## C interfaces to GALAHAD NLS

Generated by Doxygen 1.8.17

1 G <i>A</i>	ALAHAD C package nis	1
1	I.1 Introduction	1
	1.1.1 Purpose	1
	1.1.2 Authors	1
	1.1.3 Originally released	1
	1.1.4 Terminology	2
	1.1.5 Method	2
	1.1.6 Reference	3
	1.1.7 Call order	3
	1.1.8 Unsymmetric matrix storage formats	4
	1.1.8.1 Dense storage format	4
	1.1.8.2 Dense by columns storage format	4
	1.1.8.3 Sparse co-ordinate storage format	4
	1.1.8.4 Sparse row-wise storage format	4
	1.1.8.5 Sparse column-wise storage format	4
	1.1.9 Symmetric matrix storage formats	5
	1.1.9.1 Dense storage format	5
	1.1.9.2 Sparse co-ordinate storage format	5
	1.1.9.3 Sparse row-wise storage format	5
	1.1.9.4 Diagonal storage format	5
	1.1.9.5 Multiples of the identity storage format	5
	1.1.9.6 The identity matrix format	5
	1.1.9.7 The zero matrix format	5
2 Da	ita Structure Index	7
	2.1 Data Structures	7
	Data Structures	,
3 Fil	e Index	9
3	3.1 File List	9
	Ita Structure Documentation	11
4	4.1 nls_control_type Struct Reference	11
	4.1.1 Detailed Description	13
	4.1.2 Field Documentation	13
	4.1.2.1 model	14
	4.1.2.2 norm	14
	4.1.2.3 print_level	15
4	4.2 nls_inform_type Struct Reference	15
	4.2.1 Detailed Description	16
4	4.3 nls_subproblem_control_type Struct Reference	16
	4.3.1 Detailed Description	18
	4.3.2 Field Documentation	19
	4.3.2.1 model	19

4.3.2.2 norm	19
4.3.2.3 print_level	20
4.4 nls_subproblem_inform_type Struct Reference	20
4.4.1 Detailed Description	21
4.5 nls_time_type Struct Reference	21
4.5.1 Detailed Description	22
5 File Documentation	23
5.1 nls/nls.h File Reference	23
5.1.1 Function Documentation	24
5.1.1.1 nls_import()	24
5.1.1.2 nls_information()	26
5.1.1.3 nls_initialize()	26
5.1.1.4 nls_read_specfile()	27
5.1.1.5 nls_solve_reverse_with_mat()	27
5.1.1.6 nls_solve_reverse_without_mat()	30
5.1.1.7 nls_solve_with_mat()	32
5.1.1.8 nls_solve_without_mat()	35
5.1.1.9 nls_terminate()	38
6 Example Documentation	41
6.1 nlst.c	41
6.2 nlstf.c	48
Index	57

## **Chapter 1**

# GALAHAD C package nls

#### 1.1 Introduction

#### 1.1.1 Purpose

This package uses a regularization method to find a (local) unconstrained minimizer of a differentiable weighted sum-of-squares objective function

$$f(\mathbf{x}) := \frac{1}{2} \sum_{i=1}^m w_i c_i^2(\mathbf{x}) \equiv \frac{1}{2} \|\mathbf{c}(\mathbf{x})\|_W^2$$

of many variables  ${\bf x}$  involving positive weights  ${\bf w_i}$ ,  ${\bf i}=1,\dots,{\bf m}$ . The method offers the choice of direct and iterative solution of the key regularization subproblems, and is most suitable for large problems. First derivatives of the residual function c(x) are required, and if second derivatives of the  $c_i(x)$  can be calculated, they may be exploited—if suitable products of the first or second derivatives with a vector may be found but not the derivatives themselves, that can also be used to advantage.

### 1.1.2 Authors

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

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

#### 1.1.3 Originally released

October 2016, C interface August 2021.

#### 1.1.4 Terminology

The gradient  $\nabla_x f(x)$  of a function f(x) is the vector whose i-th component is  $\partial f(x)/\partial x_i$ . The Hessian  $\nabla_{xx} f(x)$  of f(x) is the symmetric matrix whose i,j-th entry is  $\partial^2 f(x)/\partial x_i \partial x_j$ . The Hessian is sparse if a significant and useful proportion of the entries are universally zero.

The algorithm used by the package is iterative. From the current best estimate of the minimizer  $x_k$ , a trial improved point  $x_k+s_k$  is sought. The correction  $s_k$  is chosen to improve a model  $m_k(s)$  of the stabilised objective function  $f_{\rho,p}(x_k+s)$  built around the objective function  $f(x_k+s)$  built around  $x_k$ . The model is the sum of two basic components, a suitable approximation  $t_k(s)$  of  $f(x_k+s)$ , another approximation of  $(\rho/r)\|x_k+s\|_r^r$  (if  $\rho>0$ ), and a regularization term  $(\sigma_k/p)\|s\|_{S_k}^p$  involving a weight  $\sigma_k$ , power p and a norm  $\|s\|_{S_k}:=\sqrt{s^TS_ks}$  for a given positive definite scaling matrix  $S_k$  that is included to prevent large corrections. The weight  $\sigma_k$  is adjusted as the algorithm progresses to ensure convergence.

The model  $t_k(s)$  is a truncated Taylor-series approximation, and this relies on being able to compute or estimate derivatives of c(x). Various models are provided, and each has different derivative requirements. We denote the m by n residual Jacobian  $J(x) \equiv \nabla_x c(x)$  as the matrix whose i,j-th component

$$J(x)_{i,j} := \partial c_i(x)/\partial x_j$$
 for  $i = 1, \dots, m$  and  $j = 1, \dots, n$ .

For a given m-vector y, the weighted-residual Hessian is the sum

$$H(x,y):=\sum_{\ell=1}^m y_\ell H_\ell(x), \text{ where } H_\ell(x)_{i,j}:=\partial^2 c_\ell(x)/\partial x_i \partial x_j \text{ for } i,j=1,\dots,n$$

is the Hessian of  $c_{\ell}(x)$ . Finally, for a given vector v, we define the residual-Hessians-vector product matrix

$$P(x,v) := (H_1(x)v, \dots, H_m(x)v).$$

The models  $t_k(s)$  provided are,

- 1. the first-order Taylor approximation  $f(x_k) + g(x_k)^T s$ , where  $g(x) = J^T(x)Wc(x)$ ,
- 2. a barely second-order approximation  $f(x_k) + g(x_k)^T s + \frac{1}{2} s^T W s$ ,
- 3. the Gauss-Newton approximation  $\frac{1}{2} ||c(x_k) + J(x_k)s||_W^2$ ,
- 4. the Newton (second-order Taylor) approximation  $f(x_k) + g(x_k)^T s + \frac{1}{2} s^T [J^T(x_k)WJ(x_k) + H(x_k,Wc(x_k))]s$ , and
- 5. the tensor Gauss-Newton approximation  $\frac{1}{2}\|c(x_k)+J(x_k)s+\frac{1}{2}s^T\cdot P(x_k,s)\|_W^2$ , where the i-th component of  $s^T\cdot P(x_k,s)$  is shorthand for the scalar  $s^TH_i(x_k)s$ , where W is the diagonal matrix of weights  $w_i$ ,  $i=1,\ldots m$ .

Access to a particular model requires that the user is either able to provide the derivatives needed ('matrix available') or that the products of these derivatives (and their transposes) with specified vectors are possible ('matrix free').

#### 1.1.5 **Method**

An adaptive regularization method is used. In this, an improvement to a current estimate of the required minimizer,  $x_k$  is sought by computing a step  $s_k$ . The step is chosen to approximately minimize a model  $t_k(s)$  of  $f_{\rho,r}(x_k+s)$  that includes a weighted regularization term  $(\sigma_k/p)\|s\|_{S_k}^p$  for some specified positive weight  $\sigma_k$ . The quality of the resulting step  $s_k$  is assessed by computing the "ratio" %  $(f_{\rho,p}(x_k)-f_{\rho,p}(x_k+s_k))/(t_k(0)-t_k(s_k))$ . ( $f(x_k)-f(x_k+s_k))/(t_k(0)-t_k(s_k))$ . The step is deemed to have succeeded if the ratio exceeds a given  $\eta_s>0$ , and in this case  $x_{k+1}=x_k+s_k$ . Otherwise  $x_{k+1}=x_k$ , and the weight is increased by powers of a given increase factor up to a given limit. If the ratio is larger than  $\eta_v\geq \eta_d$ , the weight will be decreased by powers of a given

1.1 Introduction 3

decrease factor again up to a given limit. The method will terminate as soon as  $f(x_k)$  or  $\|\nabla_x f(x_k)\|$  is smaller than a specified value.

A choice of linear, quadratic or quartic models  $t_k(s)$  is available (see the Terminology section), and normally a two-norm regularization will be used, but this may change if preconditioning is employed.

If linear or quadratic models are employed, an appropriate, approximate model minimizer is found using either a direct approach involving factorization of a shift of the model Hessian  $B_k$  or an iterative (conjugate-gradient/Lanczos) approach based on approximations to the required solution from a so-called Krlov subspace. The direct approach is based on the knowledge that the required solution satisfies the linear system of equations  $(B_k + \lambda_k I)s_k = -\nabla_x f(x_k)$  involving a scalar Lagrange multiplier  $\lambda_k$ . This multiplier is found by uni-variate root finding, using a safeguarded Newton-like process, by the GALAHAD packages RQS. The iterative approach uses the GALAHAD package GLRT, and is best accelerated by preconditioning with good approximations to the Hessian of the model using GALAHAD's PSLS. The iterative approach has the advantage that only Hessian matrix-vector products are required, and thus the Hessian  $B_k$  is not required explicitly. However when factorizations of the Hessian are possible, the direct approach is often more efficient.

When a quartic model is used, the model is itself of least-squares form, and the package calls itself recursively to approximately minimize its model. The quartic model often gives a better approximation, but at the cost of more involved derivative requirements.

#### 1.1.6 Reference

The generic adaptive cubic regularization method is described in detail in

C. Cartis, N. I. M. Gould and Ph. L. Toint, `Adaptive cubic regularisation methods for unconstrained optimization. Part I: motivation, convergence and numerical results' Mathematical Programming 127(2) (2011) 245-295,

and uses "tricks" as suggested in

N. I. M. Gould, M. Porcelli and Ph. L. Toint, "Updating the regularization parameter in the adaptive cubic regularization algorithm". Computational Optimization and Applications 53(1) (2012) 1-22.

The specific methods employed here are discussed in

N. I. M. Gould, J. A. Scott and T. Rees, `'Convergence and evaluation-complexity analysis of a regularized tensor-Newton method for solving nonlinear least-squares problems". Computational Optimization and Applications 73(1) (2019) 1–35.

#### 1.1.7 Call order

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

- nls\_initialize provide default control parameters and set up initial data structures
- nls read specfile (optional) override control values by reading replacement values from a file
- nls\_import set up problem data structures and fixed values
- · solve the problem by calling one of
  - nls\_solve\_with\_mat solve using function calls to evaluate function, gradient and Hessian values
  - nls\_solve\_without\_mat solve using function calls to evaluate function and gradient values and Hessian-vector products
  - nls\_solve\_reverse\_with\_mat solve returning to the calling program to obtain function, gradient and Hessian values, or
  - nls\_solve\_reverse\_without\_mat solve returning to the calling prorgram to obtain function and gradient values and Hessian-vector products
- nls information (optional) recover information about the solution and solution process
- nls\_terminate deallocate data structures

See Section 6.1 for examples of use.

#### 1.1.8 Unsymmetric matrix storage formats

The unsymmetric m by n Jacobian matrix  $J \equiv \nabla_x c(x)$  and the residual-Hessians-vector product matrix P(x,v) may be presented and stored in a variety of convenient input formats. Let A be J or P as appropriate.

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.

#### 1.1.8.1 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  $0 \le i \le m-1$ ,  $0 \le j \le n-1$ .

#### 1.1.8.2 Dense by columns 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  $0 \le i \le m-1$ ,  $0 \le j \le n-1$ .

#### 1.1.8.3 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.

#### 1.1.8.4 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 plus one. 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.

#### 1.1.8.5 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 plus one. 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.

1.1 Introduction 5

#### 1.1.9 Symmetric matrix storage formats

Likewise, the symmetric n by n weighted-residual Hessian matrix H=H(x,y) 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).

#### 1.1.9.1 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  $0 \le j \le i \le n-1$ .

#### 1.1.9.2 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.

#### 1.1.9.3 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 plus one. 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.

#### 1.1.9.4 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.

#### 1.1.9.5 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.

#### 1.1.9.6 The identity matrix format

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

#### 1.1.9.7 The zero matrix format

The same is true if H is the zero matrix.

# **Chapter 2**

# **Data Structure Index**

## 2.1 Data Structures

Here are the data structures with brief descriptions:

nls_control_type	. 11
nls_inform_type	. 15
nls_subproblem_control_type	. 16
nls_subproblem_inform_type	. 20
nls time type	. 21

8 Data Structure Index

# **Chapter 3**

# File Index

## 3.1 File List

Here is a list of all documented files with brief descriptions:		
nls/nls.h	23	

10 File Index

## **Chapter 4**

## **Data Structure Documentation**

## 4.1 nls\_control\_type Struct Reference

```
#include <nls.h>
```

#### **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.

• 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 maxif

the maximum number of iterations performed

int alive unit

removal of the file alive\_file from unit alive\_unit terminates execution

char alive\_file [31]

see alive\_unit

· int jacobian\_available

is the Jacobian matrix of first derivatives available (  $\geq$  2), is access only via matrix-vector products (=1) or is it not available (  $\leq$  0) ?

