





GALAHAD LMS

USER DOCUMENTATION

GALAHAD Optimization Library version 4.1

1 SUMMARY

Given a sequence of vectors $\{\mathbf{s}_k\}$ and $\{\mathbf{y}_k\}$ and scale factors δ_k , obtain the product of a limited-memory secant approximation \mathbf{H}_k (or its inverse) with a given vector, using one of a variety of well-established formulae.

ATTRIBUTES — Versions: GALAHAD_LMS_single, GALAHAD_LMS_double. Uses: GALAHAD_CLOCK, GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_LAPACK_interface, GALAHAD_BLAS_interface, GALAHAD_SPECFILE. Date: July 2014. Origin: N. I. M. Gould, Rutherford Appleton Laboratory. Language: Fortran 95 + TR 15581 or Fortran 2003.

2 HOW TO USE THE PACKAGE

Access to the package requires a USE statement such as

Single precision version

USE GALAHAD_LMS_single

Double precision version

USE GALAHAD_LMS_double

If it is required to use both modules at the same time, the derived types SMT_type, LMS_time_type, LMS_control_type, LMS_inform_type and LMS_data_type (§2.1) and the subroutines LMS_initialize, LMS_setup, LMS_form, LMS_form_shift, LMS_apply, LMS_terminate, (§2.2) and LMS_read_specfile (§2.4) must be renamed on one of the USE statements.

2.1 The derived data types

Four derived data types are accessible from the package.

2.1.1 The derived data type for holding control parameters

The derived data type LMS_control_type is used to hold controlling data. Default values may be obtained by calling LMS_initialize (see §2.2.1), while components may also be changed by calling GALAHAD_LMS_read_spec (see §2.4.1). The components of LMS_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 LMS_setup, LMS_apply and LMS_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 LMS_setup, LMS_apply 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 level of the process. If print_level ≥ 2 , this output will be increased to provide significant detail of the factorization. The default is print_level = 0.

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memory_length is a scalar variable of type default INTEGER, that is used to specify the maximum number of vectors $\{s_k\}$ and $\{y_k\}$ that will be used when building the secant approximation. Any non-positive value will be interpreted as 1. The default is memory_length = 10.

method is a scalar variable of type default INTEGER, that is used to specify the limited-memory formula that will be applied. Possible values are

- 1. A limited-memory BFGS formula will be applied.
- 2. A limited-memory symmetric rank-one formula will be applied.
- 3. The inverse of the limited-memory BFGS formula will be applied.
- 4. The inverse of the shifted limited-memory BFGS formula will be applied. This should be used instead of %method = 3 whenever a shift is planned.

Any value outside this range will be interpreted as 1. The default is method = 1.

- any_method is a scalar variable of type default LOGICAL, that must be set .TRUE. if more than one method (see %method above) is to be used and .FALSE. otherwise. The package will require more storage and may run slower if any_method is .TRUE.. The default is any_method = .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 = "".

2.1.2 The derived data type for holding timing information

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

- total is a scalar variable of type default REAL (double precision in GALAHAD_LMS_double), that gives the total CPU time spent in the package.
- setup is a scalar variable of type default REAL (double precision in GALAHAD_LMS_double), that gives the CPU time spent setting up the data structures to represent the limited-memory matrix.
- form is a scalar variable of type default REAL (double precision in GALAHAD_LMS_double), that gives the CPU time spent forming and updating the limited-memory matrix as new data arrives.
- apply is a scalar variable of type default REAL (double precision in GALAHAD_LMS_double), that gives the CPU time spent applying the matrix to given vectors.
- clock_total is a scalar variable of type default REAL (double precision in GALAHAD_LMS_double), that gives the total elapsed system clock time spent in the package.
- clock_setup is a scalar variable of type default REAL (double precision in GALAHAD_LMS_double), that gives the elapsed system clock time spent setting up the data structures to represent the limited-memory matrix.

- clock_form is a scalar variable of type default REAL (double precision in GALAHAD_LMS_double), that gives the elapsed system clock time spent forming and updating the limited-memory matrix as new data arrives.
- clock_apply is a scalar variable of type default REAL (double precision in GALAHAD_LMS_double), that gives the elapsed system clock time spent applying the matrix to given vectors. factor \mathbf{R} .

2.1.3 The derived data type for holding informational parameters

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

- status is a scalar variable of type default INTEGER, that gives the exit status of the algorithm. See §2.3 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.
- length is a scalar variable of type default INTEGER, that gives the number of pairs $\{s_k, y_k\}$ currently used to represent the limited-memory matrix
- updates_skipped is a scalar variable of type default LOGICAL, that will be .TRUE. if one or more of the current pairs $\{s_k,y_k\}$ has been ignored for stability reasons when building the current limited-memory matrix, and .FALSE. otherwise.
- time is a scalar variable of type LMS_time_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.1.2).

