NAG Library Function Document

nag_sparse_sym_chol_fac (f11jac)

1 Purpose

nag_sparse_sym_chol_fac (f11jac) computes an incomplete Cholesky factorization of a real sparse symmetric matrix, represented in symmetric coordinate storage format. This factorization may be used as a preconditioner in combination with nag_sparse_sym_chol_sol (f11jcc).

2 Specification

```
#include <nag.h>
#include <nagf11.h>

void nag_sparse_sym_chol_fac (Integer n, Integer nnz, double *a[],
     Integer *la, Integer *irow[], Integer *icol[], Integer lfill,
     double dtol, Nag_SparseSym_Fact mic, double dscale,
     Nag_SparseSym_Piv pstrat, Integer ipiv[], Integer istr[], Integer *nnzc,
     Integer *npivm, Nag_Sparse_Comm *comm, NagError *fail)
```

3 Description

This function computes an incomplete Cholesky factorization (see Meijerink and Van der Vorst (1977)) of a real sparse symmetric n by n matrix A. It is designed specifically for positive definite matrices, but may also work for some mildly indefinite cases. The factorization is intended primarily for use as a preconditioner for the symmetric iterative solver nag_sparse_sym_chol_sol (f11jcc).

The decomposition is written in the form

$$A = M + R$$

where

$$M = PLDL^{\mathrm{T}}P^{\mathrm{T}}$$

and P is a permutation matrix, L is lower triangular with unit diagonal elements, D is diagonal and R is a remainder matrix.

The amount of fill-in occurring in the factorization can vary from zero to complete fill, and can be controlled by specifying either the maximum level of fill **lfill**, or the drop tolerance **dtol**. The factorization may be modified in order to preserve row sums, and the diagonal elements may be perturbed to ensure that the preconditioner is positive definite. Diagonal pivoting may optionally be employed, either with a user-defined ordering, or using the Markowitz strategy (see Markowitz (1957)) which aims to minimize fill-in. For further details see Section 9.

The sparse matrix A is represented in symmetric coordinate storage (SCS) format (see Section 2.1.2 in the f11 Chapter Introduction). The array **a** stores all the nonzero elements of the lower triangular part of A, while arrays **irow** and **icol** store the corresponding row and column indices respectively. Multiple nonzero elements may not be specified for the same row and column index.

The preconditioning matrix M is returned in terms of the SCS representation of the lower triangular matrix

$$C = L + D^{-1} - I.$$

4 References

Chan T F (1991) Fourier analysis of relaxed incomplete factorization preconditioners *SIAM J. Sci. Statist. Comput.* **12(2)** 668–680

Markowitz H M (1957) The elimination form of the inverse and its application to linear programming *Management Sci.* **3** 255–269

Meijerink J and Van der Vorst H (1977) An iterative solution method for linear systems of which the coefficient matrix is a symmetric M-matrix *Math. Comput.* **31** 148–162

Salvini S A and Shaw G J (1995) An evaluation of new NAG Library solvers for large sparse symmetric linear systems *NAG Technical Report TR1/95*

Van der Vorst H A (1990) The convergence behaviour of preconditioned CG and CG-S in the presence of rounding errors *Lecture Notes in Mathematics* (eds O Axelsson and L Y Kolotilina) **1457** Springer–Verlag

5 Arguments

1: **n** – Integer *Input*

On entry: the order of the matrix A.

Constraint: $\mathbf{n} \geq 1$.

2: **nnz** – Integer *Input*

On entry: the number of nonzero elements in the lower triangular part of the matrix A.

Constraint: $1 < \mathbf{nnz} \leq \mathbf{n} \times (\mathbf{n} + 1)/2$.

3: **a**[**la**] – double * *Input/Output*

On entry: the nonzero elements in the lower triangular part of the matrix A, ordered by increasing row index, and by increasing column index within each row. Multiple entries for the same row and column indices are not permitted. The function nag_sparse_sym_sort (f11zbc) may be used to order the elements in this way.

On exit: the first **nnz** elements of **a** contain the nonzero elements of A and the next **nnzc** elements contain the elements of the lower triangular matrix C. Matrix elements are ordered by increasing row index, and by increasing column index within each row.

4: **la** – Integer * *Input/Output*

On entry: the dimension of the arrays **a**, **irow** and **icol**.

These arrays must be of sufficient size to store both A (**nnz** elements) and C (**nnzc** elements); for this reason the length of the arrays may be changed internally by calls to **realloc**. It is therefore *imperative* that these arrays are *allocated* using *malloc* and **not** declared as automatic arrays.

On exit: if internal allocation has taken place then **la** is set to $\mathbf{nnz} + \mathbf{nnzc}$, otherwise it remains unchanged.

Constraint: $\mathbf{la} \geq 2 \times \mathbf{nnz}$.