· int hessian\_available

is the Hessian matrix of second derivatives available (  $\geq$  2), is access only via matrix-vector products (=1) or is it not available (  $\leq$  0) ?

int model

the model used.

· int norm

the regularization norm used.

· int non monotone

non-monotone ≤ 0 monotone strategy used, anything else non-monotone strategy with this history length used

int weight\_update\_strategy

define the weight-update strategy: 1 (basic), 2 (reset to zero when very successful), 3 (imitate TR), 4 (increase lower bound), 5 (GPT)

· real\_wp\_ stop\_c\_absolute

overall convergence tolerances. The iteration will terminate when  $||c(x)||_2 \leq \text{MAX}($ . $\text{stop\_c\_absolute},$ . $\text{stop\_c\_charpoonup}$  relative  $*||c(x_{\textit{initial}})||_2$  or when the norm of the gradient,  $g = J^T(x)c(x)/||c(x)||_2$ , of  $||c(x)||_2$  satisfies  $||g||_2 \leq \text{MAX}($ . $\text{stop\_g\_absolute},$ . $\text{stop\_g\_relative} *||g_{\textit{initial}}||_2$ , or if the step is less than . $\text{stop\_s}$ 

· real wp stop c relative

see stop\_c\_absolute

real\_wp\_ stop\_g\_absolute

see stop\_c\_absolute

• real\_wp\_ stop\_g\_relative

see stop\_c\_absolute

real\_wp\_stop\_s

see stop\_c\_absolute

· real wp power

the regularization power (<2 => chosen according to the model)

real wp initial weight

initial value for the regularization weight (-ve =>  $1/\|g_0\|$ ))

· real wp minimum weight

minimum permitted regularization weight

real\_wp\_ initial\_inner\_weight

initial value for the inner regularization weight for tensor GN (-ve => 0)

real\_wp\_ eta\_successful

REAL (KIND = wp):: initial\_inner\_weight = 0.0001\_wp a potential iterate will only be accepted if the actual decrease f -  $f(x_new)$  is larger than .eta\_successful times that predicted by a quadratic model of the decrease. The regularization weight will be decreased if this relative decrease is greater than .eta\_very\_successful but smaller than .eta\_too\_ $\hookleftarrow$  successful.

• real\_wp\_ eta\_very\_successful

see eta\_successful

real\_wp\_ eta\_too\_successful

see eta\_successful

real\_wp\_ weight\_decrease\_min

on very successful iterations, the regularization weight will be reduced by the factor .weight\_decrease but no more than .weight\_decrease\_min while if the iteration is unsucceful, the weight will be increased by a factor .weight\_\to increase but no more than .weight\_increase\_max (these are delta\_1, delta\_2, delta3 and delta\_max in Gould, Porcelli and Toint, 2011)

real\_wp\_ weight\_decrease

REAL ( KIND = wp ) :: weight\_decrease = half.

real\_wp\_ weight\_increase

REAL ( KIND = wp ) :: weight\_increase = two.

real\_wp\_ weight\_increase\_max

see weight\_increase

real\_wp\_ reduce\_gap

expert parameters as suggested in Gould, Porcelli and Toint, "Updating t regularization parameter in the adaptive cubic regularization algorithm" RAL-TR-2011-007, Rutherford Appleton Laboratory, England (2011), http://epubs.stfc.ac.uk/bitstream/6181/RAL-TR-2011-007.pdf (these are denoted beta, epsilon\_chi and alpha\_max in the paper)

real\_wp\_tiny\_gap

see reduce\_gap

· real\_wp\_ large\_root

see reduce\_gap

real\_wp\_ switch\_to\_newton

if the Gauss-Newto to Newton model is specified, switch to Newton as soon as the norm of the gradient g is smaller than switch\_to\_newton

· real\_wp\_ cpu\_time\_limit

the maximum CPU time allowed (-ve means infinite)

· real\_wp\_ clock\_time\_limit

the maximum elapsed clock time allowed (-ve means infinite)

· bool subproblem direct

use a direct (factorization) or (preconditioned) iterative method to find the search direction

· bool renormalize\_weight

should the weight be renormalized to account for a change in scaling?

bool magic\_step

allow the user to perform a "magic" step to improve the objective

bool print\_obj

print values of the objective/gradient rather than ||c|| and its gradien

· 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'

• struct nls\_subproblem\_control\_type subproblem\_control

control parameters for the step-finding subproblem

#### 4.1.1 Detailed Description

control derived type as a C struct

**Examples** 

nlst.c, and nlstf.c.

#### 4.1.2 Field Documentation

#### 4.1.2.1 model

int model

the model used.

Possible values are

- 0 dynamic (not yet implemented)
- 1 first-order (no Hessian)
- · 2 barely second-order (identity Hessian)
- 3 Gauss-Newton (  $J^TJ$  Hessian)
- 4 second-order (exact Hessian)
- 5 Gauss-Newton to Newton transition
- 6 tensor Gauss-Newton treated as a least-squares model
- 7 tensor Gauss-Newton treated as a general model
- 8 tensor Gauss-Newton transition from a least-squares to a general mode

#### 4.1.2.2 norm

int norm

the regularization norm used.

The norm is defined via  $||v||^2 = v^T S v$ , and will define the preconditioner used for iterative methods. Possible values for S are

- · -3 user's own regularization norm
- -2 S = limited-memory BFGS matrix (with .PSLS\_control.lbfgs\_vectors history) (not yet implemented)
- -1 identity (= Euclidan two-norm)
- 0 automatic (not yet implemented)
- 1 diagonal,  $S = \text{diag}(\max(J^T J \text{ Hessian, .PSLS contro.min diagonal}))$
- 2 diagonal,  $S = \text{diag}(\max(\text{Hessian, .PSLS\_contro.min\_diagonal}))$
- 3 banded, S = band(Hessian) with semi-bandwidth .PSLS\_control.semi\_bandwidth
- 4 re-ordered band, P=band(order(A)) with semi-bandwidth .PSLS\_control.semi\_bandwidth
- 5 full factorization, S = Hessian, Schnabel-Eskow modification
- 6 full factorization, S = Hessian, GMPS modification (not yet implemented)
- 7 incomplete factorization of Hessian, Lin-More'
- 8 incomplete factorization of Hessian, HSL\_MI28
- 9 incomplete factorization of Hessian, Munskgaard (not yet implemented)
- 10 expanding band of Hessian (not yet implemented)

#### 4.1.2.3 print\_level

```
int print_level
```

the level of output required.

- $\leq$  0 gives no output,
- = 1 gives a one-line summary for every iteration,
- = 2 gives a summary of the inner iteration for each iteration,
- ullet  $\geq$  3 gives increasingly verbose (debugging) output

The documentation for this struct was generated from the following file:

• nls/nls.h

## 4.2 nls\_inform\_type Struct Reference

```
#include <nls.h>
```

#### **Data Fields**

· int status

return status. See NLS\_solve 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

• char bad\_eval [13]

the name of the user-supplied evaluation routine for which an error ocur

· int iter

the total number of iterations performed

• int cg\_iter

the total number of CG iterations performed

int c\_eval

the total number of evaluations of the residual function c(x)

• int j\_eval

the total number of evaluations of the Jacobian J(x) of c(x)

• int h\_eval

the total number of evaluations of the scaled Hessian H(x,y) of c(x)

int factorization\_max

the maximum number of factorizations in a sub-problem solve

int factorization\_status

the return status from the factorization

· int max entries factors

the maximum number of entries in the factors

int factorization\_integer

the total integer workspace required for the factorization

int factorization\_real

the total real workspace required for the factorization

· real\_wp\_factorization\_average

the average number of factorizations per sub-problem solve

real\_wp\_obj

the value of the objective function  $\frac{1}{2}\|c(x)\|_W^2$  at the best estimate the solution, x, determined by NLS\_solve

real\_wp\_ norm\_c

the norm of the residual  $\|c(x)\|_W$  at the best estimate of the solution x, determined by NLS\_solve

real\_wp\_ norm\_g

the norm of the gradient of  $\|c(x)\|_W$  of the objective function at the best estimate, x, of the solution determined by NLS solve

real\_wp\_ weight

the final regularization weight used

· struct nls\_time\_type time

timings (see above)

• struct nls\_subproblem\_inform\_type subproblem\_inform

inform parameters for subproblem

#### 4.2.1 Detailed Description

inform derived type as a C struct

#### **Examples**

nlst.c, and nlstf.c.

The documentation for this struct was generated from the following file:

• nls/nls.h

## 4.3 nls\_subproblem\_control\_type Struct Reference

#include <nls.h>

#### **Data Fields**

· 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.

· 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 maxit

the maximum number of iterations performed

int alive\_unit

removal of the file alive file from unit alive unit terminates execution

char alive file [31]

see alive\_unit

· int jacobian\_available

is the Jacobian matrix of first derivatives available (  $\geq$  2), is access only via matrix-vector products (=1) or is it not available ( < 0) ?

· int hessian available

is the Hessian matrix of second derivatives available (  $\geq$  2), is access only via matrix-vector products (=1) or is it not available (  $\leq$  0) ?

· int model

the model used.

int norm

the regularization norm used.

· int non monotone

 $non-monotone \leq 0$  monotone strategy used, anything else non-monotone strategy with this history length used

int weight\_update\_strategy

define the weight-update strategy: 1 (basic), 2 (reset to zero when very successful), 3 (imitate TR), 4 (increase lower bound), 5 (GPT)

real\_wp\_ stop\_c\_absolute

overall convergence tolerances. The iteration will terminate when  $||c(x)||_2 \leq \text{MAX}(.\text{stop\_c\_absolute, .stop\_c\_} \leftarrow \text{relative} * ||c(x_{\text{initial}})||_2$ , or when the norm of the gradient,  $g = J^T(x)c(x)/||c(x)||_2$ , of  $||c||_2$ , satisfies  $||g||_2 \leq \text{MAX}(.\text{stop\_g\_absolute, .stop\_g\_relative} * ||g_{\text{initial}}||_2$ , or if the step is less than .stop\_s

• real\_wp\_ stop\_c\_relative

see stop\_c\_absolute

real\_wp\_ stop\_g\_absolute

see stop\_c\_absolute

real\_wp\_ stop\_g\_relative

see stop\_c\_absolute

real\_wp\_stop\_s

see stop\_c\_absolute

· real\_wp\_ power

the regularization power (<2 => chosen according to the model)

real\_wp\_ initial\_weight

initial value for the regularization weight (-ve =>  $1/\|g_0\|$ ))

· real wp minimum weight

minimum permitted regularization weight

· real\_wp\_ initial\_inner\_weight

initial value for the inner regularization weight for tensor GN (-ve => 0)

· real wp eta successful

REAL (KIND = wp):: initial\_inner\_weight = 0.0001\_wp a potential iterate will only be accepted if the actual decrease f -  $f(x_new)$  is larger than .eta\_successful times that predicted by a quadratic model of the decrease. The regularization weight will be decreased if this relative decrease is greater than .eta\_very\_successful but smaller than .eta\_too\_ $\leftarrow$  successful.

· real\_wp\_ eta\_very\_successful

see eta successful

• real\_wp\_ eta\_too\_successful

see eta\_successful

· real\_wp\_ weight\_decrease\_min

on very successful iterations, the regularization weight will be reduced by the factor .weight\_decrease but no more than .weight\_decrease\_min while if the iteration is unsucceful, the weight will be increased by a factor .weight\_\top increase but no more than .weight\_increase\_max (these are delta\_1, delta\_2, delta3 and delta\_max in Gould, Porcelli and Toint, 2011)

real\_wp\_ weight\_decrease

REAL ( KIND = wp ) :: weight\_decrease = half.

· real\_wp\_ weight\_increase

REAL (KIND = wp) :: weight\_increase = two.

real\_wp\_ weight\_increase\_max

see weight increase

real\_wp\_ reduce\_gap

expert parameters as suggested in Gould, Porcelli and Toint, "Updating t regularization parameter in the adaptive cubic regularization algorithm" RAL-TR-2011-007, Rutherford Appleton Laboratory, England (2011), http://epubs.stfc.ac.uk/bitstream/6181/RAL-TR-2011-007.pdf (these are denoted beta, epsilon\_chi and alpha\_max in the paper)

real\_wp\_tiny\_gap

see reduce\_gap

real\_wp\_ large\_root

see reduce\_gap

· real wp switch to newton

if the Gauss-Newto to Newton model is specified, switch to Newton as soon as the norm of the gradient g is smaller than switch\_to\_newton

· real wp cpu time limit

the maximum CPU time allowed (-ve means infinite)

real\_wp\_ clock\_time\_limit

the maximum elapsed clock time allowed (-ve means infinite)

bool subproblem\_direct

use a direct (factorization) or (preconditioned) iterative method to find the search direction

· bool renormalize weight

should the weight be renormalized to account for a change in scaling?

