or 0 if the data if no failures occurred).

`max_off_diagonal_difference` is a scalar variable of type `REAL(rp_)`, that gives the maximum difference between estimated Hessian off-diagonal pairs if approximation algorithm 1, 3 or 4 has been employed and `control%average_off_diagonal` is `.TRUE.`. It will be zero otherwise.

2.3.3 The derived data type for holding problem data

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

2.4 Argument lists and calling sequences

There are four procedures for user calls (see Section 2.6 for further features):

1. The subroutine `SHA_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 `SHA_analyse` is called to analyze the sparsity pattern of the Hessian and to generate information that will be used when estimating its values.
3. The subroutine `SHA_estimate` is called to estimate the Hessian by component-wise secant approximation. This must be preceded by a call to `SHA_analyse`.
4. The subroutine `SHA_terminate` is provided to allow the user to automatically deallocate array components of the private data, allocated by `SHA_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 `SHA_initialize` cannot test for this situation, and any existing associated targets will subsequently become unreachable.

We use square brackets [] to indicate OPTIONAL arguments.

2.4.1 The initialization subroutine

Default values are provided as follows:

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

`data` is a scalar `INTENT(INOUT)` argument of type `SHA_data_type` (see Section 2.3.3). It is used to hold data about the problem being solved.

`control` is a scalar `INTENT(OUT)` argument of type `SHA_control_type` (see Section 2.3.1). On exit, `control` contains default values for the components as described in Section 2.3.1. These values should only be changed after calling `SHA_initialize`.

`inform` is a scalar `INTENT(OUT)` argument of type `SHA_inform_type` (see Section 2.3.2). A successful call to `SHA_initialize` is indicated when the component `status` has the value 0. For other return values of `status`, see Section 2.5.

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2.4.2 The analysis subroutine

The analysis phase, in which the given sparsity pattern of the Hessian is used to generate information that will be used when estimating its values, is called as follows:

```
CALL SHA_analyse( n, nz, ROW, COL, data, control, inform )
```

n is a scalar `INTENT(IN)` scalar argument of type `INTEGER(ip_)`, that must be set to n the dimension of the Hessian matrix, i.e. the number of variables in the function f . **Restrictions:** $n > 0$.

nz is a scalar `INTENT(IN)` scalar argument of type `INTEGER(ip_)`, that must be set to the number of nonzero entries on and above the diagonal of the Hessian matrix. **Restrictions:** $nz \geq 0$.

ROW and **COL** are a scalar `INTENT(IN)` rank-one array arguments of type `INTEGER(ip_)` and dimension nz , that are used to describe the sparsity structure of the Hessian matrix, $\mathbf{H}(\mathbf{x})$. They must be set so that $\text{ROW}(i)$ and $\text{COL}(i)$, $i = 1, \dots, nz$, contains the row and column indices of the nonzero elements of the **upper triangular part, including the diagonal**, of the Hessian matrix. The entries may appear in any order. **Restrictions:** $1 \leq \text{ROW}(j) \leq \text{COL}(j) \leq n$, $j = 1, \dots, nz$.

data is a scalar `INTENT(INOUT)` argument of type `SHA_data_type` (see Section 2.3.3). 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 `SHA_initialize`.

control is a scalar `INTENT(IN)` argument of type `SHA_control_type` (see Section 2.3.1). Default values may be assigned by calling `SHA_initialize` prior to the first call to `SHA_analyse`.

inform is a scalar `INTENT(INOUT)` argument of type `SHA_inform_type` (see Section 2.3.2). A successful call to `SHA_analyse` is indicated when the component `status` has the value 0. For other return values of `status`, see Section 2.5.

2.4.3 The estimation subroutine

The estimation phase, in which the nonzero entries of the Hessian are found by component-wise secant approximation, is called as follows:

```
CALL SHA_estimate( n, nz, ROW, COL, m_available, S, ls1, ls2, &
                  Y, ly1, ly2, VAL, data, control, inform[, ORDER] )
```

n, **nz**, **ROW** and **COL** are `INTENT(IN)` arguments exactly as described and input to `SHA_analyse`, and must not have been changed in the interim.

m_available is a scalar `INTENT(IN)` scalar argument of type `INTEGER(ip_)`, that should be set to the number of differences provided; ideally this will be as large as `inform%diffences_needed` as reported by `SHA_analyse`, but better still there should be a further `control%extra_differences` to allow for unlikely singularities.

S is a scalar `INTENT(IN)` rank-two array argument of type `REAL(rp_)`, and dimension $(ls1, ls2)$, that should be set on input so that the i -th entry of the k -th difference $s_i^{(k)}$ lies in $S(i, k)$.

ls1 is a scalar `INTENT(IN)` scalar argument of type `INTEGER(ip_)`, that must be set to the length of the leading dimension of **S**, and must be at least n .

ls2 is a scalar `INTENT(IN)` scalar argument of type `INTEGER(ip_)`, that must be set to the length of the trailing dimension of **S**, and must be at least `m_available`.

