

C interfaces to GALAHAD LMS

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Chapter 1

GALAHAD C package Ims

1.1 Introduction

1.1.1 Purpose

Given a sequence of vectors $\{s_k\}$ and $\{y_k\}$ and scale factors $\{\delta_k\}$, obtain the product of a limited-memory secant approximation H_k (or its inverse) with a given vector, using one of a variety of well-established formulae.

Currently, only the control and inform parameters are exposed; these are provided and used by other GALAHAD packages with C interfaces.

1.1.2 Authors

N. I. M. Gould, STFC-Rutherford Appleton Laboratory, England.

C interface, additionally J. Fowkes, STFC-Rutherford Appleton Laboratory.

Julia interface, additionally A. Montoison and D. Orban, Polytechnique Montréal.

1.1.3 Originally released

July 2014, C interface January 2022.

1.1.4 Method

Given a sequence of vectors $\{s_k\}$ and $\{y_k\}$ and scale factors $\{\delta_k\}$, a limited-memory secant approximation H_k is chosen so that $H_{\max(k-m,0)} = \delta_k I$, $H_{k-j}s_{k-j} = y_{k-j}$ and $\|H_{k-j+1} - H_{k-j}\|$ 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 H_k quickly from s_k , y_k and δ_k , and to apply it and its inverse to a given vector v. It is also possible to apply similar formulae to the `shifted" matrix $H_k + \lambda_k I$ that occurs in trust-region methods.

1.1.5 Reference

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. Mathenatical Programming, **63(2)** 129-156,

with obvious extensions.

Chapter 2

File Index

| 2 1 | Fi | le | l i | et |
|--------------|----|----|-----|----|
| Z . I | ГΙ | ıe | L | ЭL |

| Here is a list of all files with brief descriptions: | |
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Chapter 3

File Documentation

3.1 galahad_lms.h File Reference

```
#include <stdbool.h>
#include <stdint.h>
#include "galahad_precision.h"
#include "galahad_cfunctions.h"
```

Data Structures

- struct lms_control_type
- struct lms_time_type
- struct lms_inform_type

Functions

- void lms_initialize (void **data, struct lms_control_type *control, int *status)
- void Ims_information (void **data, struct Ims_inform_type *inform, int *status)
- void lms_terminate (void **data, struct lms_control_type *control, struct lms_inform_type *inform)

3.1.1 Data Structure Documentation

3.1.1.1 struct Ims_control_type

control derived type as a C struct

Data Fields

| bool | f_indexing | use C or Fortran sparse matrix indexing |
|------|---------------|-----------------------------------------|
| int | error | unit for error messages |
| int | out | unit for monitor output |
| int | print_level | controls level of diagnostic output |
| int | memory_length | limited memory length |

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Data Fields

| int | method | limited-memory formula required (others may be added in due course): |
|------|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | | 1 BFGS (default). |
| | | 2 Symmetric Rank-One (SR1). |
| | | 3 The inverse of the BFGS formula. |
| | | 4 The inverse of the shifted BFGS formula. This should be used instead of .method = 3 whenever a shift is planned. |
| bool | any_method | allow space to permit different methods if required (less efficient) |
| bool | space_critical | if space is critical, ensure allocated arrays are no bigger than needed |
| bool | deallocate_error_fatal | exit if any deallocation fails |
| char | prefix[31] | all output lines will be prefixed by prefix(2:LEN(TRIM(.prefix))-1) where prefix contains the required string enclosed in quotes, e.g. "string" or 'string' |

3.1.1.2 struct lms_time_type

time derived type as a C struct

Data Fields

| real_wp_ | total | total cpu time spent in the package |
|----------|-------------|----------------------------------------------------------------|
| real_wp_ | setup | cpu time spent setting up space for the secant approximation |
| real_wp_ | form | cpu time spent updating the secant approximation |
| real_wp_ | apply | cpu time spent applying the secant approximation |
| real_wp_ | clock_total | total clock time spent in the package |
| real_wp_ | clock_setup | clock time spent setting up space for the secant approximation |
| real_wp_ | clock_form | clock time spent updating the secant approximation |
| real_wp_ | clock_apply | clock time spent applying the secant approximation |

3.1.1.3 struct lms_inform_type

inform derived type as a C struct

Data Fields

| int | status | the return status. Possible values are: |
|----------------------|-----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | | 0 the update was successful. |
| | | -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 $s^T y>0$ has been violated and the update has been skipped. |
| | | -10. The matrix cannot be built from the current vectors {s_k} and {y_k} and values delta_k and lambda_k and the update has been skipped. |
| | | -31. A call to the function lhs_apply has been made without a prior call to lhs_form_shift or lhs_form with lambda specified when control.method = 4, or lhs_form_shift has been called when control.method = 3, or lhs_change_method has been called after control.any_method = false was specified when calling lhs_setup. |
| int | alloc_status | the status of the last attempted allocation/deallocation |
| int | length | the number of pairs (s,y) currently used to represent the limited-memory matrix. |
| bool | updates_skipped | have (s,y) pairs been skipped when forming the limited-memory matrix? |
| char | bad_alloc[81] | the name of the array for which an allocation/deallocation error occurred. |
| struct Ims_time_type | time | timings (see above) |

3.1.2 Function Documentation

3.1.2.1 Ims_initialize()

Set default control values and initialize private data

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Parameters

| in,out | data | holds private internal data |
|--------|---------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|
| out | control is a struct containing control information (see Ims_control_type) | |
| out | status | is a scalar variable of type int, that gives the exit status from the package. Possible values are (currently): |
| | | 0. The initialization was succesful. |

3.1.2.2 lms_information()

Provides output information

Parameters

| in,out | data | holds private internal data |
|--------|--------|-----------------------------------------------------------------------------------------------------------------|
| out | inform | is a struct containing output information (see Ims_inform_type) |
| out | status | is a scalar variable of type int, that gives the exit status from the package. Possible values are (currently): |
| | | 0. The values were recorded succesfully |

3.1.2.3 lms_terminate()

Deallocate all internal private storage

Parameters

| in,out | data | holds private internal data |
|--------|---------|-------------------------------------------------------------------|
| out | control | is a struct containing control information (see lms_control_type) |
| out | inform | is a struct containing output information (see lms_inform_type) |