· bool magic\_step

allow the user to perform a "magic" step to improve the objective

bool print\_obj

print values of the objective/gradient rather than ||c|| and its gradien

· 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'

#### 4.3.1 Detailed Description

control derived type as a C struct

#### 4.3.2 Field Documentation

#### 4.3.2.1 model

int model

the model used.

Possible values are

- 0 dynamic (not yet implemented)
- 1 first-order (no Hessian)
- 2 barely second-order (identity Hessian)
- 3 Gauss-Newton (  $J^TJ$  Hessian)
- 4 second-order (exact Hessian)
- 5 Gauss-Newton to Newton transition
- · 6 tensor Gauss-Newton treated as a least-squares model
- 7 tensor Gauss-Newton treated as a general model
- 8 tensor Gauss-Newton transition from a least-squares to a general mode

#### 4.3.2.2 norm

int norm

the regularization norm used.

The norm is defined via  $||v||^2 = v^T S v$ , and will define the preconditioner used for iterative methods. Possible values for S are

- -3 user's own regularization norm
- -2 S = limited-memory BFGS matrix (with .PSLS\_control.lbfgs\_vectors history) (not yet implemented)
- -1 identity (= Euclidan two-norm)
- 0 automatic (not yet implemented)
- 1 diagonal,  $S = \text{diag}(\max(J^T J \text{ Hessian, .PSLS\_contro.min\_diagonal}))$
- 2 diagonal,  $S = \text{diag}(\text{max}(\text{Hessian}, .PSLS\_\text{contro.min\_diagonal}))$
- 3 banded, S = band(Hessian) with semi-bandwidth .PSLS\_control.semi\_bandwidth
- 4 re-ordered band, P=band(order(A)) with semi-bandwidth .PSLS\_control.semi\_bandwidth
- 5 full factorization, S = Hessian, Schnabel-Eskow modification
- 6 full factorization, S = Hessian, GMPS modification (not yet implemented)
- 7 incomplete factorization of Hessian, Lin-More'
- 8 incomplete factorization of Hessian, HSL\_MI28
- 9 incomplete factorization of Hessian, Munskgaard (not yet implemented)
- 10 expanding band of Hessian (not yet implemented)

#### 4.3.2.3 print\_level

```
int print_level
```

the level of output required.

- $\leq$  0 gives no output,
- = 1 gives a one-line summary for every iteration,
- = 2 gives a summary of the inner iteration for each iteration,
- ullet  $\geq$  3 gives increasingly verbose (debugging) output

The documentation for this struct was generated from the following file:

• nls/nls.h

## 4.4 nls\_subproblem\_inform\_type Struct Reference

```
#include <nls.h>
```

#### **Data Fields**

· int status

return status. See NLS\_solve 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

• char bad\_eval [13]

the name of the user-supplied evaluation routine for which an error ocur

· int iter

the total number of iterations performed

• int cg\_iter

the total number of CG iterations performed

int c\_eval

the total number of evaluations of the residual function c(x)

• int j\_eval

the total number of evaluations of the Jacobian J(x) of c(x)

• int h\_eval

the total number of evaluations of the scaled Hessian H(x,y) of c(x)

· int factorization max

the maximum number of factorizations in a sub-problem solve

int factorization\_status

the return status from the factorization

· int max entries factors

the maximum number of entries in the factors

int factorization\_integer

the total integer workspace required for the factorization

· int factorization\_real

the total real workspace required for the factorization

real\_wp\_ factorization\_average

the average number of factorizations per sub-problem solve

real\_wp\_obj

the value of the objective function  $\frac{1}{2}\|c(x)\|_W^2$  at the best estimate the solution, x, determined by NLS\_solve

· real wp norm c

the norm of the residual  $||c(x)||_W$  at the best estimate of the solution x, determined by NLS\_solve

real\_wp\_ norm\_g

the norm of the gradient of  $||c(x)||_W$  of the objective function at the best estimate, x, of the solution determined by NLS\_solve

· real\_wp\_ weight

the final regularization weight used

struct nls\_time\_type time

timings (see above)

## 4.4.1 Detailed Description

inform derived type as a C struct

The documentation for this struct was generated from the following file:

• nls/nls.h

## 4.5 nls\_time\_type Struct Reference

#include <nls.h>

#### **Data Fields**

· real sp total

the total CPU time spent in the package

real\_sp\_ preprocess

the CPU time spent preprocessing the problem

real\_sp\_ analyse

the CPU time spent analysing the required matrices prior to factorizatio

real\_sp\_ factorize

the CPU time spent factorizing the required matrices

real\_sp\_ solve

the CPU time spent computing the search direction

real\_wp\_ clock\_total

the total clock time spent in the package

real\_wp\_ clock\_preprocess

the clock time spent preprocessing the problem

real\_wp\_ clock\_analyse

the clock time spent analysing the required matrices prior to factorizat

real\_wp\_ clock\_factorize

the clock time spent factorizing the required matrices

real\_wp\_ clock\_solve

the clock time spent computing the search direction

## 4.5.1 Detailed Description

time derived type as a C struct

The documentation for this struct was generated from the following file:

• nls/nls.h

## **Chapter 5**

## **File Documentation**

#### 5.1 nls/nls.h File Reference

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

#### **Data Structures**

- struct nls\_subproblem\_control\_type
- struct nls control type
- struct nls\_time\_type
- struct nls\_subproblem\_inform\_type
- struct nls\_inform\_type

#### **Functions**

- void nls initialize (void \*\*data, struct nls control type \*control, struct nls inform type \*inform)
- void nls\_read\_specfile (struct nls\_control\_type \*control, const char specfile[])
- void nls\_import (struct nls\_control\_type \*control, void \*\*data, int \*status, int n, int m, const char J\_type[], int J\_ne, const int J\_row[], const int J\_col[], const int J\_ptr[], const char H\_type[], int H\_ne, const int H\_row[], const int H\_col[], const int H\_ptr[], const char P\_type[], int P\_ne, const int P\_row[], const int P\_col[], const int P\_ptr[], const real\_wp\_w[])
- void nls\_solve\_with\_mat (void \*\*data, void \*userdata, int \*status, int n, int m, real\_wp\_ x[], real\_wp\_ c[], real\_wp\_ g[], int(\*eval\_c)(int, int, const real\_wp\_[], real\_wp\_[], const void \*), int j\_ne, int(\*eval\_j)(int, int, int, const real\_wp\_[], real\_wp\_[], const void \*), int h\_ne, int(\*eval\_h)(int, int, int, const real\_wp\_[], const real\_wp\_[], real\_wp\_[], const void \*), int p\_ne, int(\*eval\_hprods)(int, int, int, const real\_wp\_[], const real\_wp\_[], real\_wp\_[], bool, const void \*))
- void nls\_solve\_without\_mat (void \*\*data, void \*userdata, int \*status, int n, int m, real\_wp\_x[], real\_wp\_c[], real\_wp\_g[], int(\*eval\_c)(int, int, const real\_wp\_[], const void \*), int(\*eval\_jprod)(int, int, const real\_wp\_[], const bool, real\_wp\_[], const real\_wp\_[], bool, const void \*), int(\*eval\_hprod)(int, int, const real\_wp\_[], const real\_wp\_[], const real\_wp\_[], bool, const void \*), int p\_ne, int(\*eval\_hprods)(int, int, int, const real\_wp\_[], const real\_wp\_[], real\_wp\_[], bool, const void \*))
- void nls\_solve\_reverse\_with\_mat (void \*\*data, int \*status, int \*eval\_status, int n, int m, real\_wp\_ x[], real—
   \_wp\_ c[], real\_wp\_ g[], int j\_ne, real\_wp\_ J\_val[], const real\_wp\_ y[], int h\_ne, real\_wp\_ H\_val[], real\_wp\_
   v[], int p\_ne, real\_wp\_ P\_val[])
- void nls\_solve\_reverse\_without\_mat (void \*\*data, int \*status, int \*eval\_status, int n, int m, real\_wp\_ x[], real\_wp\_ c[], real\_wp\_ g[], bool \*transpose, real\_wp\_ u[], real\_wp\_ v[], real\_wp\_ y[], int p\_ne, real\_wp\_ P val[])
- void nls\_information (void \*\*data, struct nls\_inform\_type \*inform, int \*status)
- void nls\_terminate (void \*\*data, struct nls\_control\_type \*control, struct nls\_inform\_type \*inform)

24 File Documentation

#### 5.1.1 Function Documentation

#### 5.1.1.1 nls\_import()

```
void nls_import (
            struct nls_control_type * control,
             void ** data,
             int * status,
             int n,
             int m,
             const char J_type[],
            int J_ne,
            const int J_row[],
            const int J_{col[]},
             const int J_ptr[],
             const char H_type[],
             int H_ne,
             const int H_row[],
             const int H_col[],
             const int H_ptr[],
             const char P_type[],
             int P_ne,
             const int P_row[],
             const int P_col[],
             const int P_ptr[],
             const real_wp_ w[] )
```

Import problem data into internal storage prior to solution.

in	control	is a atrust whose members provide control paramters for the remaining presedures (see
T11	Control	is a struct whose members provide control paramters for the remaining proedures (see
		nls_control_type)
in,out	data	holds private internal data
in,out	status	<ul> <li>is a scalar variable of type int, that gives the exit status from the package. Possible values are:</li> <li>1. The import was successful, and the package is ready for the solve phase</li> <li>-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 page of the offending array are hold in inform allocations.</li> </ul>
		<ul> <li>containing the name of the offending array are held in inform.alloc_status and inform.bad_alloc respectively.</li> <li>-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.</li> <li>-3. The restrictions n &gt; 0, m &gt; 0 or requirement that J/H/P_type contains its relevant string 'dense', 'dense_by_columns', 'coordinate', 'sparse_by_rows', 'sparse_by_columns', 'diagonal' or 'absent' has been violated.</li> </ul>
in	n	is a scalar variable of type int, that holds the number of variables.
in	m	is a scalar variable of type int, that holds the number of residuals.

25

	T	
in	J_type	is a one-dimensional array of type char that specifies the symmetric storage scheme used for the Jacobian, \bf\$J\bf\$. It should be one of 'coordinate', 'sparse_by_rows', 'dense' or 'absent', the latter if access to the Jacobian is via matrix-vector products; lower or upper case variants are allowed.
in	J_ne	is a scalar variable of type int, that holds the number of entries in \bf\$J\bf\$ in the sparse co-ordinate storage scheme. It need not be set for any of the other schemes.
in	J_row	is a one-dimensional array of size J_ne and type int, that holds the row indices of \bf\$J\bf\$ in the sparse co-ordinate storage scheme. It need not be set for any of the other schemes, and in this case can be NULL.
in	J_col	is a one-dimensional array of size J_ne and type int, that holds the column indices of \bf\$J\bf\$ in either the sparse co-ordinate, or the sparse row-wise storage scheme. It need not be set when the dense or diagonal storage schemes are used, and in this case can be NULL.
in	J_ptr	is a one-dimensional array of size $n+1$ and type int, that holds the starting position of each row of $J$ , as well as the total number of entries plus one, in the sparse row-wise storage scheme. It need not be set when the other schemes are used, and in this case can be NULL.
in	H_type	is a one-dimensional array of type char that specifies the symmetric storage scheme used for the Hessian, $H$ . It should be one of 'coordinate', 'sparse_by_rows', 'dense', 'diagonal' or 'absent', the latter if access to $H$ is via matrix-vector products; lower or upper case variants are allowed.
in	H_ne	is a scalar variable of type int, that holds the number of entries in the lower triangular part of $H$ in the sparse co-ordinate storage scheme. It need not be set for any of the other three schemes.
in	H_row	is a one-dimensional array of size $H_n$ e and type int, that holds the row indices of the lower triangular part of $H$ in the sparse co-ordinate storage scheme. It need not be set for any of the other three schemes, and in this case can be NULL.
in	H_col	is a one-dimensional array of size $H_n$ e and type int, that holds the column indices of the lower triangular part of $H$ in either the sparse co-ordinate, or the sparse row-wise storage scheme. It need not be set when the dense or diagonal storage schemes are used, and in this case can be NULL.
in	H_ptr	is a one-dimensional array of size $n+1$ and type int, that holds the starting position of each row of the lower triangular part of $H$ , as well as the total number of entries plus one, in the sparse row-wise storage scheme. It need not be set when the other schemes are used, and in this case can be NULL.
in	P_type	is a one-dimensional array of type char that specifies the symmetric storage scheme used for the residual-Hessians-vector product matrix, $P$ . It should be one of 'coordinate', 'sparse_by_columns', 'dense_by_columns' or 'absent', the latter if access to $P$ is via matrix-vector products; lower or upper case variants are allowed.
in	P_ne	is a scalar variable of type int, that holds the number of entries in $P$ in the sparse co-ordinate storage scheme. It need not be set for any of the other schemes.
in	P_row	is a one-dimensional array of size P_ne and type int, that holds the row indices of $P$ in either the sparse co-ordinate, or the sparse column-wise storage scheme. It need not be set when the dense storage scheme is used, and in this case can be NULL.
in	P_col	is a one-dimensional array of size $P$ _ne and type int, that holds the row indices of $P$ in the sparse co-ordinate storage scheme. It need not be set for any of the other schemes, and in this case can be NULL.
in	P_ptr	is a one-dimensional array of size $m+1$ and type int, that holds the starting position of each row of $P$ , as well as the total number of entries plus one, in the sparse row-wise storage scheme. It need not be set when the other schemes are used, and in this case can be NULL.
in	W	is a one-dimensional array of size m and type double, that holds the values $w$ of the weights on the residuals in the least-squares objective function. It need not be set if the weights are all ones, and in this case can be NULL

26 File Documentation

## Examples

nlst.c, and nlstf.c.