Y is a scalar `INTENT(IN)` rank-two array argument of type `REAL(rp_)`, and dimension $(ly1, ly2)$, that should be set on input so that the i -th entry of the k -th difference $y_i^{(k)}$ lies in $Y(i, k)$.

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`ly1` is a scalar `INTENT(IN)` scalar argument of type `INTEGER(ip_)`, that must be set to the length of the leading dimension of `Y`, and must be at least `n`.

`ly2` is a scalar `INTENT(IN)` scalar argument of type `INTEGER(ip_)`, that must be set to the length of the trailing dimension of `Y`, and must be at least `m_available`.

`VAL` is a scalar `INTENT(OUT)` rank-one array argument of type `REAL(rp_)`, and dimension `nz`, that will be set on output to the non-zeros of the Hessian approximation **B** in the order defined by the list stored in `ROW` and `COL`.

`data` is a scalar `INTENT(INOUT)` argument of type `SHA_data_type` (see Section 2.3.3). 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 `SHA_analyse`.

`control` is a scalar `INTENT(IN)` argument of type `SHA_control_type` (see Section 2.3.1) exactly as for `SHA_analyse`.

`inform` is a scalar `INTENT(INOUT)` argument of type `SHA_inform_type` (see Section 2.3.2) exactly as for `SHA_analyse`. A successful call to `SHA_estimate` is indicated when the component `status` has the value 0. For other return values of `status`, see Section 2.5.

`ORDER` is an `OPTIONAL` scalar `INTENT(IN)` rank-one array argument of type default integer and dimension `m_available`, that can be set to the preferred order of access of the differences stored in `S` and `Y`. The calculation of each row of the Hessian approximation **B** depends on the number of nonzeros in the row, and `ORDER` allows the user to specify the order in which the columns of `S` and `Y` are accessed to determine these row values. If `ORDER` is `PRESENT` the i -th accessed column will be `ORDER(i)`. Otherwise the columns will be accessed in their natural order $i, i = 1, \dots, m_available$.

2.4.4 The termination subroutine

All previously allocated arrays are deallocated as follows:

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

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

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

`inform` is a scalar `INTENT(OUT)` argument of type `SHA_inform_type` exactly as for `SHA_analyse`. Only the component `status` will be set on exit, and a successful call to `SHA_terminate` is indicated when this component `status` has the value 0. For other return values of `status`, see Section 2.5.

2.5 Warning and error messages

A positive value of `inform%status` on exit from `SHA_estimate` provides a warning. Possible values are:

1. Insufficient data pairs (s_i, y_i) have been provided, as `m` is too small. The returned **B** is likely not fully accurate.

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

- 1. An allocation error occurred. A message indicating the offending array is written on unit `control%error`, and the returned allocation status and a string containing the name of the offending array are held in `inform%alloc_status` and `inform%bad_alloc`, respectively.

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- 2. A deallocation error occurred. A message indicating the offending array is written on unit `control%error` and the returned allocation status and a string containing the name of the offending array are held in `inform%alloc_status` and `inform%bad_alloc`, respectively.
- 3. One or more of the restrictions $n > 0$, $n_z \geq 0$, $1 \leq \text{ROW}(j) \leq \text{COL}(j) \leq n$, $j = 1, \dots, n_z$, has been violated.
- 10. The LAPACK dense linear equation solver used to find the values of the rows of **B** has failed.
- 31. `SHA_estimate` has been called before `SHA_analyse`.

2.6 Further features

In this section, we describe an alternative means of setting control parameters, that is components of the variable `control` of type `SHA_control_type` (see Section 2.3.1), by reading an appropriate data specification file using the subroutine `SHA_read_specfile`. This facility is useful as it allows a user to change SHA control parameters without editing and recompiling programs that call `SHA`.

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

```
( .. lines ignored by SHA_read_specfile .. )
  BEGIN SHA
    keyword      value
    .....
    keyword      value
  END
( .. lines ignored by SHA_read_specfile .. )
```

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

and

```
END SHA SPECIFICATION
```

are acceptable. Furthermore, between the "BEGIN SHA" 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".

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The specification file must be open for input when `SHA_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 `SHA_read_specfile`.