2.1.4 The derived data type for holding problem data

The derived data type LMS_data_type is used to hold all the data for the problem and the workspace arrays used to construct the multi-level incomplete factorization between calls of LMS procedures. This data should be preserved, untouched, from the initial call to LMS_initialize to the final call to LMS_terminate.

2.2 Argument lists and calling sequences

There are seven procedures for user calls (see §2.4 for further features):

- 1. The subroutine LMS_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 LMS_setup is called to set up the data structures needed to represent the limited-memory matrix \mathbf{H}_k or its inverse.
- 3. The subroutine LMS_form is called to form the limited-memory matrix \mathbf{H}_k or its inverse as new data $(\mathbf{s}_k, \mathbf{y}_k, \delta_k)$ arrives. The matrix $\mathbf{H}_k + \lambda_k \mathbf{I}$ or its inverse for a specified shift λ_k may be formed instead.
- 4. The subroutine LMS_form_shift is called to update the inverse of the limited-memory matrix $\mathbf{H}_k + \lambda_k \mathbf{I}$ when a new shift λ_k is required.
- 5. The subroutine LMS_change_method is called to build the limited-memory matrices \mathbf{H}_k , $\mathbf{H}_k + \lambda_k \mathbf{I}$ or their inverse for a new method from the current data.

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6. The subroutine LMS_apply is called to form the product $\mathbf{u} = \mathbf{H}_k \mathbf{v}$, $\mathbf{u} = (\mathbf{H}_k + \lambda_k \mathbf{I})\mathbf{v}$, $\mathbf{u} = \mathbf{H}_k^{-1}\mathbf{v}$ or $\mathbf{u} = (\mathbf{H}_k + \lambda_k \mathbf{I})^{-1}\mathbf{v}$ for a given vector \mathbf{v} .

7. The subroutine LMS_terminate is provided to allow the user to automatically deallocate array components of the private data, allocated by LMS_setup at the end of the solution process.

We use square brackets [] to indicate OPTIONAL arguments.

2.2.1 The initialization subroutine

Default values are provided as follows:

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

- data is a scalar INTENT (INOUT) argument of type LMS_data_type (see §2.1.4). It is used to hold data about the problem being solved.
- control is a scalar INTENT (OUT) argument of type LMS_control_type (see §2.1.1). On exit, control contains default values for the components as described in §2.1.1. These values should only be changed after calling LMS_initialize.
- inform is a scalar INTENT (OUT) argument of type LMS_inform_type (see Section 2.1.3). A successful call to LMS_initialize is indicated when the component status has the value 0. For other return values of status, see Section 2.3.

2.2.2 The subroutine for setting up the required data structures

The data structures needed to represent the limited-memory matrix \mathbf{H}_k or its inverse are set up as follows:

```
CALL LMS_setup( n, data, control, inform )
```

- is a scalar INTENT (IN) argument of type default INTEGER, that must be set to the dimension of the limited-memory matrix required. **Restriction:** $n \ge 1$.
- data is a scalar INTENT (INOUT) argument of type LMS_data_type (see §2.1.4). It is used to hold data about the factors obtained. It must not have been altered by the user since the last call to LMS_initialize.
- control is a scalar INTENT (IN) argument of type LMS_control_type (see §2.1.1). Default values may be assigned by calling LMS_initialize prior to the first call to LMS_setup.
- inform is a scalar INTENT (OUT) argument of type LMS_inform_type (see §2.1.3). A successful call to LMS_setup is indicated when the component status has the value 0. For other return values of status, see §2.3.

2.2.3 The subroutine for updating the limited memory matrix

The required limited memory matrix is updated to accommodate the incoming triple $(\mathbf{s}_k, \mathbf{y}_k, \delta_k)$ as follows:

```
CALL LMS_form( S, Y, delta, data, control, inform[, lambda] )
```

- is an INTENT (IN) rank-1 array of type REAL (double precision in GALAHAD_LMS_double) and length at least as large as the value n as set on input to LMS_setup, whose first n components must hold the incoming vector \mathbf{s}_k .
- is an INTENT (IN) rank-1 array of type REAL (double precision in GALAHAD_LMS_double) and length at least as large as the value n as set on input to LMS_setup, whose first n components must hold the incoming vector \mathbf{y}_k . **Restriction:** the update will be skipped for for limited-memory BFGS methods if the inner product $\mathbf{s}_k^T \mathbf{y}_k <= 0$.
- delta is an INTENT(IN) REAL (double precision in GALAHAD_LMS_double) scalar that must hold the value δ_k . Restriction: the update will be skipped if delta ≤ 0 .