## 5.1.1.2 nls\_information()

#### Provides output information

#### **Parameters**

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

nlst.c, and nlstf.c.

## 5.1.1.3 nls\_initialize()

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 nls_control_type)
out	inform	is a struct containing output information (see nls_inform_type)

## Examples

nlst.c, and nlstf.c.

5.1 nls/nls.h File Reference 27

#### 5.1.1.4 nls\_read\_specfile()

Read the content of a specification file, and assign values associated with given keywords to the corresponding control parameters

#### **Parameters**

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

#### 5.1.1.5 nls\_solve\_reverse\_with\_mat()

```
void nls_solve_reverse_with_mat (
             void ** data,
             int * status,
             int * eval_status,
             int n_{i}
             int m_{*}
             real_wp_ x[],
             real_wp_ c[],
             real_wp_ g[],
             int j_ne,
             real_wp_ J_val[],
             const real_wp_ y[],
             int h_ne,
             real_wp_ H_val[],
             real_wp_v[],
             int p_ne,
             real_wp_ P_val[] )
```

Find a local minimizer of a given function using a trust-region method.

This call is for the case where  $H=\nabla_{xx}f(x)$  is provided specifically, but function/derivative information is only available by returning to the calling procedure

in,out	data	holds private internal data
--------	------	-----------------------------

28 File Documentation

#### **Parameters**

in, out status is a scalar variable of type int, that gives the entry and exit status from the package. On initial entry, status must be set to 1. Possible exit are: · 0. The import was succesful · -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. The restriction n > 0 or requirement that type contains its relevant string 'dense', 'coordinate', 'sparse\_by\_rows', 'diagonal' or 'absent' has been violated. • -9. The analysis phase of the factorization failed; the return status from the factorization package is given in the component inform.factor\_status • -10. The factorization failed; the return status from the factorization package is given in the component inform.factor status. • -11. The solution of a set of linear equations using factors from the factorization package failed; the return status from the factorization package is given in the component inform factor status. • -16. The problem is so ill-conditioned that further progress is impossible. • -17. The step is too small to make further impact. • -18. Too many iterations have been performed. This may happen if control.maxit is too small, but may also be symptomatic of a badly scaled problem. • -19. The CPU time limit has been reached. This may happen if control.cpu time limit is too small, but may also be symptomatic of a badly scaled problem. • -82. The user has forced termination of solver by removing the file named control.alive file from unit unit control.alive unit. • 2. The user should compute the vector of residuals c(x) at the point xindicated in x and then re-enter the function. The required value should be set in c, and eval status should be set to 0. If the user is unable to evaluate c(x)— for instance, if the function is undefined at x— the user need not set c, but should then set eval status to a non-zero value. • 3. The user should compute the Jacobian of the vector of residual functions,  $\nabla_x c(x)$ , at the point x indicated in x and then re-enter the function. The I-th component of the Jacobian stored according to the scheme specified for the remainder of J in the earlier call to nls\_import should be set in J\_val[I], for I = 0, ..., J\_ne-1 and eval\_status should be set to 0. If the user is unable to

evaluate a component of J — for instance, if a component of the matrix is

undefined at x — the user need not set J val, but should then set

eval status to a non-zero value.

5.1 nls/nls.h File Reference 29

	status	(continued)
		• 4. The user should compute the matrix $H=\sum_{i=1}^m v_i \nabla_{xx} c_i(x)$ of weighted residual Hessian evaluated at $\mathbf{x}=x$ and $\mathbf{v}=v$ and then re-enter the function. The l-th component of the matrix stored according to the scheme specified for the remainder of $H$ in the earlier call to nls_import should be set in H_val[I], for I = 0,, H_ne-1 and eval_status should be set to 0. If the user is unable to evaluate a component of $H$ — for instance, if a component of the matrix is undefined at $x$ — the user need not set H_val, but should then set eval_status to a non-zero value. <b>Note</b> that this return will not happen if the Gauss-Newton model is selected.
		• 7. The user should compute the entries of the matrix $P$ , whose i-th column is the product $\nabla_{xx}c_i(x)v$ between $\nabla_{xx}c_i(x)$ , the Hessian of the i-th component of the residual $c(x)$ at $\mathbf{x}=x$ , and $\mathbf{v}=v$ and then re-enter the function. The I-th component of the matrix stored according to the scheme specified for the remainder of $P$ in the earlier call to nls_import should be set in P_val[I], for I = 0,, P_ne-1 and eval_status should be set to 0. If the user is unable to evaluate a component of $P$ — for instance, if a component of the matrix is undefined at $x$ — the user need not set P_val, but should then set eval_status to a non-zero value. <b>Note</b> that this return will not happen if either the Gauss-Newton or Newton models is selected.
in,out	eval_status	is a scalar variable of type int, that is used to indicate if objective function/gradient/Hessian values can be provided (see above)
in	n	is a scalar variable of type int, that holds the number of variables
in	m	is a scalar variable of type int, that holds the number of residuals.
in,out	X	is a one-dimensional array of size n and type double, that holds the values $x$ of the
,		optimization variables. The j-th component of x, j = 0,, n-1, contains $x_j$ .
in,out	С	is a one-dimensional array of size m and type double, that holds the residual $c(x)$ . The i-th component of c, j = 0,, n-1, contains $c_j(x)$ . See status = 2, above, for more details.
in,out	g	is a one-dimensional array of size n and type double, that holds the gradient $g=\nabla_x f(x)$ of the objective function. The j-th component of g, j = 0, , n-1, contains $g_j$ .
in	j_ne	is a scalar variable of type int, that holds the number of entries in the Jacobian matrix $J$ .
in	J_val	is a one-dimensional array of size ne and type double, that holds the values of the entries of the Jacobian matrix $J$ in any of the available storage schemes. See status = 3, above, for more details.
in,out	У	is a one-dimensional array of size m and type double, that is used for reverse communication. See status = 4 above for more details.
in	h_ne	is a scalar variable of type int, that holds the number of entries in the lower triangular part of the Hessian matrix ${\cal H}.$
in	H_val	is a one-dimensional array of size ne and type double, that holds the values of the entries of the lower triangular part of the Hessian matrix $H$ in any of the available storage schemes. See status = 4, above, for more details.
in,out	V	is a one-dimensional array of size n and type double, that is used for reverse communication. See status = 7, above, for more details.
in	p_ne	is a scalar variable of type int, that holds the number of entries in the residual-Hessians-vector product matrix, ${\cal P}.$
in	P_val	is a one-dimensional array of size ne and type double, that holds the values of the entries of the residual-Hessians-vector product matrix, $P$ . See status = 7, above, for more details.

30 File Documentation

#### Examples

nlst.c, and nlstf.c.

#### 5.1.1.6 nls\_solve\_reverse\_without\_mat()

```
void nls_solve_reverse_without_mat (
    void ** data,
    int * status,
    int * eval_status,
    int n,
    int m,
    real_wp_ x[],
    real_wp_ g[],
    bool * transpose,
    real_wp_ u[],
    real_wp_ v[],
    real_wp_ y[],
    int p_ne,
    real_wp_ P_val[] )
```

Find a local minimizer of a given function using a trust-region method.

This call is for the case where access to  $H=\nabla_{xx}f(x)$  is provided by Hessian-vector products, but function/derivative information is only available by returning to the calling procedure.

in,out	data	holds private internal data
in,out	status	is a scalar variable of type int, that gives the entry and exit status from the package.
		On initial entry, status must be set to 1.  Possible exit are:  • 0. The import was succesful
		<ul> <li>-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.</li> </ul>
		<ul> <li>-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.</li> </ul>
		<ul> <li>-3. The restriction n &gt; 0 or requirement that type contains its relevant string 'dense', 'coordinate', 'sparse_by_rows', 'diagonal' or 'absent' has been violated.</li> </ul>
		<ul> <li>-9. The analysis phase of the factorization failed; the return status from the factorization package is given in the component inform.factor_status</li> </ul>

5.1 nls/nls.h File Reference 31

	status	(continued)
		<ul> <li>-10. The factorization failed; the return status from the factorization package is given in the component inform.factor_status.</li> </ul>
		<ul> <li>-11. The solution of a set of linear equations using factors from the factorization package failed; the return status from the factorization package is given in the component inform.factor_status.</li> </ul>
		-16. The problem is so ill-conditioned that further progress is impossible.
		<ul> <li>-17. The step is too small to make further impact.</li> </ul>
		<ul> <li>-18. Too many iterations have been performed. This may happen if control.maxit is too small, but may also be symptomatic of a badly scaled problem.</li> </ul>
		<ul> <li>-19. The CPU time limit has been reached. This may happen if control.cpu_time_limit is too small, but may also be symptomatic of a badly scaled problem.</li> </ul>
		-82. The user has forced termination of solver by removing the file named control.alive_file from unit unit control.alive_unit.
		• 2. The user should compute the vector of residuals $c(x)$ at the point $x$ indicated in x and then re-enter the function. The required value should be set in c, and eval_status should be set to 0. If the user is unable to evaluate $c(x)$ — for instance, if the function is undefined at $x$ — the user need not set c, but should then set eval_status to a non-zero value.
		• 5. The user should compute the sum $u+\nabla_x c(x)v$ (if tranpose is false) or $u+(\nabla_x c(x))^Tv$ (if tranpose is true) between the product of the Jacobian $\nabla_x c(x)$ or its tranpose with the vector $\mathbf{v}=v$ and the vector $\mathbf{u}=\$u$ , and then re-enter the function. The result should be set in $\mathbf{u}$ , and eval_status should be set to 0. If the user is unable to evaluate the sum — for instance, if the Jacobian is undefined at $x$ — the user need not set $\mathbf{u}$ , but should then set eval_status to a non-zero value.
		• 6. The user should compute the sum $u+\sum_{i=1}^m y_i \nabla_{xx} c_i(x)v$ between the product of the weighted residual Hessian $H=\sum_{i=1}^m y_i \nabla_{xx} c_i(x)$ evaluated at $\mathbf{x}=x$ and $\mathbf{y}=y$ with the vector $\mathbf{v}=v$ and the the vector $\mathbf{u}=\$u$ , and then re-enter the function. The result should be set in $\mathbf{u}$ , and eval_status should be set to 0. If the user is unable to evaluate the sum — for instance, if the weifghted residual Hessian is undefined at $x$ — the user need not set $\mathbf{u}$ , but should then set eval_status to a non-zero value.
		• 7. The user should compute the entries of the matrix $P$ , whose i-th column is the product $\nabla_{xx}c_i(x)v$ between $\nabla_{xx}c_i(x)$ , the Hessian of the i-th component of the residual $c(x)$ at $x=x$ , and $v=v$ and then re-enter the function. The I-th component of the matrix stored according to the scheme specified for the remainder of $P$ in the earlier call to nls_import should be set in P_val[i], for $I=0,\ldots,P_ne-1$ and eval_status should be set to 0. If the user is unable to evaluate a component of $P$ —for instance, if a component of the matrix is undefined at $x$ —the user need not set P_val, but should then set eval_status to a non-zero value. <b>Note</b> that this return will not happen if either the Gauss-Newton or Newton models is selected.
in,out	eval_status	is a scalar variable of type int, that is used to indicate if objective function/gradient/Hessian values can be provided (see above)

32 File Documentation

#### **Parameters**

in	n	is a scalar variable of type int, that holds the number of variables
in	m	is a scalar variable of type int, that holds the number of residuals.
in,out	Х	is a one-dimensional array of size n and type double, that holds the values $x$ of the optimization variables. The j-th component of x, j = 0,, n-1, contains $x_j$ .
in,out	С	is a one-dimensional array of size m and type double, that holds the residual $c(x)$ . The i-th component of c, j = 0,, n-1, contains $c_j(x)$ . See status = 2, above, for more details.
in,out	g	is a one-dimensional array of size n and type double, that holds the gradient $g=\nabla_x f(x)$ of the objective function. The j-th component of g, j = 0, , n-1, contains $g_j$ .
out	transpose	is a scalar variable of type bool, that indicates whether the product with Jacobian or its transpose should be obtained when status=5.
in,out	u	is a one-dimensional array of size $max(n,m)$ and type double, that is used for reverse communication. See status = 5,6 above for more details.
in,out	V	is a one-dimensional array of size $max(n,m)$ and type double, that is used for reverse communication. See status = 5,6,7 above for more details.
in,out	У	is a one-dimensional array of size m and type double, that is used for reverse communication. See status = 6 above for more details.
in	p_ne	is a scalar variable of type int, that holds the number of entries in the residual-Hessians-vector product matrix, ${\cal P}.$
in	P_val	is a one-dimensional array of size P_ne and type double, that holds the values of the entries of the residual-Hessians-vector product matrix, $P$ . See status = 7, above, for more details.

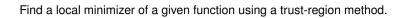
## **Examples**

nlst.c, and nlstf.c.

