

### C interfaces to GALAHAD

Jari Fowkes and Nick Gould STFC Rutherford Appleton Laboratory Sun Apr 16 2023

GALAHAD C package fit	1
1.1 Introduction	1
1.1.1 Purpose	1
1.1.2 Authors	1
1.1.3 Originally released	1
File Index	3
2.1 File List	3
File Documentation	5
3.1 galahad_fit.h File Reference	5
3.1.1 Data Structure Documentation	5
3.1.1.1 struct fit_control_type	5
3.1.1.2 struct fit_inform_type	6

### **Chapter 1**

## **GALAHAD C packages**

#### 1.1 Introduction

GALAHAD is foremost a modern fortran library of packages designed to solve continuous optimization problems, with a particular emphasis on those that involve a large number of unknowns. Since many application programs or applications are written in other languages, of late there has been a considerable effort to provide interfaces to GALAHAD. Thus there are Matlab interfaces, and here we provide details of those to C using the standardized ISO C support now provided within fortran.

#### 1.1.1 Main authors

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

D. Orban, Polytechnique Montréal, Canada,

D. P. Robinson, Leheigh University, USA,

Ph. L. Toint, The University of Namur, Belgium,

J. Fowkes, STFC-Rutherford Appleton Laboratory, England, and

A. Montoison, Polytechnique Montréal, Canada.

GALAHAD provides packages as named for the following problems:

- fdc determine consistency and redundancy of linear systems (link)
- lpa linear programming using an active-set method (link)
- · lpb linear programming using an interior-point method (link)
- wcp linear feasibility using an interior-point method (link)
- · blls bound-constrained linear least-squares problems using a gradient-projection method (link)
- bllsb bound-constrained linear-least-squares using an interior-point method (in preparation)
- slls simplex-constrained linear least-squares problems using a gradient-projection method (link)
- presolve simplify quadratic programs prior to solution (link)
- bgp bound-constrained convex quadratic programming using a gradient-projection method (link)
- bqpb bound-constrained convex quadratic programming using an interior-point method (link)
- Isqp linear and separable quadratic programming using an interior-point method (link)

- cqp convex quadratic programming using an interior-point method (link)
- dqp convex quadratic programming using a dual active-set method (link)
- eqp equality-constrained quadratic programming using an iterative method (link)
- trs the trust-region subproblem using matrix factorization (link)
- gltr the trust-region subproblem using matrix-vector products (link)
- rgs the regularized quadratic subproblem using matrix factorization (link)
- glrt the regularized quadratic subproblem using matrix-vector products (link)
- dps the trust-region and regularized quadratic subproblems in a diagonalising norm (link)
- lstr the least-squares trust-region subproblem using matrix-vector products (link)
- Isrt the regularized least-squares subproblem using matrix-vector products (link)
- I2rt the regularized linear  $l_2$  norm subproblem using matrix-vector products (link)
- qpa general quadratic programming using an active-set method (link)
- qpb general quadratic programming using an interior-point method (link)
- tru unconstrained optimization using a trust-region method (link)
- · arc unconstrained optimization using a regularization method (link)
- nls least-squares optimization using a regularization method (link)
- trb bound-constrained optimization using a gradient-projection trust-region method (link)
- ugo univariate global optimization (link)
- · bgo multivariate global optimization in a box using a multi-start trust-region method (link)
- dgo multivariate global optimization in a box using a deterministic partition-and-bound method (link)
- nlsb bound-constrained least-squares optimization using a gradient-projection regularization method (in preparation)
- lancelot general constrained optimization using an augmented Lagrangian method (interface in preparation)
- fisqp general constrained optimization using an SQP method (in preparation)

In addition, there are packages for solving a variety of required sub tasks, and most specifically interface routines to external solvers for solving linear equations:

- · uls unsymmetric linear systems (link)
- sls symmetric linear systems (link)
- sbls symmetric block linear systems (link)
- psls preconditioners for symmetric linear systems (link)

C interfaces to all of these are underway, and each will be released once it is ready. If **you** have a particular need, please let us know, and we will raise its priority!

Interface header files are in \$GALAHAD/include; that for a package named pack will be in the file galahad\_pack.h. PDF documentation for pack will be in pack\_c.pdf in the directory, and there is a man page entry in the file pack\_c.3 in \$GALAHAD/man/man3.

1.2 Further topics 3

### 1.2 Further topics

#### 1.2.1 Unsymmetric matrix storage formats

An unsymmetric m by n matrix A may be presented and stored in a variety of convenient input formats.

Both C-style (0 based) and fortran-style (1-based) indexing is allowed. Choose control.f\_indexing as false for C style and true for fortran style; the discussion below presumes C style, but add 1 to indices for the corresponding fortran version.

Wrappers will automatically convert between 0-based (C) and 1-based (fortran) array indexing, so may be used transparently from C. This conversion involves both time and memory overheads that may be avoided by supplying data that is already stored using 1-based indexing.