- data is a scalar INTENT (INOUT) argument of type LMS_data_type (see §2.1.4). It is used to hold data about the factors obtained. It must not have been altered by the user since the last call to LMS_setup.
- control is a scalar INTENT(IN) argument of type LMS_control_type (see §2.1.1). Default values may be assigned by calling LMS_initialize prior to the first call to LMS_setup.
- inform is a scalar INTENT (OUT) argument of type LMS_inform_type (see §2.1.3). A successful call to LMS_setup is indicated when the component status has the value 0. For other return values of status, see §2.3.
- lambda is an OPTIONAL, INTENT(IN) REAL (double precision in GALAHAD_LMS_double)scalar that if present will be used to specify the shift λ_k that is used by the limited memory methods defined by control%method = 1, 2 or 4. **Restriction:** the update will be skipped if lambda < 0 for these methods.

2.2.4 The subroutine for shifting the limited-memory matrix

The required limited memory matrix is updated to accommodate the shift λ_k as follows—this call is mandatory when control%method = 4 if λ_k was not set during the call to LMS_form:

```
CALL LMS_form_shift( lambda, data, control, inform )
```

- lambda is an INTENT(IN) REAL (double precision in GALAHAD_LMS_double)scalar that must hold the value λ_k . Restriction: the update will be skipped if lambda < 0 or if control%method = 3.
- data is a scalar INTENT (INOUT) argument of type LMS_data_type (see §2.1.4). It is used to hold data about the factors obtained. It must not have been altered by the user since the last call to LMS_form.
- control is a scalar INTENT(IN) argument of type LMS_control_type (see §2.1.1). Default values may be assigned by calling LMS_initialize prior to the first call to LMS_setup.
- inform is a scalar INTENT (OUT) argument of type LMS_inform_type (see §2.1.3). A successful call to LMS_setup is indicated when the component status has the value 0. For other return values of status, see §2.3.

2.2.5 The subroutine for changing the method defining the limited-memory matrix

The required limited memory matrix is updated to accommodate the shift λ_k as follows—this call is only permitted if control%any_method = .TRUE. was set when LMS_setup was originally called:

```
CALL LMS_change_method( data, control, inform, lambda )
```

- data is a scalar INTENT (INOUT) argument of type LMS_data_type (see §2.1.4). It is used to hold data about the factors obtained. It must not have been altered by the user since the last call to LMS_form.
- control is a scalar INTENT(IN) argument of type LMS_control_type (see §2.1.1). Default values may be assigned by calling LMS_initialize prior to the first call to LMS_setup.
- inform is a scalar INTENT (OUT) argument of type LMS_inform_type (see §2.1.3). A successful call to LMS_setup is indicated when the component status has the value 0. For other return values of status, see §2.3.
- lambda is an OPTIONAL, INTENT(IN) REAL (double precision in GALAHAD_LMS_double)scalar that if present will be used to specify the shift λ_k that is used by the limited memory methods defined by control%method = 1, 2 or 4. **Restriction:** the update will be skipped if lambda < 0 for these methods.

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2.2.6 The subroutine for applying the limited-memory formula to a vector

Given the vector **v**, the required limited-memory formula, as specified in the most recent call to LMS_form, LMS_form_shift or LMS_change_method, is applied to **v** as follows:

```
CALL LMS_apply( V, U, data, control, inform )
```

- V is a rank-one INTENT (IN) array of type default REAL that must be set on entry to hold the components of the vector v.
- U is a rank-one INTENT (OUT) array of type default REAL that will be set on exit to the result of applying the required limited-memory formula to v.
- data is a scalar INTENT (INOUT) argument of type LMS_data_type (see §2.1.4). It is used to hold data about the factors obtained. It must not have been altered by the user since the last call to LMS_setup.
- control is a scalar INTENT (IN) argument of type LMS_control_type (see §2.1.1). Default values may be assigned by calling LMS_initialize prior to the first call to LMS_setup.
- inform is a scalar INTENT (OUT) argument of type LMS_inform_type (see §2.1.3). A successful call to LMS_apply is indicated when the component status has the value 0. For other return values of status, see §2.3.

2.2.7 The termination subroutine

All previously allocated arrays are deallocated as follows:

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

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

control is a scalar INTENT (IN) argument of type LMS_control_type exactly as for LMS_setup.

inform is a scalar INTENT (OUT) argument of type LMS_inform_type exactly as for LMS_setup. Only the component status will be set on exit, and a successful call to LMS_terminate is indicated when this component status has the value 0. For other return values of status, see §2.3.