### 5.1.1.7 nls\_solve\_with\_mat()

```
void nls_solve_with_mat (
             void ** data,
             void * userdata,
             int * status,
            int n,
            int m_{r}
            real_wp_ x[],
            real_wp_ c[],
             real_wp_ g[],
             int(*)(int, int, const real_wp_[], real_wp_[], const void *) eval_c,
             int j_ne,
             int(*)(int, int, int, const real_wp_[], real_wp_[], const void *) eval_j,
             int h_ne,
             int(*)(int, int, int, const real_wp_[], const real_wp_[], real_wp_[], const void
*) eval_h,
            int p_ne,
             int(*)(int, int, int, const real_wp_[], const real_wp_[], real_wp_[], bool, const
void *) eval_hprods )
```

5.1 nls/nls.h File Reference 33



This call is for the case where  $H=\nabla_{xx}f(x)$  is provided specifically, and all function/derivative information is available by function calls.

#### **Parameters**

in,out	data	holds private internal data
in	userdata	is a structure that allows data to be passed into the function and derivative evaluation programs.
in, out	status	is a scalar variable of type int, that gives the entry and exit status from the package.  On initial entry, status must be set to 1.  Possible exit are:  • 0. The import was succesful  • -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. The restriction n > 0 or requirement that type contains its relevant string 'dense', 'coordinate', 'sparse_by_rows', 'diagonal' or 'absent' has been violated.  • -9. The analysis phase of the factorization failed; the return status from the factorization package is given in the component inform.factor_status  • -10. The factorization failed; the return status from the factorization package is given in the component inform.factor_status.  • -11. The solution of a set of linear equations using factors from the factorization package failed; the return status from the factorization package is given in the component inform.factor_status.  • -16. The problem is so ill-conditioned that further progress is impossible.  • -17. The step is too small to make further impact.  • -18. Too many iterations have been performed. This may happen if control.maxit is too small, but may also be symptomatic of a badly scaled problem.  • -19. The CPU time limit has been reached. This may happen if control.cup_time_limit is too small, but may also be symptomatic of a badly scaled problem.  • -82. The user has forced termination of solver by removing the file named control.alive_file from unit unit control.alive_unit.
in	n	is a scalar variable of type int, that holds the number of variables.
in	m	is a scalar variable of type int, that holds the number of residuals.
in,out	X	is a one-dimensional array of size n and type double, that holds the values $x$ of the optimization variables. The j-th component of x, j = 0,, n-1, contains $x_j$ .
out	С	is a one-dimensional array of size m and type double, that holds the residual $c(x)$ . The i-th component of c, j = 0, , n-1, contains $c_j(x)$ .
out	g	is a one-dimensional array of size n and type double, that holds the gradient $g=\nabla_x f(x)$ of the objective function. The j-th component of g, j = 0,, n-1, contains $g_j$ .

#### **Parameters**

	eval_c	is a user-supplied function that must have the following signature: $ \begin{array}{ccccccccccccccccccccccccccccccccccc$
in	j_ne	structure userdata.  is a scalar variable of type int, that holds the number of entries in the Jacobian matrix $J$ .
	eval_j	is a user-supplied function that must have the following signature: $ \begin{array}{l} \text{int eval\_j(int n, int m, int jne, const double x[], double j[], const void } \\ \text{*userdata} )                                  $
		Data may be passed into eval_j via the structure userdata.
in	h_ne	is a scalar variable of type int, that holds the number of entries in the lower triangular part of the Hessian matrix $H$ if it is used.
	eval_h	is a user-supplied function that must have the following signature:
in	p_ne	is a scalar variable of type int, that holds the number of entries in the residual-Hessians-vector product matrix $P$ if it is used.
	eval_hprods	is an optional user-supplied function that may be NULL. If non-NULL, it must have the following signature: $ \begin{array}{lll} & \text{int eval\_hprods(int n, int m, int pne, const double x[], const double v[], } \\ & \text{double p[], bool got\_h, } \\ & \text{const void *userdata)}); \\ & \text{The entries of the matrix $P$, whose i-th column is the product $\nabla_{xx}c_i(x)v$ between $\nabla_{xx}c_i(x)$, the Hessian of the i-th component of the residual $c(x)$ at $x=x$, and $v=v$ must be returned in p and the function return value set to 0. If the evaluation is impossible at $x$, return should be set to a nonzero value. Data may be passed into eval\_hprods via the structure userdata. \\ \end{aligned}$

#### Examples

nlst.c, and nlstf.c.

#### 5.1.1.8 nls\_solve\_without\_mat()

```
real_wp_ g[],
    int(*)(int, int, const real_wp_[], real_wp_[], const void *) eval_c,
    int(*)(int, int, const real_wp_[], const bool, real_wp_[], const real_wp_[],
bool, const void *) eval_jprod,
    int(*)(int, int, const real_wp_[], const real_wp_[], real_wp_[], const real_wp_←

[], bool, const void *) eval_hprod,
    int p_ne,
    int(*)(int, int, int, const real_wp_[], const real_wp_[], real_wp_[], bool, const
void *) eval_hprods)
```

Find a local minimizer of a given function using a trust-region method.

This call is for the case where access to  $H = \nabla_{xx} f(x)$  is provided by Hessian-vector products, and all function/derivative information is available by function calls.

#### **Parameters**

	in,out	data	holds private internal data
Ī	in	userdata	is a structure that allows data to be passed into the function and derivative
			evaluation programs.

5.1 nls/nls.h File Reference 37

#### **Parameters**

in,out	status	is a scalar variable of type int, that gives the entry and exit status from the package.  On initial entry, status must be set to 1.
		Possible exit are:
		0. The import was succesful
		<ul> <li>-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.</li> </ul>
		<ul> <li>-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.</li> </ul>
		<ul> <li>-3. The restriction n &gt; 0 or requirement that type contains its relevant string 'dense', 'coordinate', 'sparse_by_rows', 'diagonal' or 'absent' has been violated.</li> </ul>
		-9. The analysis phase of the factorization failed; the return status from the factorization package is given in the component inform.factor_status
		<ul> <li>-10. The factorization failed; the return status from the factorization package is given in the component inform.factor_status.</li> </ul>
		<ul> <li>-11. The solution of a set of linear equations using factors from the factorization package failed; the return status from the factorization package is given in the component inform.factor_status.</li> </ul>
		-16. The problem is so ill-conditioned that further progress is impossible.
		-17. The step is too small to make further impact.
		<ul> <li>-18. Too many iterations have been performed. This may happen if control.maxit is too small, but may also be symptomatic of a badly scaled problem.</li> </ul>
		<ul> <li>-19. The CPU time limit has been reached. This may happen if control.cpu_time_limit is too small, but may also be symptomatic of a badly scaled problem.</li> </ul>
		-82. The user has forced termination of solver by removing the file named control.alive_file from unit unit control.alive_unit.
in	n	is a scalar variable of type int, that holds the number of variables
in	m	is a scalar variable of type int, that holds the number of residuals.
in,out	X	is a one-dimensional array of size n and type double, that holds the values $x$ of the optimization variables. The j-th component of x, j = 0,, n-1, contains $x_j$ .
out	С	is a one-dimensional array of size m and type double, that holds the residual $c(x)$ . The i-th component of c, j = 0,, n-1, contains $c_j(x)$ .
out	g	is a one-dimensional array of size n and type double, that holds the gradient $g=\nabla_x f(x)$ of the objective function. The j-th component of g, j = 0, , n-1, contains $g_j$ .

#### **Parameters**

	eval c	is a user-supplied function that must have the following signature:
		int eval_c( int n, const double x[], double c[], const void *userdata ) The componnts of the residual function $c(x)$ evaluated at x= $x$ must be assigned to c,
		and the function return value set to 0. If the evaluation is impossible at x, return
		should be set to a nonzero value. Data may be passed into eval_c via the structure userdata.
	aval inrad	
	eval_jprod	<pre>is a user-supplied function that must have the following signature: int eval_jprod( int n, int m, const double x[], bool transpose, double u[],     const double v[], bool got_j,     const void *userdata )</pre>
		The sum $u + \nabla_x c(x)v$ (if tranpose is false) or The sum $u + (\nabla_x c(x))^T v$ (if
		tranpose is true) bewteen the product of the Jacobian $\nabla_x c_i(x)$ or its tranpose with
		the vector $\mathbf{v} = v$ and the vector $\mathbf{\$} u$ must be returned in $\mathbf{u}$ , and the function return
		value set to 0. If the evaluation is impossible at x, return should be set to a nonzero
		value. Data may be passed into eval_jprod via the structure userdata.
	eval_hprod	<pre>is a user-supplied function that must have the following signature: int eval_hprod( int n, int m, const double x[], const double y[], double     u[], const double v[], bool got_h,     const void *userdata )</pre>
		The sum $u + \sum_{i=1}^m y_i \nabla_{xx} c_i(x) v$ of the product of the weighted residual Hessian $H = \sum_{i=1}^m y_i \nabla_{xx} c_i(x)$ evaluated at $x = x$ and $y = y$ with the vector $v = v$ and the
		vector $\$u$ must be returned in u, and the function return value set to 0. If the
		evaluation is impossible at x, return should be set to a nonzero value. The
		Hessians have already been evaluated or used at x if got_h is true. Data may be
		passed into eval_hprod via the structure userdata.
in	p_ne	is a scalar variable of type int, that holds the number of entries in the
		residual-Hessians-vector product matrix $P$ if it is used.
	eval_hprods	is an optional user-supplied function that may be NULL. If non-NULL, it must have
		<pre>the following signature: int eval_hprods( int n, int m, int p_ne, const double x[], const double     v[], double pval[], bool got_h,     const void *userdata )</pre>
		The entries of the matrix $P$ , whose i-th column is the product $\nabla_{xx}c_i(x)v$ between
		$\nabla_{xx}c_i(x)$ , the Hessian of the i-th component of the residual $c(x)$ at $x=x$ , and $v=y$
		must be returned in pval and the function return value set to 0. If the evaluation is impossible at x, return should be set to a nonzero value. Data may be passed into
		eval_hprods via the structure userdata.

#### Examples

nlst.c, and nlstf.c.

#### 5.1.1.9 nls\_terminate()

Deallocate all internal private storage

#### **Parameters**

i	.n,out	data	holds private internal data
0	ut	control	is a struct containing control information (see nls_control_type)
0	ut	inform	is a struct containing output information (see nls_inform_type)

### Examples

nlst.c, and nlstf.c.

## **Chapter 6**

# **Example Documentation**

#### 6.1 nlst.c

This is an example of how to use the package both when the matrices (Jacobian, Hessian, residual-Hessians-vector product) are directly available and when their product with vectors may be found. Both function call evaluations and returns to the calling program to find the required values are illustrated. A variety of supported Hessian storage formats are shown.

Notice that C-style indexing is used, and that this is flaggeed by setting control.f\_indexing to false. In addition, see how parameters may be passed into the evaluation functions via userdata.

```
/* nlst.c */
/* Full test for the NLS C interface using C sparse matrix indexing */
#include <stdio.h>
#include <math.h>
#include "nls.h"
#define max(a,b)
({ __typeof__ (a) _a = (a); \
    _typeof__ (b) _b = (b); \
    _a > _b ? _a : _b; })
// Custom userdata struct
struct userdata_type {
  double p;
};
// Function prototypes
int res( int n, int m, const double x[], double c[], const void * );
int jac( int n, int m, int jne, const double x[], double jval[], const void *);
int hess( int n, int m, int hne, const double x[], const double y[],
         double hval[], const void \star );
double pval[], bool got_h, const void * );
int jac_dense( int n, int m, int jne, const double x[], double jval[],
              const void * );
int hess_dense( int n, int m, int hne, const double x[], const double y[],
               double hval[], const void \star );
int rhessprods_dense( int n, int m, int pne, const double x[],
                     const double v[], double pval[], bool got_h,
                     const void * );
int main(void) {
    // Derived types
    void *data;
    struct nls_control_type control;
    struct nls_inform_type inform;
// Set user data
    struct userdata_type userdata;
    userdata.p = 1.0;
```

```
// Set problem data
    int n = 2; // # variables int m = 3; // # residuals
    int j_ne = 5; // Jacobian elements
int h_ne = 2; // Hesssian elements
    int p_ne = 2; // residual-Hessians-vector products elements
    int J_row[] = {0, 1, 1, 2, 2}; // Jacobian J int J_col[] = {0, 0, 1, 0, 1}; //
    int J_ptr[] = {0, 1, 3, 5}; // row pointers
int H row[] = {0, 1}; // Hessian H
    int H_row[] = \{0, 1\};
    int H_col[] = {0, 1};
                                    // NB lower triangle
    int H_ptr[] = {0, 1, 2};
int P_row[] = {0, 1};
                                    // row pointers
                                    // residual-Hessians-vector product matrix
    int P_ptr[] = {0, 1, 2, 2};
                                   // column pointers
    // Set storage
    double g[n]; // gradient
double c[m]; // residual
double y[m]; // multipliers
    double W[] = \{1.0, 1.0, 1.0\}; // weights
    char st;
    int status;
    printf(" C sparse matrix indexing\n\n");
// Initialize NLS
        nls_initialize( &data, &control, &inform );
        // Set user-defined control options
        control.f_indexing = false; // C sparse matrix indexing
        //control.print_level = 1;
        control.jacobian_available = 2;
        control.hessian_available = 2;
        control.model = 6;
        double x[] = \{1.5, 1.5\}; // starting point double W[] = \{1.0, 1.0, 1.0\}; // weights
        switch(d){
            case 1: // sparse co-ordinate storage
                st = 'C';
                nls_import( &control, &data, &status, n, m,
                h_ne, hess, p_ne, rhessprods );
            case 2: // sparse by rows
st = 'R';
                "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
                nls_solve_with_mat( &data, &userdata, &status,
                                     n, m, x, c, g, res, j_ne, jac,
                                     h_ne, hess, p_ne, rhessprods );
                break;
            case 3: // dense
                st = 'D';
                nls_import( &control, &data, &status, n, m,
                             "dense", j_ne, NULL, NULL, NULL, "dense", h_ne, NULL, NULL, NULL, NULL, "dense", p_ne, NULL, NULL, NULL, W );
                nls_solve_with_mat(&data, &userdata, &status,
                                     n, m, x, c, g, res, j_ne, jac_dense,
                                      h_ne, hess_dense, p_ne, rhessprods_dense );
            break;
case 4: // diagonal
st = 'I';
                "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
                nls_solve_with_mat( &data, &userdata, &status,
                                     n, m, x, c, g, res, j_ne, jac,
h_ne, hess, p_ne, rhessprods );
                break;
            case 5: // access by products
    st = 'P';
                "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
                nls_solve_without_mat( &data, &userdata, &status,
                                         n, m, x, c, g, res, jacprod,
                                         hessprod, p_ne, rhessprods );
                break:
        }
```