5: **irow**[**la**] – Integer * *Input/Output*
6: **icol**[**la**] – Integer * *Input/Output*

On entry: the row and column indices of the nonzero elements supplied in **a**.

Constraints:

irow and **icol** must satisfy the following constraints (which may be imposed by a call to nag_sparse_sym_sort (f11zbc)):;
$1 \leq \mathbf{irow}[i] \leq \mathbf{n}$ and $1 \leq \mathbf{icol}[i] \leq \mathbf{n}$, for $i = 0, 1, \ldots, \mathbf{nnz} - 1$;

irow$[i-1] <$ **irow**$[i]$ or **irow**$[i-1] =$ **irow**$[i]$ and **icol**$[i-1] <$ **icol**$[i]$, for $i = 1, 2, \ldots,$ **nnz** $- 1$.

On exit: the row and column indices of the nonzero elements returned in **a**.

7: **lfill** – Integer *Input*

On entry: if **lfill** ≥ 0 its value is the maximum level of fill allowed in the decomposition (see Section 9.1). A negative value of **lfill** indicates that **dtol** will be used to control the fill instead.

8: **dtol** – double *Input*

On entry: if **lfill** < 0 then **dtol** is used as a drop tolerance to control the fill-in (see Section 9.1). Otherwise **dtol** is not referenced.

Constraint: if **lfill** < 0, **dtol** ≥ 0.0.

9: **mic** – Nag_SparseSym_Fact *Input*

On entry: indicates whether or not the factorization should be modified to preserve row sums (see Section 9.2).

mic = Nag_SparseSym_ModFact
The factorization is modified (MIC).

mic = Nag_SparseSym_UnModFact
The factorization is not modified.

Constraint: **mic** = Nag_SparseSym_ModFact or Nag_SparseSym_UnModFact.

10: **dscale** – double *Input*

On entry: the diagonal scaling argument. All diagonal elements are multiplied by the factor (1 + **dscale**) at the start of the factorization. This can be used to ensure that the preconditioner is positive definite. See Section 9.2.

11: **pstrat** – Nag_SparseSym_Piv *Input*

On entry: specifies the pivoting strategy to be adopted as follows:

if **pstrat** = Nag_SparseSym_NoPiv then no pivoting is carried out;

if **pstrat** = Nag_SparseSym_MarkPiv then diagonal pivoting aimed at minimizing fill-in is carried out, using the Markowitz strategy;

if **pstrat** = Nag_SparseSym_UserPiv then diagonal pivoting is carried out according to the user-defined input value of **ipiv**.

Suggested value: **pstrat** = Nag_SparseSym_MarkPiv.

Constraint: **pstrat** = Nag_SparseSym_NoPiv, Nag_SparseSym_MarkPiv or Nag_SparseSym_UserPiv.

12: **ipiv**[**n**] – Integer *Input/Output*

On entry: if **pstrat** = Nag_SparseSym_UserPiv, then **ipiv**$[i-1]$ must specify the row index of the diagonal element used as a pivot at elimination stage i. Otherwise **ipiv** need not be initialized.

Constraint: if **pstrat** = Nag_SparseSym_UserPiv, then **ipiv** must contain a valid permutation of the integers on $[1, \mathbf{n}]$.

On exit: the pivot indices. If **ipiv**$[i-1] = j$ then the diagonal element in row j was used as the pivot at elimination stage i.

13: **istr**[$\mathbf{n}+\mathbf{1}$] – Integer *Output*

On exit: **istr**[i] -1, for $i = 0, 1, \ldots, \mathbf{n}-1$, is the starting address in the arrays **a**, **irow** and **icol** of row i of the matrix C. **istr**[**n**] -1 is the address of the last nonzero element in C plus one.

14: **nnzc** – Integer * *Output*

On exit: the number of nonzero elements in the lower triangular matrix C.

15: **npivm** – Integer * *Output*

On exit: the number of pivots which were modified during the factorization to ensure that M was positive definite. The quality of the preconditioner will generally depend on the returned value of **npivm**. If **npivm** is large the preconditioner may not be satisfactory. In this case it may be advantageous to call nag_sparse_sym_chol_fac (f11jac) again with an increased value of either **lfill** or **dscale**.

16: **comm** – Nag_Sparse_Comm * *Input/Output*

On entry/exit: a pointer to a structure of type Nag_Sparse_Comm whose members are used by the iterative solver.

17: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

6 Error Indicators and Warnings

NE_2_INT_ARG_LT

On entry, **la** $= \langle value \rangle$ while **nnz** $= \langle value \rangle$. These arguments must satisfy **la** $\geq 2 \times$ **nnz**.

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_BAD_PARAM

On entry, argument **mic** had an illegal value.

On entry, argument **pstrat** had an illegal value.

