C interfaces to GALAHAD LSRT

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Chapter 1

GALAHAD C package lsrt

1.1 Introduction

1.1.1 Purpose

Given a real m by n matrix A, a real m vector b and scalars $\sigma > 0$ and $p \geq 2$, this package finds an **approximate minimizer of the regularised linear-least-squares objective function** $\frac{1}{2}\|Ax - b\|_2^2 + \frac{1}{p}\sigma\|x\|_2^p$**.** This problem commonly occurs as a subproblem in nonlinear optimization calculations involving cubic regularisation, and may be used to regularise the solution of under-determined or ill-conditioned linear least-squares problems. The method may be suitable for large m and/or n as no factorization involving A is required. Reverse communication is used to obtain matrix-vector products of the form $u + Av$ and $v + A^T u$.

1.1.2 Authors

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1.1.3 Originally released

November 2007, C interface December 2021.

1.1.4 Terminology

The required solution x necessarily satisfies the optimality condition $A^T(Ax - b) + \lambda x = 0$, where the multiplier $\lambda = \sigma\|x\|_2^{p-2}$.

1.1.5 Method

The method is iterative. Starting with the vector $u_1 = b$, a bi-diagonalisation process is used to generate the vectors v_k and $u_k + 1$ so that the n by k matrix $V_k = (v_1 \dots v_k)$ and the m by $(k + 1)$ matrix $U_k = (u_1 \dots u_{k+1})$ together satisfy

$$AV_k = U_{k+1}B_k \text{ and } b = \|b\|_2 U_{k+1}e_1$$

where B_k is $(k+1)$ by k and lower bi-diagonal, U_k and V_k have orthonormal columns and e_1 is the first unit vector. The solution sought is of the form $x_k = V_k y_k$, where y_k solves the bi-diagonal regularised least-squares problem

$$(1) \quad \min \|B_k y - \|b\|e_1\|_2 + \frac{1}{p}\sigma\|y\|_2^p.$$

To minimize (1), the optimality conditions

$$(B_k^T(B_k y(\lambda) - \|b\|e_1) + \lambda y(\lambda) = 0,$$

where $\lambda = \sigma\|y(\lambda)\|_2^{p-2}\|$, are used as the basis of an iteration. The vector $y(\lambda)$ is equivalently the solution to the regularised least-squares problem

$$(2) \quad \min \left\| \begin{pmatrix} B_k \\ \lambda^{\frac{1}{2}} I \end{pmatrix} y - \|b\|e_1 \right\|_2 .$$

Thus, given an estimate $\lambda \geq 0$, (2) may be efficiently solved to give $y(\lambda)$. It is then simply a matter of adjusting λ (for example by a Newton-like process) to solve the scalar nonlinear equation

$$(3) \quad \theta(\lambda) \equiv \|y(\lambda)\|_2^{p-2} - \frac{\lambda}{\sigma} = 0.$$

In practice (3) is reformulated, and a more rapidly converging iteration is used. Having found y_k, a second pass in which $x_k = V_k y_k$ is regenerated is needed—this need only be done once x_k has implicitly deemed to be sufficiently close to optimality. As this second pass is an additional expense, a record is kept of the optimal objective function values for each value of k, and the second pass is only performed so far as to ensure a given fraction of the final optimal objective value. Large savings may be made in the second pass by choosing the required fraction to be significantly smaller than one.

Special code is used in the special case $p = 2$, as in this case a single pass suffices.

1.1.6 Reference

A complete description of the un- and quadratically-regularised cases is given by

C. C. Paige and M. A. Saunders, LSQR: an algorithm for sparse linear equations and sparse least squares. ACM Transactions on Mathematical Software, 8(1):43–71, 1982

and

C. C. Paige and M. A. Saunders, ALGORITHM 583: LSQR: an algorithm for sparse linear equations and sparse least squares. ACM Transactions on Mathematical Software, 8(2):195–209, 1982.

Additional details on the Newton-like process needed to determine λ and other details are described in

C. Cartis, N. I. M. Gould and Ph. L. Toint, Trust-region and other regularisation of linear least-squares problems. BIT 49(1):21-53 (2009).

1.1.7 Call order

To solve a given problem, functions from the lsrt package must be called in the following order:

- lsrt_initialize - provide default control parameters and set up initial data structures
- lsrt_read_specfile (optional) - override control values by reading replacement values from a file
- lsrt_import_control - import control parameters prior to solution
- lsrt_solve_problem - solve the problem by reverse communication, a sequence of calls are made under control of a status parameter, each exit either asks the user to provide additional informaton and to re-enter, or reports that either the solution has been found or that an error has occurred
- lsrt_information (optional) - recover information about the solution and solution process
- lsrt_terminate - deallocate data structures

See Section 4.1 for an example of use.