6.1 nlst.c 43

```
nls_information( &data, &inform, &status );
         if(inform.status == 0){
             st, inform.iter, inform.obj, inform.status);
         }else{
            printf("%c: NLS_solve exit status = %li\n", st, inform.status);
         // Delete internal workspace
        nls_terminate( &data, &control, &inform );
    printf("\n tests reverse-communication options\n\n");
    // reverse-communication input/output
    int eval_status;
    double u[max(m,n)], v[max(m,n)];
    double J_val[j_ne], J_dense[m*n];
    double H_{val[h_ne]}, H_{dense[n*(n+1)/2]}, H_{diag[n]};
    double P_val[p_ne], P_dense[m*n];
    bool transpose;
    bool got_j = false;
bool got_h = false;
    for ( int d=1; d <= 5; d++) {</pre>
// for( int d=1; d <= 4; d++) {
         // Initialize NLS
        nls_initialize( &data, &control, &inform );
         // Set user-defined control options
         control.f_indexing = false; // C sparse matrix indexing
         //control.print_level = 1;
         control.jacobian_available = 2;
        control.hessian_available = 2;
control.model = 6;
        double x[] = \{1.5, 1.5\}; // starting point double W[] = \{1.0, 1.0, 1.0\}; // weights
         switch(d){
             case 1: // sparse co-ordinate storage
   st = 'C';
                  nls_import( &control, &data, &status, n, m,
                               "coordinate", j_ne, J_row, J_col, NULL,
"coordinate", h_ne, H_row, H_col, NULL,
"sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
                  while(true){ // reverse-communication loop
                    nls_solve_reverse_with_mat( &data, &status, &eval_status,
                                                   n, m, x, c, g, j_ne, J_val, y, h_ne, H_val, v, p_ne, P_val);
                    if(status == 0){ // successful termination
                    }else if(status < 0){ // error exit</pre>
                        break;
                    }else if(status == 2){ // evaluate c
                        eval_status = res( n, m, x, c, &userdata );
                    }else if(status == 3){ // evaluate J
                    eval_status = jac( n, m, j_ne, x, J_val, &userdata );
}else if(status == 4){ // evaluate H
                    eval_status = hess( n, m, h_ne, x, y, H_val, &userdata );
}else if(status == 7) { // evaluate P
                        eval_status = rhessprods( n, m, p_ne, x, v, P_val, got_h, &userdata );
                       printf(" the value %li of status should not occur\n",
                          status);
                        break:
                    }
             case 2: // sparse by rows
                  st = 'R';
                  "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
                  while(true){ // reverse-communication loop
                    nls_solve_reverse_with_mat( &data, &status, &eval_status,
                                                    n, m, x, c, g, j_ne, J_val, y, h_ne, H_val, v, p_ne, P_val);
                    if(status == 0){ // successful termination
                          break;
                    }else if(status < 0){ // error exit</pre>
                        break;
                    }else if(status == 2){ // evaluate c
                    eval_status = res( n, m, x, c, &userdata );
}else if(status == 3){ // evaluate J
                    eval_status = jac( n, m, j_ne, x, J_val, &userdata );
}else if(status == 4){ // evaluate H
                        eval_status = hess( n, m, h_ne, x, y, H_val, &userdata );
                    }else if(status == 7) { // evaluate P
                        eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                                      got h. &userdata );
```

```
}else{
         printf(" the value %li of status should not occur\n",
           status);
         break;
      }
    break;
case 3: // dense
    st = 'D';
   while(true){ // reverse-communication loop
      nls_solve_reverse_with_mat( &data, &status, &eval_status,
                                  n, m, x, c, g, j_ne, J_dense, y, h_ne, H_dense, v, p_ne, P_dense);
      if(status == 0) { // successful termination
           break;
      }else if(status < 0){ // error exit</pre>
         break;
      }else if(status == 2){ // evaluate c
      eval_status = res( n, m, x, c, &userdata ); }else if(status == 3){ // evaluate J
         eval_status = jac_dense( n, m, j_ne, x, J_dense,
                                   &userdata );
      }else if(status == 4){ // evaluate H
          eval_status = hess_dense( n, m, h_ne, x, y, H_dense,
                                    &userdata );
      }else if(status == 7) { // evaluate P
          eval_status = rhessprods_dense( n, m, p_ne, x, v, P_dense,
                                          got_h, &userdata );
         printf(" the value %1i of status should not occurn",
           status);
          break;
      }
    break;
case 4: // diagonal
    st = 'I';
   while(true){ // reverse-communication loop
     nls_solve_reverse_with_mat( &data, &status, &eval_status,
                                  n, m, x, c, g, j_ne, J_val, y,
h_ne, H_diag, v, p_ne, P_val );
      if(status == 0){ // successful termination
           break;
      }else if(status < 0){ // error exit</pre>
          break;
      }else if(status == 2){ // evaluate c
      eval_status = res( n, m, x, c, &userdata );
}else if(status == 3){ // evaluate J
         eval_status = jac( n, m, j_ne, x, J_val, &userdata );
      }else if(status == 4){ // evaluate H
          eval_status = hess( n, m, h_ne, x, y, H_diag, &userdata );
      }else if(status == 7) { // evaluate P
         eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                    got h, &userdata );
      }else{
         printf(" the value %1i of status should not occur\n",
           status);
          break;
      }
    }
    break:
case 5: // access by products
    st = 'P';
    control.print_level = 1;
   while(true){ // reverse-communication loop
     nls_solve_reverse_without_mat( &data, &status, &eval_status,
                                     n, m, x, c, g, &transpose,
                                     u, v, y, p_ne, P_val);
      if(status == 0){ // successful termination
           break;
      }else if(status < 0){ // error exit</pre>
         break;
      }else if(status == 2){ // evaluate c
      eval_status = res( n, m, x, c, &userdata );
}else if(status == 5){ // evaluate u + J v or u + J'v
```

6.1 nlst.c 45

```
eval_status = jacprod( n, m, x, transpose, u, v, got_j,
                                            &userdata );
               }else if(status == 6){ // evaluate u + H v
                   eval\_status = hessprod(n, m, x, y, u, v, got\_h,
                                             &userdata );
               }else if(status == 7){ // evaluate P
                   eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                               got_h, &userdata );
                   printf(" the value %1i of status should not occur\n",
                     status);
                   break:
              }
            break;
    nls_information( &data, &inform, &status );
    if (inform.status == 0) {
        printf("%c:%6i iterations. Optimal objective value = %5.2f"
                " status = %1i\n",
                st, inform.iter, inform.obj, inform.status);
    }else{
        printf("%c: NLS_solve exit status = %li\n", st, inform.status);
    // Delete internal workspace
    nls_terminate( &data, &control, &inform );
printf("\n basic tests of models used, direct acces\n\n");
for( int model=3; model <= 8; model++) {</pre>
    // Initialize NLS
    nls initialize ( &data, &control, &inform );
    // Set user-defined control options
    control.f_indexing = false; // C sparse matrix indexing
    //control.print_level = 1;
    control.jacobian_available = 2;
    control.hessian_available = 2;
    control.model = model;
    double x[] = \{1.5, 1.5\}; // starting point
    double W[] = \{1.0, 1.0, 1.0\}; // weights
   nls_solve_with_mat(&data, &userdata, &status,
                         n, m, x, c, g, res, j_ne, jac,
                         h_ne, hess, p_ne, rhessprods );
    nls_information( &data, &inform, &status );
    if(inform.status == 0){
        printf(" %li:%6i iterations. Optimal objective value = %5.2f"
    status = %1i\n",
                model, inform.iter, inform.obj, inform.status);
        printf(" %i: NLS_solve exit status = %li\n", model, inform.status);
    // Delete internal workspace
    nls terminate ( &data, &control, &inform );
printf("\n basic tests of models used, access by <math>products\n");
for( int model=3; model <= 8; model++) {</pre>
    // Initialize NLS
    nls_initialize( &data, &control, &inform );
// Set user-defined control options
    control.f_indexing = false; // C sparse matrix indexing
    //control.print_level = 1;
    control.jacobian_available = 2;
    control.hessian_available = 2;
    \label{eq:control.model} \begin{array}{l} \texttt{model}: \\ \texttt{double} \ x[] = \{1.5, 1.5\}; \ // \ \texttt{starting point} \\ \texttt{double} \ W[] = \{1.0, \ 1.0, \ 1.0\}; \ // \ \texttt{weights} \end{array}
    "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
    nls_solve_without_mat( &data, &userdata, &status,
                            n, m, x, c, g, res, jacprod,
hessprod, p_ne, rhessprods );
    nls_information( &data, &inform, &status );
    if(inform.status == 0){
        printf("P%1i:%6i iterations. Optimal objective value = %5.2f" status = %1i\n",
                model, inform.iter, inform.obj, inform.status);
    }else{
       printf("P%i: NLS_solve exit status = %1i\n", model, inform.status);
    // Delete internal workspace
    nls_terminate( &data, &control, &inform );
}
```

```
printf("\n basic tests of models used, reverse access\n\n");
for( int model=3; model <= 8; model++) {</pre>
    // Initialize NLS
    nls_initialize( &data, &control, &inform );
    // Set user-defined control options
control.f_indexing = false; // C sparse matrix indexing
    //control.print_level = 1;
    control.jacobian_available = 2;
    control.hessian_available = 2;
   "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
    while (true) { // reverse-communication loop
      nls_solve_reverse_with_mat( &data, &status, &eval_status,
                                      n, m, x, c, g, j_ne, J_val, y, h_ne, H_val, v, p_ne, P_val);
      if(status == 0){ // successful termination
             break;
       }else if(status < 0){ // error exit</pre>
          break:
       }else if(status == 2){ // evaluate c
       eval_status = res( n, m, x, c, &userdata );
}else if(status == 3){ // evaluate J
       eval_status = jac( n, m, j_ne, x, J_val, &userdata );
}else if(status == 4){ // evaluate H
          eval_status = hess( n, m, h_ne, x, y, H_val, &userdata );
       }else if(status == 7){ // evaluate P
           eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                        got_h, &userdata );
          printf(" the value %1i of status should not occur\n",
             status);
           break;
    nls_information( &data, &inform, &status );
    if(inform.status == 0){
        printf("P%1i:%6i iterations. Optimal objective value = %5.2f" status = %1i\n",
                model, inform.iter, inform.obj, inform.status);
        printf(" %i: NLS_solve exit status = %li\n", model, inform.status);
    // Delete internal workspace
    nls_terminate( &data, &control, &inform );
printf("\n basic tests of models used, reverse access by products\n\n");
for( int model=3; model <= 8; model++) {</pre>
    // Initialize NLS
    nls_initialize( &data, &control, &inform );
// Set user-defined control options
    control.f_indexing = false; // C sparse matrix indexing
    //control.print_level = 1;
    control.jacobian_available = 2;
    control.hessian_available = 2;
    control.model = model;
double x[] = {1.5,1.5}; // starting point
double W[] = {1.0, 1.0, 1.0}; // weights
    nls_import( &control, &data, &status, n, m, "absent", j_ne, NULL, NULL, NULL, "absent", h_ne, NULL, NULL, NULL,
                  "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
    while(true){ // reverse-communication loop
      nls_solve_reverse_without_mat( &data, &status, &eval_status,
                                          n, m, x, c, q, &transpose,
                                          u, v, y, p_ne, P_val );
       if(status == 0){ // successful termination
             break;
       }else if(status < 0){ // error exit</pre>
          break:
       }else if(status == 2){ // evaluate c
       eval_status = res( n, m, x, c, &userdata );
}else if(status == 5){ // evaluate u + J v or u + J'v
           eval_status = jacprod( n, m, x, transpose, u, v, got_j,
                                     &userdata );
       }else if(status == 6) { // evaluate u + H v
          eval_status = hessprod( n, m, x, y, u, v, got_h,
                                      &userdata );
       }else if(status == 7) { // evaluate P
           eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                        got_h, &userdata );
           printf(" the value %1i of status should not occur\n",
```