NE_INT_2

On entry, **nnz** $= \langle value \rangle$, **n** $= \langle value \rangle$.
Constraint: $1 \leq$ **nnz** $\leq$ **n** $\times (\mathbf{n}+1)/2$.

NE_INT_ARG_LT

On entry, **n** $= \langle value \rangle$.
Constraint: **n** ≥ 1.

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

NE_INVALID_ROW_PIVOT

On entry, **pstrat** = Nag_SparseSym_UserPiv and the array **ipiv** does not represent a valid permutation of integers in $[1, \mathbf{n}]$. An input value of **ipiv** is either out of range or repeated.

NE_REAL_INT_ARG_CONS

On entry, **dtol** = ⟨*value*⟩ and **lfill** = ⟨*value*⟩. These arguments must satisfy **dtol** ≥ 0.0 if **lfill** < 0.

NE_SYMM_MATRIX_DUP

A nonzero element has been supplied which does not lie in the lower triangular part of the matrix A, is out of order, or has duplicate row and column indices, i.e., one or more of the following constraints has been violated:

$1 \leq \mathbf{irow}[i] \leq \mathbf{n}$ and $1 \leq \mathbf{icol}[i] \leq \mathbf{n}$, for $i = 0, 1, \ldots, \mathbf{nnz} - 1$.

$\mathbf{irow}[i-1] < \mathbf{irow}[i]$, or

$\mathbf{irow}[i-1] = \mathbf{irow}[i]$ and $\mathbf{icol}[i-1] < \mathbf{icol}[i]$, for $i = 1, 2, \ldots, \mathbf{nnz} - 1$.
Call nag_sparse_sym_sort (f11zbc) to reorder and sum or remove duplicates.

7 Accuracy

The accuracy of the factorization will be determined by the size of the elements that are dropped and the size of any modifications made to the diagonal elements. If these sizes are small then the computed factors will correspond to a matrix close to A. The factorization can generally be made more accurate by increasing **lfill**, or by reducing **dtol** with **lfill** < 0. If nag_sparse_sym_chol_fac (f11jac) is used in combination with nag_sparse_sym_chol_sol (f11jcc), the more accurate the factorization the fewer iterations will be required. However, the cost of the decomposition will also generally increase.

8 Parallelism and Performance

nag_sparse_sym_chol_fac (f11jac) is not threaded in any implementation.

9 Further Comments

The time taken for a call to nag_sparse_sym_chol_fac (f11jac) is roughly proportional to $\mathbf{nnzc}^2/\mathbf{n}$.

9.1 Control of Fill-in

If **lfill** ≥ 0 the amount of fill-in occurring in the incomplete factorization is controlled by limiting the maximum **level** of fill-in to **lfill**. The original nonzero elements of A are defined to be of level 0. The fill level of a new nonzero location occurring during the factorization is defined as:

$$k = \max(k_e, k_c) + 1,$$

where k_e is the level of fill of the element being eliminated, and k_c is the level of fill of the element causing the fill-in.

If **lfill** < 0 the fill-in is controlled by means of the **drop tolerance dtol**. A potential fill-in element a_{ij} occurring in row i and column j will not be included if:

$$|a_{ij}| < \mathbf{dtol} \times \sqrt{|a_{ii} a_{jj}|}.$$

For either method of control, any elements which are not included are discarded if **mic** = Nag_SparseSym_UnModFact, or subtracted from the diagonal element in the elimination row if **mic** = Nag_SparseSym_ModFact.

9.2 Choice of Parameters

There is unfortunately no choice of the various algorithmic arguments which is optimal for all types of symmetric matrix, and some experimentation will generally be required for each new type of matrix encountered.

If the matrix A is not known to have any particular special properties the following strategy is recommended. Start with **lfill** = 0, **mic** = Nag_SparseSym_UnModFact and **dscale** = 0.0. If the value returned for **npivm** is significantly larger than zero, i.e., a large number of pivot modifications were required to ensure that M was positive definite, the preconditioner is not likely to be satisfactory. In this case increase either **lfill** or **dscale** until **npivm** falls to a value close to zero. Once suitable values of **lfill** and **dscale** have been found try setting **mic** = Nag_SparseSym_ModFact to see if any improvement can be obtained by using **modified** incomplete Cholesky.

nag_sparse_sym_chol_fac (f11jac) is primarily designed for positive definite matrices, but may work for some mildly indefinite problems. If **npivm** cannot be satisfactorily reduced by increasing **lfill** or **dscale** then A is probably too indefinite for this function.

If A has non-positive off-diagonal elements, is nonsingular, and has only non-negative elements in its inverse, it is called an 'M-matrix'. It can be shown that no pivot modifications are required in the incomplete Cholesky factorization of an M-matrix (Meijerink and Van der Vorst (1977)). In this case a good preconditioner can generally be expected by setting **lfill** $= 0$, **mic** = Nag_SparseSym_ModFact and **dscale** $= 0.0$.