Chapter 2

File Index

2.1 File List

Here is a list of all files with brief descriptions:

Chapter 3

File Documentation

3.1 lsrt.h File Reference

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

Data Structures

- struct lsrt_control_type
- struct lsrt_inform_type

Functions

- void lsrt_initialize (void **data, struct lsrt_control_type *control, int *status)
- void lsrt_read_specfile (struct lsrt_control_type *control, const char specfile[ ])
- void lsrt_import_control (struct lsrt_control_type *control, void **data, int *status)
- void lsrt_solve_problem (void **data, int *status, int m, int n, const real_wp_ power, const real_wp_ weight, real_wp_ x[ ], real_wp_ u[ ], real_wp_ v[ ])
- void lsrt_information (void **data, struct lsrt_inform_type *inform, int *status)
- void lsrt_terminate (void **data, struct lsrt_control_type *control, struct lsrt_inform_type *inform)

3.1.1 Data Structure Documentation

3.1.1.1 struct lsrt_control_type

control derived type as a C struct

Examples

lsrtt.c.

Data Fields

bool	f_indexing	use C or Fortran sparse matrix indexing
int	error	error and warning diagnostics occur on stream error
int	out	general output occurs on stream out
int	print_level	the level of output required is specified by print_level
int	start_print	any printing will start on this iteration
int	stop_print	any printing will stop on this iteration
int	print_gap	the number of iterations between printing
int	itmin	the minimum number of iterations allowed (-ve = no bound)
int	itmax	the maximum number of iterations allowed (-ve = no bound)
int	bitmax	the maximum number of Newton inner iterations per outer iteration allowed (-ve = no bound)
int	extra_vectors	the number of extra work vectors of length n used
int	stopping_rule	the stopping rule used: 0=1.0, 1=norm step, 2=norm step/sigma (NOT USED)
int	freq	frequency for solving the reduced tri-diagonal problem (NOT USED)
real_wp_	stop_relative	the iteration stops successfully when $\|\|A^{\wedge}Tr\|\|$ is less than max(stop_relative $*$ $\|\|A^{\wedge}Tr$ initial $\|\|$, stop_absolute)
real_wp_	stop_absolute	see stop_relative
real_wp_	fraction_opt	an estimate of the solution that gives at least .fraction_opt times the optimal objective value will be found
real_wp_	time_limit	the maximum elapsed time allowed (-ve means infinite)
bool	space_critical	if .space_critical true, every effort will be made to use as little space as possible. This may result in longer computation time
bool	deallocate_error_fatal	if .deallocate_error_fatal is true, any array/pointer deallocation error will terminate execution. Otherwise, computation will continue
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 lsrt_inform_type

inform derived type as a C struct

Examples

lsrtt.c.

Data Fields

int	status	return status. See lsrt_solve_problem for details
int	alloc_status	the status of the last attempted allocation/deallocation
char	bad_alloc[81]	the name of the array for which an allocation/deallocation error ocurred
int	iter	the total number of iterations required
int	iter_pass2	the total number of pass-2 iterations required
int	biters	the total number of inner iterations performed
int	biter_min	the smallest number of inner iterations performed during an outer iteration
int	biter_max	the largest number of inner iterations performed during an outer iteration

Data Fields

real_wp_	obj	the value of the objective function
real_wp_	multiplier	the multiplier, $\lambda = sigma\|\|x\|\|^(p-2)$
real_wp_	x_norm	the Euclidean norm of x
real_wp_	r_norm	the Euclidean norm of $Ax - b$
real_wp_	Atr_norm	the Euclidean norm of $A^T(Ax - b) + \lambda x$
real_wp_	biter_mean	the average number of inner iterations performed during an outer iteration

3.1.2 Function Documentation

3.1.2.1 lsrt_initialize()

```
void lsrt_initialize (
            void ** data,
            struct lsrt_control_type * control,
            int * status )
```

Set default control values and initialize private data

Parameters

in,out	*data*	holds private internal data
out	*control*	is a struct containing control information (see lsrt_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 import was succesful.

Examples

lsrtt.c.

3.1.2.2 lsrt_read_specfile()

```
void lsrt_read_specfile (
            struct lsrt_control_type * control,
            const char specfile[] )
```

Read the content of a specification file, and assign values associated with given keywords to the corresponding control parameters. By default, the spcification file will be named RUNLSRT.SPC and lie in the current directory. Refer to Table 2.1 in the fortran documentation provided in $GALAHAD/doc/lsrt.pdf for a list of keywords that may be set.

Parameters

in,out	*control*	is a struct containing control information (see lsrt_control_type)
in	*specfile*	is a character string containing the name of the specification file

3.1.2.3 lsrt_import_control()

```
void lsrt_import_control (
            struct lsrt_control_type * control,
            void ** data,
            int * status )
```

Import control parameters prior to solution.

Parameters

in	*control*	is a struct whose members provide control paramters for the remaining prcedures (see lsrt_control_type)
in,out	*data*	holds private internal data
in,out	*status*	is a scalar variable of type int, that gives the exit status from the package. Possible values are (currently): • 1. The import was succesful, and the package is ready for the solve phase

Examples

lsrtt.c.