6.1 nlst.c 47

```
status);
           }
         nls_information( &data, &inform, &status );
          if (inform.status == 0) {
             printf("P%1i:%6i iterations. Optimal objective value = %5.2f"
                       " status = %1i\n",
                       model, inform.iter, inform.obj, inform.status);
          }else{
             printf("P%i: NLS_solve exit status = %li\n", model, inform.status);
          // Delete internal workspace
         nls_terminate( &data, &control, &inform );
// compute the residuals
int res( int n, int m, const double x[], double c[], const void *userdata ){
    struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
    double p = myuserdata->p;
  printf(" in res\n");
       printf( "n, m = %6i %6i\n", n, m);
       printf( "X = %12.4e %12.4e\n", x[0], x[1]);
    c[0] = pow(x[0], 2.0) + p;
    c[1] = x[0] + pow(x[1], 2.0);

c[2] = x[0] - x[1];
      printf( "C = %12.4e %12.4e %12.4e\n", c[0], c[1], c[2]);
    return 0;
// compute the Jacobian
int jac( int n, int m, int jne, const double x[], double jval[],
          const void *userdata ) {
     struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
      printf( "X = 12.4e 12.4e n", x[0], x[1]);
     jval[4] = - 1.0;
printf( "J = %12.4e %12.4e %12.4e %12.4e %12.4e\n",
             jval[0], jval[1], jval[2], jval[3], jval[4]);
    return 0:
// compute the Hessian
int hess( int n, int m, int hne, const double x[], const double y[], double hval[], const void *userdata ){
     struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
    hval[0] = 2.0 * y[0];
hval[1] = 2.0 * y[1];
     return 0:
// compute Jacobian-vector products
int jacprod( int n, int m, const double x[], const bool transpose, double u[],
    const double v[], bool got_j, const void *userdata ){
struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
printf( "X in = %12.4e %12.4e\n", x[0], x[1]);
printf( " transpose %d\n", transpose);
       printf(transpose ? "transpose is true\n" : "transpose is false\n");
     if (transpose) {
       printf("transpose\n");
u[0] = u[0] + 2.0 * x[0] * v[0] + v[1] + v[2];
u[1] = u[1] + 2.0 * x[1] * v[1] - v[2];
    }else{
         printf("not transpose\n");
         printf( "U in = %12.4e %12.4e %12.4e\n", u[0], u[1], u[2]);
printf( "V in = %12.4e %12.4e\n", v[0], v[1]);
      u[0] = u[0] + 2.0 * x[0] * v[0];

u[1] = u[1] + v[0] + 2.0 * x[1] * v[1];

u[2] = u[2] + v[0] - v[1];
         printf( "U in = 12.4e 12.4e 12.4e n", u[0], u[1], u[2]);
     return 0;
// compute Hessian-vector products
struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
     u[0] = u[0] + 2.0 * y[0] * v[0];

u[1] = u[1] + 2.0 * y[1] * v[1];
     return 0:
// compute residual-Hessians-vector products
int rhessprods (int n, int m, int pne, const double x[], const double v[],
                   double pval[], bool got_h, const void *userdata ){
     struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
    pval[0] = 2.0 * v[0];
pval[1] = 2.0 * v[1];
```

```
return 0;
// scale v
u[0] = v[0];
   u[1] = v[1];
   return 0;
// compute the dense Jacobian
struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
   jval[0] = 2.0 * x[0];
   jval[1] = 0.0;
   jval[2] = 1.0;
   jval[3] = 2.0 * x[1];
jval[4] = 1.0;
   jval[5] = -1.0;
   return 0;
// compute the dense Hessian
struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
   hval[0] = 2.0 * y[0];
   hval[1] = 0.0;
   hval[2] = 2.0 * y[1];
   return 0:
// compute dense residual-Hessians-vector products
int rhessprods_dense( int n, int m, int pne, const double x[],
                 const double v[], double pval[], bool got_h,
                 const void *userdata ) {
   struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
   pval[0] = 2.0 * v[0];
pval[1] = 0.0;
   pval[2] = 0.0;
   pval[3] = 2.0 * v[1];
   pval[4] = 0.0;
   pval[5] = 0.0;
   return 0:
```

This is the same example, but now fortran-style indexing is used.

```
/\star Full test for the NLS interface using Fortran sparse matrix indexing \star/
#include <stdio.h>
#include <math.h>
#include "nls.h"
#define max(a,b)
({ __typeof__ (a) _a = (a); \ _typeof__ (b) _b = (b); \ _a > _b ? _a : _b; })
// Custom userdata struct
struct userdata_type {
   double p;
// Function prototypes
int res( int n, int m, const double x[], double c[], const void \star );
const double v[], bool got_h, const void \star );
int rhessprods( int n, int m, int pne, const double x[], const double v[], double pval[], bool got_h, const void *); int scale( int n, int m, const double x[], double u[],
              const double v[], const void \star );
int jac_dense( int n, int m, int jne, const double x[], double jval[],
                  const void * );
int hess_dense( int n, int m, int hne, const double x[], const double y[], double hval[], const void \star ); int rhessprods_dense( int n, int m, int pne, const double x[],
                           const double v[], double pval[], bool got_h,
```

```
const void * );
int main(void) {
     // Derived types
    void *data;
    struct nls_control_type control;
    struct nls_inform_type inform;
    // Set user data
    struct userdata_type userdata;
    userdata.p = 1.0;
     // Set problem data
    int n = 2; // # variables int m = 3; // # residuals
    int j_ne = 5; // Jacobian elements
int h_ne = 2; // Hesssian elements
    int p_ne = 2; // residual-Hessians-vector products elements
    int J_row[] = {1, 2, 2, 3, 3}; // Jacobian J
int J_col[] = {1, 1, 2, 1, 2}; //
    int J_ptr[] = {1, 2, 4, 6};
int H_row[] = {1, 2};
                                           // row pointers
                                           // Hessian H
    int H_{col[]} = \{1, 2\};
                                           // NB lower triangle
    int H_ptr[] = {1, 2, 3};
int P_row[] = {1, 2};
                                           // row pointers
// residual-Hessians-vector product matrix
                                          // column pointers
    int P_ptr[] = \{1, 2, 3, 3\};
    // Set storage
    double g[n]; // gradient
    double c[m]; // residual
    double y[m]; // multipliers
    double W[] = \{1.0, 1.0, 1.0\}; // weights
    char st;
    int status:
    printf(" Fortran sparse matrix indexing\n\n");
    printf(" tests options for all-in-one storage format\n\n");
      or( int d=1; d <= 5; d++){
// for( int d=5; d <= 5; d++){
          // Initialize NLS
         nls_initialize( &data, &control, &inform );
          // Set user-defined control options
         control.f_indexing = true; // Fortran sparse matrix indexing
          //control.print_level = 1;
          control.jacobian_available = 2;
         control.hessian_available = 2;
         \label{eq:control.model} \begin{array}{l} \texttt{control.model} = \texttt{6;} \\ \texttt{double} \ x[] = \{1.5, 1.5\}; \ // \ \texttt{starting point} \\ \texttt{double} \ W[] = \{1.0, \ 1.0, \ 1.0\}; \ // \ \texttt{weights} \\ \end{array}
         switch(d) {
               case 1: // sparse co-ordinate storage
                   st = 'C';
                   nls_import( &control, &data, &status, n, m,
                                   "coordinate", j_ne, J_row, J_col, NULL,
"coordinate", h_ne, H_row, H_col, NULL,
"sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
                   nls_solve_with_mat( &data, &userdata, &status,
                                            n, m, x, c, g, res, j_ne, jac,
                                            h_ne, hess, p_ne, rhessprods );
              break;
case 2: // sparse by rows
st = 'R';
                   break;
              case 3: // dense
    st = 'D';
                   nls_import( &control, &data, &status, n, m,
                                   "dense", j_ne, NULL, NULL, NULL, NULL, "dense", h_ne, NULL, NULL, NULL,
                                   "dense", p_ne, NULL, NULL, NULL, W );
                   nls_solve_with_mat( &data, &userdata, &status,
                                            n, m, x, c, g, res, j_ne, jac_dense,
h_ne, hess_dense, p_ne, rhessprods_dense );
                   break;
               case 4: // diagonal
                   st = 'I';
                   "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
nls_solve_with_mat( &data, &userdata, &status,
                                            n, m, x, c, g, res, j_ne, jac,
                                            h_ne, hess, p_ne, rhessprods );
               break;
case 5: // access by products
    st = 'P';
```

```
nls_import( &control, &data, &status, n, m,
                                 "absent", j_ne, NULL, NULL, NULL, NULL, NULL, NULL, NULL, NULL, NULL,
                                 "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
                  nls_solve_without_mat( &data, &userdata, &status,
                                             n, m, x, c, q, res, jacprod,
                                              hessprod, p_ne, rhessprods );
         nls_information( &data, &inform, &status );
         if (inform.status == 0) {
             printf("%c:%6i iterations. Optimal objective value = %5.2f"
                      " status = %1i\n",
                      st, inform.iter, inform.obj, inform.status);
         }else{
             printf("%c: NLS_solve exit status = %1i\n", st, inform.status);
         // Delete internal workspace
         nls_terminate( &data, &control, &inform );
    printf("\n tests reverse-communication options\n\n");
     // reverse-communication input/output
    int eval status;
    double u[max(m,n)], v[max(m,n)];
double J_val[j_ne], J_dense[m*n];
double H_val[h_ne], H_dense[n*(n+1)/2], H_diag[n];
    double P_val[p_ne], P_dense[m*n];
    bool transpose;
    bool got_j = false;
bool got_h = false;
for( int d=1; d <= 5; d++) {
// for( int d=1; d <= 4; d++) {</pre>
         // Initialize NLS
         nls_initialize( &data, &control, &inform );
         // Set user-defined control options
         control.f_indexing = true; // Fortran sparse matrix indexing
         //control.print_level = 1;
         control.jacobian_available = 2;
         control.hessian_available = 2;
         control.model = 6;
         double x[] = \{1.5, 1.5\}; // starting point double W[] = \{1.0, 1.0, 1.0\}; // weights
         switch(d){
              case 1: // sparse co-ordinate storage
                  st = 'C';
                  nls_import( &control, &data, &status, n, m,
                  "coordinate", j_ne, J_row, J_col, NULL,
"coordinate", h_ne, H_row, H_col, NULL,
"sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
while (true) { // reverse-communication loop
                    nls_solve_reverse_with_mat( &data, &status, &eval_status,
                                                      n, m, x, c, g, j_ne, J_val, y,
                                                      h_ne, H_val, v, p_ne, P_val );
                     if(status == 0){ // successful termination
                           break:
                     }else if(status < 0){ // error exit</pre>
                         break;
                     }else if(status == 2){ // evaluate c
                     eval_status = res( n, m, x, c, &userdata );
}else if(status == 3){ // evaluate J
                     eval_status = jac( n, m, j_ne, x, J_val, &userdata );
}else if(status == 4){ // evaluate H
                         eval_status = hess( n, m, h_ne, x, y, H_val, &userdata );
                     }else if(status == 7) { // evaluate P
                          eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                                        got_h, &userdata );
                         printf(" the value %1i of status should not occur\n",
                           status);
                         break;
              break;
case 2: // sparse by rows
st = 'R';
                  "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
                  while(true){ // reverse-communication loop
                    nls_solve_reverse_with_mat( &data, &status, &eval_status,
                                                      n, m, x, c, g, j_ne, J_val, y, h_ne, H_val, v, p_ne, P_val);
                     if(status == 0){ // successful termination
                     break;
}else if(status < 0){ // error exit</pre>
                         break:
```