2.3 Warning and error messages

A negative value of inform% status on exit from LMS_setup, LMS_apply or LMS_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 n > 0, delta > 0, lambda ≥ 0 or $\mathbf{s}^T \mathbf{y} > 0$ has been violated and the update has been skipped.
- -10. The matrix cannot be built from the current vectors $\{\mathbf{s}_k\}$ and $\{\mathbf{y}_k\}$ and values δ_k and λ_k and the update has been skipped.

-31. A call to subroutine LMS_apply has been made without a prior call to LMS_form_shift or LMS_form with lambda specified when control%method = 4, or LMS_form_shift has been called when control%method = 3, or LMS_change_method has been called after control%any_method = .FALSE. was specified when calling LMS_setup.

2.4 Further features

In this section, we describe an alternative means of setting control parameters, that is components of the variable control of type LMS_control_type (see §2.1.1), by reading an appropriate data specification file using the subroutine LMS_read_specifile. This facility is useful as it allows a user to change LMS control parameters without editing and recompiling programs that call LMS.

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

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

```
( .. lines ignored by LMS_read_specfile .. )
BEGIN LMS
    keyword value
    .....
    keyword value
END
( .. lines ignored by LMS_read_specfile .. )
```

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

and

END LMS SPECIFICATION
```

are acceptable. Furthermore, between the "BEGIN LMS" 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 LMS_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 LMS_read_specfile.

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2.4.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
CALL LMS_read_specfile( control, device )
```

control is a scalar INTENT (INOUT) argument of type LMS_control_type (see §2.1.1). Default values should have already been set, perhaps by calling LMS_initialize. On exit, individual components of control may have been changed according to the commands found in the specifile. Specifile commands and the component (see §2.1.1) 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
limited-memory-length	%memory_length	integer
limited-memory-method	%method	integer
allow-any-method	%any_method	logical
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
output-line-prefix	%prefix	character

Table 2.1: Specifle commands and associated components of control.

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

2.5 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 , statistics concerning the formation of ${\bf R}$ as well as warning and error messages will be reported.

3 GENERAL INFORMATION

Use of common: None.

Workspace: Provided automatically by the module.

Other routines called directly: None.

Other modules used directly: LMS calls the GALAHAD packages GALAHAD_CLOCK, GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_LAPACK_interface, GALAHAD_BLAS_interface and GALAHAD_SPECFILE,

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

Restrictions: n > 0, delta > 0, $lambda \ge 0$.

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

4 METHOD

Given a sequence of vectors $\{\mathbf{s}_k\}$ and $\{\mathbf{y}_k\}$ and scale factors δ_k , a limited-memory secant approximation \mathbf{H}_k is chosen so that $\mathbf{H}_{\max(k-m,0)} = \delta_k \mathbf{I}$, $\mathbf{H}_{k-j}\mathbf{s}_{k-j} = \mathbf{y}_{k-j}$ and $\|\mathbf{H}_{k-j+1} - \mathbf{H}_{k-j}\|$ is "small" for $j = \min(k-1,m-1),\ldots,0$. Different ways of quantifying "small" distinguish different methods, but the crucial observation is that it is possible to construct \mathbf{H}_k quickly from $\{\mathbf{s}_k\}$, $\{\mathbf{y}_k\}$ and δ_k , and to apply it and its inverse to a given vector \mathbf{v} . It is also possible to apply similar formulae to the "shifted" matrix $\mathbf{H}_k + \lambda_k \mathbf{I}$ that occurs in trust-region methods.

References:

The basic methods are those given by

R. H. Byrd, J. Nocedal and R. B. Schnabel (1994) "Representations of quasi-Newton matrices and their use in limited memory methods". Mathematical Programming **63**(2) 129–156,

with obvious extensions.