3.1.2.4 lsrt_solve_problem()

```
void lsrt_solve_problem (
            void ** data,
            int * status,
            int m,
            int n,
            const real_wp_ power,
            const real_wp_ weight,
            real_wp_ x[],
            real_wp_ u[],
            real_wp_ v[] )
```

Solve the regularized least-squuares problem using reverse communication.

Parameters

in,out	*data*	holds private internal data

Parameters

`in,out`	*status*	is a scalar variable of type int, that gives the entry and exit status from the package. This must be set to • 1. on initial entry. Set u (below) to b for this entry. Possible exit values are: • 0. the solution has been found • 2. The user must perform the operation $$u := u + Av,$$ and recall the function. The vectors u and v are available in the arrays u and v (below) respectively, and the result u must overwrite the content of u. No argument except u should be altered before recalling the function • 3. The user must perform the operation $$v := v + A^T u,$$ and recall the function. The vectors u and v are available in the arrays u and v (below) respectively, and the result v must overwrite the content of v. No argument except v should be altered before recalling the function • 4. The user must reset u (below) to b are recall the function. No argument except u should be altered before recalling the function • -1. an array allocation has failed • -2. an array deallocation has failed • -3. one or more of n, m, power or weight violates allowed bounds • -18. the iteration limit has been exceeded • -25. status is negative on entry
`in`	*m*	is a scalar variable of type int, that holds the number of equations (i.e., rows of A), $m > 0$
`in`	*n*	is a scalar variable of type int, that holds the number of variables (i.e., columns of A), $n > 0$
`in`	*power*	is a scalar of type double, that holds the regularization power, $p \geq 2$
`in`	*weight*	is a scalar of type double, that holds the regularization weight, $\sigma > 0$
`in,out`	*x*	is a one-dimensional array of size n and type double, that holds the solution x. The j-th component of x, j = 0, ... , n-1, contains x_j.
`in,out`	*u*	is a one-dimensional array of size m and type double, that should be used and reset appropriately when status = 1 to 5 as directed by status.
`in,out`	*v*	is a one-dimensional array of size n and type double, that should be used and reset appropriately when status = 1 to 5 as directed by status.

Examples

lsrtt.c.

3.1.2.5 lsrt_information()

```
void lsrt_information (
             void ** data,
             struct lsrt_inform_type * inform,
             int * status )
```

Provides output information

Parameters

in,out	*data*	holds private internal data
out	*inform*	is a struct containing output information (see lsrt_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

Examples

lsrtt.c.

3.1.2.6 lsrt_terminate()

```
void lsrt_terminate (
             void ** data,
             struct lsrt_control_type * control,
             struct lsrt_inform_type * inform )
```

Deallocate all internal private storage

Parameters

in,out	*data*	holds private internal data
out	*control*	is a struct containing control information (see lsrt_control_type)
out	*inform*	is a struct containing output information (see lsrt_inform_type)

Examples

lsrtt.c.

Chapter 4

Example Documentation

4.1 lsrtt.c

This is an example of how to use the package to solve a regularized quadratic problem. The use of default and non-default scaling matrices, and restarts with a larger regularization weight are illustrated.

```
/* lsrtt.c */
/* Full test for the LSRT C interface */
#include <stdio.h>
#include <math.h>
#include "lsrt.h"
int main(void) {
    // Derived types
    void *data;
    struct lsrt_control_type control;
    struct lsrt_inform_type inform;
    // Set problem data
    int n = 50; // dimensions
    int m = 2 * n;
    int status;
    double power = 3.0;
    double weight = 1.0;
    double x[n];
    double u[m];
    double v[n];
    // Initialize lsrt
    lsrt_initialize( &data, &control, &status );
    status = 1;
    control.print_level = 0;
    lsrt_import_control( &control, &data, &status );
    for( int i = 0; i < m; i++) u[i] = 1.0; // b = 1
    // iteration loop to find the minimizer with A^T = (I:diag(1:n))
    while(true){ // reverse-communication loop
      lsrt_solve_problem( &data, &status, m, n, power, weight, x, u, v );
      if ( status == 0 ) { // successful termination
          break;
      } else if ( status < 0 ) { // error exit
          break;
      } else if ( status == 2 ) { // form u <- u + A * v
        for( int i = 0; i < n; i++) {
          u[i] = u[i] + v[i];
          u[n+i] = u[n+i] + (i+1)*v[i];
        }
      } else if ( status == 3 ) { // form v <- v + A^T * u
        for( int i = 0; i < n; i++) v[i] = v[i] + u[i] + (i+1) * u[n+i];
      } else if ( status == 4 ) { // restart
        for( int i = 0; i < m; i++) u[i] = 1.0;
      }else{
          printf(" the value %1i of status should not occur\n",
            status);
          break;
      }
    }
    lsrt_information( &data, &inform, &status );
    printf("lsrt_solve_problem exit status = %i,"
           " f = %.2f\n", inform.status, inform.obj );
    // Delete internal workspace
    lsrt_terminate( &data, &control, &inform );
}
```

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