}else if(status == 2){ // evaluate c

```
eval_status = res( n, m, x, c, &userdata );
}else if(status == 3){ // evaluate J
                    eval_status = jac( n, m, j_ne, x, J_val, &userdata );
}else if(status == 4){ // evaluate H
                        eval_status = hess( n, m, h_ne, x, y, H_val, &userdata );
                    }else if(status == 7) { // evaluate P
                        eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                                    got_h, &userdata );
                       printf(" the value %1i of status should not occur\n",
                         status);
                        break;
             break;
case 3: // dense
st = 'D';
                 nls_import( &control, &data, &status, n, m,
                               "dense", j_ne, NULL, NULL, NULL,
"dense", h_ne, NULL, NULL, NULL,
"dense", p_ne, NULL, NULL, NULL, W );
                 while(true){ // reverse-communication loop
                   if(status == 0){ // successful termination
                         break;
                    }else if(status < 0){ // error exit</pre>
                        break:
                    }else if(status == 2){ // evaluate c
                    eval_status = res( n, m, x, c, &userdata );
}else if(status == 3){ // evaluate J
                        eval_status = jac_dense( n, m, j_ne, x, J_dense,
                                                    &userdata );
                    }else if(status == 4) { // evaluate H
                        eval_status = hess_dense( n, m, h_ne, x, y, H_dense,
                                                     &userdata );
                    }else if(status == 7) { // evaluate P
                       eval_status = rhessprods_dense( n, m, p_ne, x, v, P_dense,
                                                            got_h, &userdata );
                    lelse(
                       printf(" the value %1i of status should not occur\n",
                          status);
                        break;
                   }
             break;
case 4: // diagonal
st = 'I';
                 "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W ); while(true){ // reverse-communication loop
                   nls_solve_reverse_with_mat( &data, &status, &eval_status,
                                                  n, m, x, c, g, j_ne, J_val, y,
                                                   h_ne, H_diag, v, p_ne, P_val );
                    if(status == 0){ // successful termination
                          break;
                    }else if(status < 0){ // error exit</pre>
                       break;
                    }else if(status == 2){ // evaluate c
                    eval_status = res( n, m, x, c, &userdata );
}else if(status == 3){ // evaluate J
                    eval_status = jac( n, m, j_ne, x, J_val, &userdata );
}else if(status == 4){ // evaluate H
                        eval_status = hess( n, m, h_ne, x, y, H_diag, &userdata );
                    }else if(status == 7) { // evaluate P
                        eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                                     got_h, &userdata );
                       printf(" the value %li of status should not occur\n",
                          status);
                        break;
                   }
                 break;
             case 5: // access by products
    st = 'P';
                 control.print_level = 1;
11
                 nls_import( &control, &data, &status, n, m,
                               "absent", j_ne, NULL, NULL, NULL, NULL, "absent", h_ne, NULL, NULL, NULL,
                               "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
                 while(true){ // reverse-communication loop
                   nls_solve_reverse_without_mat( &data, &status, &eval_status,
```

```
n, m, x, c, q, &transpose,
                                              u, v, y, p_ne, P_val );
              if(status == 0){ // successful termination
                    break;
              }else if(status < 0){ // error exit</pre>
                  break:
              }else if(status == 2){ // evaluate c
                  eval\_status = res(n, m, x, c, &userdata);
              else if(status == 5) { // evaluate u + J v or u + J'v}
                  eval\_status = jacprod(n, m, x, transpose, u, v, got\_j,
                                         &userdata );
              }else if(status == 6){ // evaluate u + H v
                  eval_status = hessprod( n, m, x, y, u, v, got_h,
                                           &userdata );
              }else if(status == 7) { // evaluate P
                  eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                             got_h, &userdata );
              }else{
                 printf(" the value %1i of status should not occur\n",
                   status);
              }
            break:
   nls_information( &data, &inform, &status );
    if(inform.status == 0){
       printf("%:%6: %6i iterations. Optimal objective value = %5.2f"  
" status = %1i\n",
               st, inform.iter, inform.obj, inform.status);
    }else{
       printf("%c: NLS_solve exit status = %1i\n", st, inform.status);
    // Delete internal workspace
    nls_terminate( &data, &control, &inform );
printf("\n basic tests of models used, direct acces\n\n");
for( int model=3; model <= 8; model++) {</pre>
    // Initialize NLS
    nls_initialize( &data, &control, &inform );
    // Set user-defined control options
    control.f_indexing = true; // Fortran sparse matrix indexing
    //control.print_level = 1;
    control.jacobian_available = 2;
    control.hessian_available = 2;
    control.model = model;
   double x[] = \{1.5, 1.5\}; // \text{ starting point double } W[] = \{1.0, 1.0, 1.0\}; // \text{ weights}
   "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
    nls_solve_with_mat( &data, &userdata, &status,
                        n, m, x, c, g, res, j_ne, jac,
h_ne, hess, p_ne, rhessprods );
   nls_information( &data, &inform, &status );
    if(inform.status == 0){
       printf(" %1i:%6i iterations. Optimal objective value = %5.2f"
               " status = %1i\n",
               model, inform.iter, inform.obj, inform.status);
    lelse(
       printf(" %i: NLS_solve exit status = %1i\n", model, inform.status);
    // Delete internal workspace
    nls_terminate( &data, &control, &inform );
printf("\n basic tests of models used, access by products\n\n");\\
for( int model=3; model <= 8; model++) {</pre>
    // Initialize NLS
   nls_initialize( &data, &control, &inform );
    // Set user-defined control options
    control.f_indexing = true; // Fortran sparse matrix indexing
    //control.print_level = 1;
    control.jacobian_available = 2;
   control.hessian_available = 2;
control.model = model;
    double x[] = \{1.5, 1.5\}; // starting point
    double W[] = \{1.0, 1.0, 1.0\}; // weights
   nls_solve_without_mat( &data, &userdata, &status,
                           n, m, x, c, g, res, jacprod,
                           hessprod, p_ne, rhessprods );
   nls_information( &data, &inform, &status );
    if (inform.status == 0) {
```

```
printf("P%1i:%6i iterations. Optimal objective value = %5.2f"
                 " status = %1i\n",
                model, inform.iter, inform.obj, inform.status);
    }else{
        printf("P%i: NLS_solve exit status = %li\n", model, inform.status);
    // Delete internal workspace
    nls_terminate( &data, &control, &inform );
printf("\n basic tests of models used, reverse access\n\n");
for( int model=3; model <= 8; model++) {</pre>
    // Initialize NLS
    nls_initialize( &data, &control, &inform );
    // Set user-defined control options
    control.f_indexing = true; // Fortran sparse matrix indexing
    //control.print_level = 1;
    control.jacobian_available = 2;
    control.hessian_available = 2;
    control.model = model;
    double x[] = \{1.5, 1.5\}; // starting point
    double W[] = \{1.0, 1.0, 1.0\}; // weights
    "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
while(true){ // reverse-communication loop
      nls_solve_reverse_with_mat( &data, &status, &eval_status,
                                     n, m, x, c, g, j_ne, J_val, y, h_ne, H_val, v, p_ne, P_val);
      if(status == 0){ // successful termination
            break:
       }else if(status < 0){ // error exit</pre>
          break;
       }else if(status == 2){ // evaluate c
      eval_status = res( n, m, x, c, &userdata );
}else if(status == 3){ // evaluate J
      eval_status = jac( n, m, j_ne, x, J_val, &userdata );
}else if(status == 4){ // evaluate H
           eval_status = hess( n, m, h_ne, x, y, H_val, &userdata );
       }else if(status == 7) { // evaluate P
           eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                        got_h, &userdata );
      lelse(
          printf(" the value %li of status should not occur\n",
            status);
      }
    nls_information( &data, &inform, &status );
    if (inform.status == 0) {
        printf("P%1i:%6i iterations. Optimal objective value = %5.2f"
                " status = %1i\n",
                model, inform.iter, inform.obj, inform.status);
    }else{
        printf(" %i: NLS_solve exit status = %1i\n", model, inform.status);
    // Delete internal workspace
    nls_terminate( &data, &control, &inform );
printf("\n basic tests of models used, reverse access by products\n\n");
for( int model=3; model <= 8; model++) {
    // Initialize NLS</pre>
    nls_initialize( &data, &control, &inform );
    // Set user-defined control options
    control.f_indexing = true; // Fortran sparse matrix indexing
    //control.print_level = 1;
    control.jacobian_available = 2;
    control.hessian_available = 2;
    control.model = model;
    double x[] = \{1.5, 1.5\}; // starting point double W[] = \{1.0, 1.0, 1.0\}; // weights
    nls_import( &control, &data, &status, n, m,
                 "absent", j_ne, NULL, NULL, NULL, "absent", h_ne, NULL, NULL, NULL, NULL,
    "sparse_by_columns", p_ne, P_row, NULL, P_ptr, W );
while(true){ // reverse-communication loop
      nls_solve_reverse_without_mat( &data, &status, &eval_status,
                                         n, m, x, c, g, &transpose,
                                         u, v, y, p_ne, P_val );
      if(status == 0){ // successful termination
            break;
       }else if(status < 0){ // error exit</pre>
          break;
       }else if(status == 2){ // evaluate c
      eval_status = res( n, m, x, c, &userdata );
}else if(status == 5) { // evaluate u + J v or u + J'v
           eval_status = jacprod( n, m, x, transpose, u, v, got_j,
```

```
&userdata );
          }else if(status == 6){ // evaluate u + H v
               eval\_status = hessprod(n, m, x, y, u, v, got\_h,
                                        &userdata );
          }else if(status == 7) { // evaluate P
               eval_status = rhessprods( n, m, p_ne, x, v, P_val,
                                          got_h, &userdata );
              printf(" the value %1i of status should not occur\n",
                status);
               break:
          }
        nls_information( &data, &inform, &status );
        if(inform.status == 0){
            model, inform.iter, inform.obj, inform.status);
            printf("P%i: NLS_solve exit status = %1i\n", model, inform.status);
         // Delete internal workspace
        nls_terminate( &data, &control, &inform );
// compute the residuals
int res( int n, int m, const double x[], double c[], const void *userdata ){
    struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
    double p = myuserdata->p;
printf(" in res\n");
printf( "n, m = %6i %6i\n", n, m );
printf( "X = %12.4e %12.4e\n", x[0], x[1]);
    c[0] = pow(x[0], 2.0) + p;
    c[1] = x[0] + pow(x[1], 2.0);
    c[2] = x[0] - x[1];
printf( "C = %12.4e %12.4e %12.4e\n", c[0], c[1], c[2]);
    return 0;
// compute the Jacobian
int jac( int n, int m, int jne, const double x[], double jval[],
         const void *userdata ) {
    struct userdata_type *myuserdata = ( struct userdata_type * ) userdata; printf( "X = %12.4e %12.4e\n", x[0], x[1]);
    jval[0] = 2.0 * x[0];
    jval[1] = 1.0;
    jval[2] = 2.0 * x[1];
    jval[3] = 1.0;
   jval[4] = - 1.0;
printf( "J = %12.4e %12.4e %12.4e %12.4e %12.4e\n",
            jval[0], jval[1], jval[2], jval[3], jval[4]);
    return 0;
// compute the Hessian
hval[0] = 2.0 * y[0];
    hval[1] = 2.0 * y[1];
    return 0;
// compute Jacobian-vector products
printf( "X in = %12.4e %12.4e\n", x[0], x[1]);
printf( " transpose %d\n", transpose);
printf(transpose ? "transpose is true\n" : "transpose is false\n");
    if (transpose) {
      printf("transpose\n");

u[0] = u[0] + 2.0 * x[0] * v[0] + v[1] + v[2];

u[1] = u[1] + 2.0 * x[1] * v[1] - v[2];
    }else{
        u[0] = u[0] + 2.0 * x[0] * v[0];

u[1] = u[1] + v[0] + 2.0 * x[1] * v[1];

u[2] = u[2] + v[0] - v[1];
        printf( "U in = %12.4e %12.4e %12.4e\n", u[0], u[1], u[2]);
    return 0;
// compute Hessian-vector products
int hessprod( int n, int m, const double x[], const double y[], double u[],
              const double v[], bool got_h, const void *userdata ){
    struct userdata_type *myuserdata = ( struct userdata_type * ) userdata; u[0] = u[0] + 2.0 * y[0] * v[0];
```

```
u[1] = u[1] + 2.0 * y[1] * v[1];
// compute residual-Hessians-vector products
pval[0] = 2.0 * v[0];
   pval[1] = 2.0 * v[1];
   return 0;
// scale v
struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
   u[0] = v[0];
u[1] = v[1];
   return 0;
// compute the dense Jacobian
struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
   jval[0] = 2.0 * x[0];

jval[1] = 0.0;
    jval[2] = 1.0;
    jval[3] = 2.0 * x[1];
   jval[4] = 1.0;
jval[5] = - 1.0;
   return 0;
// compute the dense Hessian
int hess_dense( int n, int m, int hne, const double x[], const double y[],
              double hval[], const void *userdata ){
   struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
hval[0] = 2.0 * y[0];
hval[1] = 0.0;
hval[2] = 2.0 * y[1];
   return 0;
// compute dense residual-Hessians-vector products
const void *userdata ) {
   struct userdata_type *myuserdata = ( struct userdata_type * ) userdata;
   pval[0] = 2.0 * v[0];
   pval[1] = 0.0;
pval[2] = 0.0;
   pval[3] = 2.0 * v[1];
pval[4] = 0.0;
   pval[5] = 0.0;
   return 0;
```

## Index

```
model
                                                              nls_subproblem_control_type, 19
     nls_control_type, 13
     nls_subproblem_control_type, 19
nls.h
     nls_import, 24
     nls_information, 26
     nls_initialize, 26
     nls_read_specfile, 26
     nls_solve_reverse_with_mat, 27
     nls_solve_reverse_without_mat, 30
     nls solve with mat, 32
     nls_solve_without_mat, 35
     nls_terminate, 38
nls/nls.h, 23
nls_control_type, 11
     model, 13
     norm, 14
     print_level, 14
nls_import
     nls.h, 24
nls_inform_type, 15
nls information
     nls.h, 26
nls_initialize
     nls.h, 26
nls_read_specfile
     nls.h, 26
nls_solve_reverse_with_mat
     nls.h, 27
nls_solve_reverse_without_mat
     nls.h, 30
nls_solve_with_mat
     nls.h, 32
nls_solve_without_mat
     nls.h, 35
nls_subproblem_control_type, 16
     model, 19
     norm, 19
     print_level, 19
nls_subproblem_inform_type, 20
nls terminate
     nls.h, 38
nls_time_type, 21
norm
     nls_control_type, 14
     nls_subproblem_control_type, 19
print_level
     nls_control_type, 14
```