2.6.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
CALL SHA_read_specfile( control, device )
```

`control` is a scalar `INTENT(INOUT)` argument of type `SHA_control_type` (see Section 2.3.1). Default values should have already been set, perhaps by calling `SHA_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 2.3.1) 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
approximation-algorithm	%approximation_algorithm	integer
dense-linear-solver	%dense_linear_solver	integer
extra-differences	%extra_differences	integer
maximum-degree-considered-sparse	%sparse_row	integer
maximum-recursion-levels	%recursion_max	integer
recursion-entries-required	%recursion_entries_required	integer
average-off-diagonals	%average_off_diagonals	logical
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
output-line-prefix	%prefix	character

Table 2.1: Specfile commands and associated components of `control`.

`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`.

2.7 Information printed

If `control%print_level` is positive, information about errors encountered will be printed on unit `control%out`.

3 GENERAL INFORMATION

Use of common: None.

Workspace: Provided automatically by the module.

Other routines called directly: None.

Other modules used directly: `SHA_solve` calls the GALAHAD packages `GALAHAD_SYMBOLS`, `GALAHAD_SPECFILE` and `GALAHAD_NLPT`.

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

Restrictions: $0 < n$, $0 \leq nz$, $1 \leq \text{ROW}(j) \leq \text{COL}(j) \leq n$, $j = 1, \dots, nz$.

Portability: Fortran 2003. The package is thread-safe.

4 METHOD

The package computes the entries in the each row of \mathbf{B} one at a time. The entries b_{ij} in row i may be chosen to

$$\underset{b_{i,j}}{\text{minimize}} \sum_{k \in I_i} \left[\sum_{\text{nonzeros } j} b_{i,j} s_j^{(k)} - y_i^{(k)} \right]^2, \quad (4.1)$$

where I_i is ideally chosen to be sufficiently large so that (4.1) has a unique minimizer. Since this requires that there are at least as many $(\mathbf{s}^{(k)}, \mathbf{y}^{(k)})$ pairs as the maximum number of nonzeros in any row, this may be prohibitive in some cases. We might then be content with a minimum-norm (under-determined) least-squares solution; each row may then be processed in parallel. Or, we may take advantage of the symmetry of the Hessian, and note that if we have already found the values in row j , then the value $b_{i,j} = b_{j,i}$ in (4.1) is known before we process row i . Thus by ordering the rows and exploiting symmetry we may reduce the numbers of unknowns in future unprocessed rows.

In the analysis phase, we order the rows by constructing the connectivity graph—a graph comprising nodes 1 to n and edges connecting nodes i and j if $h_{i,j}$ is everywhere nonzero—of $\mathbf{H}(\mathbf{x})$. The nodes are ordered by increasing degree (that is, the number of edges emanating from the node) using a bucket sort. The row chosen to be ordered next corresponds to a node of minimum degree, the node is removed from the graph, the degrees updated efficiently, and the process repeated until all rows have been ordered. This often leads to a significant reduction in the numbers of unknown values in each row as it is processed in turn, but numerical rounding can lead to inaccurate values in some cases. A useful remedy is to process all rows for which there are sufficient $(\mathbf{s}^{(k)}, \mathbf{y}^{(k)})$ as before, and then process the remaining rows taking into account the symmetry. That is, the rows and columns are rearranged so that the matrix is in block form

$$\mathbf{B} = \begin{pmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{12}^T & \mathbf{B}_{22} \end{pmatrix},$$

the $(\mathbf{B}_{11} \ \mathbf{B}_{12})$ rows are processed without regard for symmetry but give the 2, 1 block \mathbf{B}_{12}^T , and finally the 2, 2 block \mathbf{B}_{22} is processed knowing \mathbf{B}_{12}^T again without respecting symmetry. The rows in blocks $(\mathbf{B}_{11} \ \mathbf{B}_{12})$ and \mathbf{B}_{22} may be computed in parallel. It is also possible to generalise this so that \mathbf{B} is decomposed into r blocks, and the blocks processed one at a time recursively using the symmetry from previous rows. More details of the precise algorithms (Algorithms 2.1–2.4) are given in the reference below. The linear least-squares problems (4.1) themselves are solved by a choice of LAPACK packages.

Reference:

The method is described in detail in

J. M. Fowkes, N. I. M. Gould and J. A. Scott, Approximating large-scale Hessians using secant equations. Preprint P-2024-001, Rutherford Appleton Laboratory.

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5 EXAMPLES OF USE

Suppose we wish to estimate the Hessian matrix whose values at a given \mathbf{x} are

$$\mathbf{H}(\mathbf{x}) = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 6 & 0 & 0 & 0 \\ 3 & 0 & 7 & 0 & 0 \\ 4 & 0 & 0 & 8 & 0 \\ 5 & 0 & 0 & 0 & 9 \end{pmatrix}$$

and that we have (artificially) sampled the matrix via $\mathbf{y}^{(k)} = \mathbf{H}(\mathbf{x})\mathbf{s}^{(k)}$ along random vectors $\mathbf{s}^{(k)}$ for $k = 1, \dots, k_s$; a suitable value for k_s is returned by SHA_analyse. Then we may recover $\mathbf{H}(\mathbf{x})$ as follows:

```
! THIS VERSION: GALAHAD 4.1 - 2023-08-19 AT 15:40 GMT.
PROGRAM GALAHAD_SHA_EXAMPLE
USE GALAHAD_SHA_double ! double precision version
USE GALAHAD_RAND_double
IMPLICIT NONE
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 ) ! set precision
TYPE ( SHA_data_type ) :: data
TYPE ( SHA_control_type ) :: control
TYPE ( SHA_inform_type ) :: inform
INTEGER :: i, j, k, k_s, l
REAL ( KIND = wp ) :: v
INTEGER, ALLOCATABLE, DIMENSION( : ) :: ORDER
REAL ( KIND = wp ), ALLOCATABLE, DIMENSION( : , : ) :: S, Y
TYPE ( RAND_seed ) :: seed
INTEGER, PARAMETER :: n = 5, nz = 9 ! set problem data
INTEGER :: ROW( nz ), COL( nz )
REAL ( KIND = wp ) :: VAL( nz ), VAL_est( nz )
ROW = ( / 1, 1, 1, 1, 1, 2, 3, 4, 5 / ) ! N.B. upper triangle only
COL = ( / 1, 2, 3, 4, 5, 2, 3, 4, 5 / )
VAL = ( / 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0 / ) ! artificial values
CALL SHA_initialize( data, control, inform ) ! initialize
control%approximation_algorithm = 2 ! symmetric approximation
CALL SHA_analyse( n, nz, ROW, COL, data, control, inform ) ! analyse sparsity
IF ( inform%status /= 0 ) THEN ! Failure
  WRITE( 6, "( ' return with nonzero status ', I0, ' from SHA_analyse' )" ) &
    inform%status ; STOP
END IF
WRITE( 6, "( 1X, I0, ' differences are needed,', &
& ' one or more extra might help' )" ) inform%differences_needed
control%extra_differences = 1 ! use as many differences as required + 1
k_s = inform%differences_needed + control%extra_differences
! artificial setup: compute random s_i and then form y_i = Hessian * s_i
ALLOCATE( S( n, k_s ), Y( n, k_s ), ORDER( k_s ) )
CALL RAND_initialize( seed )
DO k = 1, k_s
  DO i = 1, n ! choose random S
    CALL RAND_random_real( seed, .FALSE., S( i, k ) )
    CALL RAND_random_real( seed, .FALSE., Y( i, k ) )
    Y( i, k ) = Y( i, k ) * 0.001
  END DO
  Y( : n, k ) = 0.0_wp ! form Y = H * S
DO l = 1, nz
```

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```

      i = ROW( 1 ) ; j = COL( 1 ) ; v = VAL( 1 )
      Y( i, k ) = Y( i, k ) + v * S( j, k )
      IF ( i /= j ) Y( j, k ) = Y( j, k ) + v * S( i, k )
    END DO
    ORDER( k ) = k_s - k + 1 ! pick the (s,y) vectors in reverse order
  END DO
! approximate the Hessian
CALL SHA_estimate( n, nz, ROW, COL, k_s, S, n, k_s, Y, n, k_s, VAL_est,      &
                  data, control, inform, ORDER = ORDER )
IF ( inform%status /= 0 ) THEN ! Failure
  WRITE( 6, "( ' return with nonzero status ', I0, ' from SHA_estimate' )" ) &
    inform%status ; STOP
ELSE
  WRITE( 6, "( /, ' Successful run with ', I0,                                &
    & ' differences, estimated matrix:' )" ) k_s
  DO l = 1, nz
    WRITE( 6, "( ' (row,col,val) = (', I0, ', ', I0, ', ', ES9.2, ')' )" ) &
      ROW( l ), COL( l ), VAL_est( l )
  END DO
END IF
CALL SHA_terminate( data, control, inform ) ! Delete internal workspace
END PROGRAM GALAHAD_SHA_EXAMPLE

```

The code produces the following output:

2 differences are needed, one or more extra might help

Successful run with 3 differences, estimated matrix:

```

(row,col,val) = (1,1, 1.00E+00)
(row,col,val) = (1,2, 2.00E+00)
(row,col,val) = (1,3, 3.00E+00)
(row,col,val) = (1,4, 4.00E+00)
(row,col,val) = (1,5, 5.00E+00)
(row,col,val) = (2,2, 6.00E+00)
(row,col,val) = (3,3, 7.00E+00)
(row,col,val) = (4,4, 8.00E+00)
(row,col,val) = (5,5, 9.00E+00)

```

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