5 EXAMPLE OF USE

Suppose that we generate random vectors $\{\mathbf{s}_k\}$ and $\{\mathbf{y}_k\}$ and scale factors δ_k , that we build the limited-memory BFGS matrix \mathbf{H}_k and its inverse \mathbf{H}_k^{-1} and that we apply \mathbf{H}_k and then \mathbf{H}_k^{-1} to a given vector \mathbf{v} . Suppose further, that at some stage, we instead apply the inverse $(\mathbf{H}_k + \lambda_k \mathbf{I})^{-1}$ with $\lambda_k = 0$. Then we may use the following code; of course since we have the identities $\mathbf{v} = \mathbf{H}_k^{-1}(\mathbf{H}_k \mathbf{v})$ and $\mathbf{v} = (\mathbf{H}_k + \lambda_k \mathbf{I})^{-1}(\mathbf{H}_k \mathbf{v})$ when $\lambda_k = 0$, we expect to recover the original \mathbf{v} after every step:

```
! THIS VERSION: GALAHAD 2.6 - 12/06/2014 AT 15:30 GMT.
  PROGRAM GALAHAD LMS example
  USE GALAHAD_LMS_double
                                             ! double precision version
  USE GALAHAD_rand_double
  IMPLICIT NONE
  INTEGER, PARAMETER :: wp = KIND( 1.0D+0 ) ! set precision
  INTEGER, PARAMETER :: n = 5, m = 3
  TYPE ( LMS_data_type ) :: data, data2
  TYPE ( LMS_control_type ) :: control, control2
  TYPE ( LMS_inform_type ) :: inform, inform2
  REAL ( KIND = wp ), DIMENSION( n ) :: S, Y, U, V
  INTEGER :: iter, fail
  REAL (KIND = wp) :: delta, lambda
  TYPE ( RAND_seed ) :: seed
  CALL RAND_initialize ( seed ) ! Initialize the random generator word
  CALL LMS_initialize( data, control, inform ) ! initialize data
  control%memory_length = m ! set the memory length
  control2 = control
  control%method = 1 ! start with L-BFGS
  CALL LMS_setup( n, data, control, inform )
  control2%method = 3 ! then inverse L-BFGS
  control2%any_method =.TRUE. ! allow the 2nd update to change method
  CALL LMS_setup( n, data2, control2, inform2 )
  fail = 0 ! count the failures
  DO iter = 1, 5 * n
    IF ( iter == 3 * n ) THEN ! switch to inverse shifted L-BFGS
      CALL LMS_setup( n, data, control, inform )
      control2\mbox{method} = 4
      CALL LMS_setup( n, data2, control2, inform2 )
```

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```
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```

```
CALL RAND_random_real( seed, .FALSE., S ) ! pick random S, Y and delta
    CALL RAND_random_real( seed, .FALSE., Y )
    IF ( DOT_PRODUCT( S, Y ) < 0.0_wp ) Y = - Y ! ensure that S^T Y is positive
    CALL RAND_random_real( seed, .TRUE., delta )
    CALL LMS_form( S, Y, delta, data, control, inform ) ! update the model
    IF ( inform%status /= 0 ) THEN
      WRITE( 6, "( ' update error, status = ', IO )" ) inform%status
      fail = fail + 1 ; CYCLE
    END IF
    V = 1.0_wp ! form the first product with the vector ones
    CALL LMS_apply( V, U, data, control, inform ) ! form the required product
    IF ( inform%status /= 0 ) THEN
      WRITE(6, "('apply error, status = ', I0)") inform%status
      fail = fail + 1 ; CYCLE
    END IF
    CALL LMS_form( S, Y, delta, data2, control2, inform2 ) ! update model 2
    IF ( inform2%status /= 0 ) THEN
      WRITE( 6, "( ' update error, status = ', IO )" ) inform2%status
      fail = fail + 1; CYCLE
    IF ( control2%method == 4 ) THEN
      lambda = 0.0_wp ! apply the shifted L_BFGS (inverse) with zero shift
      CALL LMS_form_shift( lambda, data2, control2, inform2 )
      IF ( inform2%status /= 0 ) THEN
        WRITE(6, "(' update error, status = ', I0)") inform2%status
        fail = fail + 1 ; CYCLE
      END IF
    END IF
! note, the preceeding two calls could have been condensed as
    CALL LMS_form( S, Y, delta, data2, control2, inform2, lambda = 0.0_wp)
    CALL LMS_apply( U, V, data2, control2, inform2 ) ! form the new product
    IF ( inform2\$status /= 0 ) THEN
      WRITE( 6, "( 'apply error, status = ', I0 )" ) inform2%status
      fail = fail + 1; CYCLE
    END IF
    IF ( MAXVAL( ABS( V - 1.0 wp ) ) > 0.00001 wp ) fail = fail + 1
  END DO
  IF ( fail == 0 ) THEN ! check for overall success
    WRITE( 6, "( ' no failures ' )" )
  ELSE
    WRITE( 6, "( I0, ' failures ')" ) fail
  CALL LMS_terminate( data, control, inform ) ! delete internal workspace
  CALL LMS_terminate( data2, control2, inform2 )
  END PROGRAM GALAHAD_LMS_example
```

This produces the following output:

no failures