#### 1.2.1.1 Dense storage format

The matrix A 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. In this case, component n\*i+j of the storage array A\_val will hold the value  $A_{ij}$  for  $0 \le i \le m-1$ ,  $0 \le j \le n-1$ .

#### 1.2.1.2 Dense storage format

The matrix A is stored as a compact dense matrix by columns, that is, the values of the entries of each column in turn are stored in order within an appropriate real one-dimensional array. In this case, component m\*j+i of the storage array A\_val will hold the value  $A_{ij}$  for  $0 \le i \le m-1$ ,  $0 \le j \le n-1$ .

#### 1.2.1.3 Sparse co-ordinate storage format

Only the nonzero entries of the matrices are stored. For the l-th entry,  $0 \le l \le ne-1$ , of A, its row index i, column index j and value  $A_{ij}$ ,  $0 \le i \le m-1$ ,  $0 \le j \le n-1$ , are stored as the l-th components of the integer arrays A\_row and A\_col and real array A\_val, respectively, while the number of nonzeros is recorded as A\_ne = ne.

#### 1.2.1.4 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 A the i-th component of the integer array A\_ptr holds the position of the first entry in this row, while A\_ptr(m) holds the total number of entries. The column indices j,  $0 \le j \le n-1$ , and values  $A_{ij}$  of the nonzero entries in the i-th row are stored in components I = A\_ptr(i), . . . , A\_ptr(i+1)-1,  $0 \le i \le m-1$ , of the integer array A\_col, and real array A\_val, respectively. For sparse matrices, this scheme almost always requires less storage than its predecessor.

#### 1.2.1.5 Sparse column-wise storage format

Once again only the nonzero entries are stored, but this time they are ordered so that those in column j appear directly before those in column j+1. For the j-th column of A the j-th component of the integer array A\_ptr holds the position of the first entry in this column, while A\_ptr(n) holds the total number of entries. The row indices i,  $0 \le i \le m-1$ , and values  $A_{ij}$  of the nonzero entries in the j-th columnsare stored in components I = A\_ptr(j), ..., A\_ptr(j+1)-1,  $0 \le j \le n-1$ , of the integer array A\_row, and real array A\_val, respectively. As before, for sparse matrices, this scheme almost always requires less storage than the co-ordinate format.

C interfaces to GALAHAD GALAHAD

### 1.2.2 Symmetric matrix storage formats

Likewise, a symmetric n by n matrix H may be presented and stored in a variety of formats. But crucially symmetry is exploited by only storing values from the lower triangular part (i.e, those entries that lie on or below the leading diagonal).

#### 1.2.2.1 Dense storage format

The matrix 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 H is symmetric, only the lower triangular part (that is the part  $H_{ij}$  for  $0 \le j \le i \le n-1$ ) need be held. In this case the lower triangle should be stored by rows, that is component i\*i/2+j of the storage array H\_val will hold the value  $H_{ij}$  (and, by symmetry,  $h_{ji}$ ) for  $0 \le j \le i \le n-1$ .

#### 1.2.2.2 Sparse co-ordinate storage format

Only the nonzero entries of the matrices are stored. For the l-th entry,  $0 \le l \le ne-1$ , of H, its row index i, column index j and value  $h_{ij}$ ,  $0 \le j \le i \le n-1$ , are stored as the l-th components of the integer arrays H\_row and H\_col and real array H\_val, respectively, while the number of nonzeros is recorded as H\_ne = ne. Note that only the entries in the lower triangle should be stored.

#### 1.2.2.3 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 H the i-th component of the integer array H\_ptr holds the position of the first entry in this row, while H\_ptr(n) holds the total number of entries. The column indices j,  $0 \le j \le i$ , and values  $H_{ij}$  of the entries in the i-th row are stored in components I = H\_ptr(i), ..., H\_ptr(i+1)-1 of the integer array H\_col, and real array H\_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.

#### 1.2.2.4 Diagonal storage format

If H is diagonal (i.e.,  $h_{ij}=0$  for all  $0 \le i \ne j \le n-1$ ) only the diagonals entries  $h_{ii}$ ,  $0 \le i \le n-1$  need be stored, and the first n components of the array H\_val may be used for the purpose.

#### 1.2.2.5 Multiples of the identity storage format

If H is a multiple of the identity matrix, (i.e.,  $H=\alpha I$  where I is the n by n identity matrix and  $\alpha$  is a scalar), it suffices to store  $\alpha$  as the first component of H\_val.

#### 1.2.2.6 The identity matrix format

If H is the identity matrix, no values need be stored.

#### 1.2.2.7 The zero matrix format

The same is true if H is the zero matrix.

# **Chapter 2**

## File Index

### 2.1 File List

Here is a list of all files with brief descriptions:	
galahad.h	??

6 File Index

# **Chapter 3**

## **File Documentation**

3.1 galahad.h File Reference

8 File Documentation