For certain mesh-based problems involving M-matrices it can be shown in theory that setting **mic** = Nag_SparseSym_ModFact, and choosing **dscale** appropriately can reduce the order of magnitude of the condition number of the preconditioned matrix as a function of the mesh steplength (Chan (1991)). In practise this property often holds even with **dscale** $= 0.0$, although an improvement in condition can result from increasing **dscale** slightly (Van der Vorst (1990)).

Some illustrations of the application of nag_sparse_sym_chol_fac (f11jac) to linear systems arising from the discretization of two-dimensional elliptic partial differential equations, and to random-valued randomly structured symmetric positive definite linear systems, can be found in Salvini and Shaw (1995).

9.3 Direct Solution of Positive Definite Systems

Although it is not their primary purpose, nag_sparse_sym_chol_fac (f11jac) and nag_sparse_sym_pre con_ichol_solve (f11jbc) may be used together to obtain a **direct** solution to a symmetric positive definite linear system. To achieve this the call to nag_sparse_sym_precon_ichol_solve (f11jbc) should be preceded by a **complete** Cholesky factorization

$$A = PLDL^{\mathrm{T}}P^{\mathrm{T}} = M.$$

A complete factorization is obtained from a call to nag_sparse_sym_chol_fac (f11jac) with **lfill** < 0 and **dtol** $= 0.0$, provided **npivm** $= 0$ on exit. A nonzero value of **npivm** indicates that A is not positive definite, or is ill-conditioned. A factorization with nonzero **npivm** may serve as a preconditioner, but will not result in a direct solution. It is therefore **essential** to check the output value of **npivm** if a direct solution is required.

The use of nag_sparse_sym_chol_fac (f11jac) and nag_sparse_sym_precon_ichol_solve (f11jbc) as a direct method is illustrated in Section 10 in nag_sparse_sym_precon_ichol_solve (f11jbc).

10 Example

This example program reads in a symmetric sparse matrix A and calls nag_sparse_sym_chol_fac (f11jac) to compute an incomplete Cholesky factorization. It then outputs the nonzero elements of both A and $C = L + D^{-1} - I$. The call to nag_sparse_sym_chol_fac (f11jac) has **lfill** $= 0$, **mic** = Nag_SparseSym_UnModFact, **dscale** $= 0.0$ and **pstrat** = Nag_SparseSym_MarkPiv, giving an unmodified zero-fill factorization of an unperturbed matrix, with Markowitz diagonal pivoting.

10.1 Program Text

```
/* nag_sparse_sym_chol_fac (f11jac) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 *
 */
```

```
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nag_string.h>
#include <nagf11.h>

int main(void)
{
  double dtol;
  double *a;
  double dscale;
  Integer *irow, *icol;
  Integer *ipiv, nnzc, *istr;
  Integer exit_status = 0, i, n, lfill, npivm;
  Integer nnz;
  Integer num;
  char nag_enum_arg[40];
  Nag_SparseSym_Piv pstrat;
  Nag_SparseSym_Fact mic;
  Nag_Sparse_Comm comm;
  NagError fail;

  INIT_FAIL(fail);

  printf("nag_sparse_sym_chol_fac (f11jac) Example Program Results\n\n");

  /* Skip heading in data file */
#ifdef _WIN32
  scanf_s("%*[^\n]");
#else
  scanf("%*[^\n]");
#endif

  /* Read algorithmic parameters */
#ifdef _WIN32
  scanf_s("%" NAG_IFMT "", &n);
#else
  scanf("%" NAG_IFMT "", &n);
#endif
#ifdef _WIN32
  scanf_s("%*[^\n]");
#else
  scanf("%*[^\n]");
#endif
#ifdef _WIN32
  scanf_s("%" NAG_IFMT "%*[^\n]", &nnz);
#else
  scanf("%" NAG_IFMT "%*[^\n]", &nnz);
#endif
#ifdef _WIN32
  scanf_s("%" NAG_IFMT "%lf%*[^\n]", &lfill, &dtol);
#else
  scanf("%" NAG_IFMT "%lf%*[^\n]", &lfill, &dtol);
#endif
#ifdef _WIN32
  scanf_s("%39s%lf%*[^\n]", nag_enum_arg, (unsigned)_countof(nag_enum_arg),
          &dscale);
#else
  scanf("%39s%lf%*[^\n]", nag_enum_arg, &dscale);
#endif
  /* nag_enum_name_to_value (x04nac).
   * Converts NAG enum member name to value
   */
  mic = (Nag_SparseSym_Fact) nag_enum_name_to_value(nag_enum_arg);
#ifdef _WIN32
  scanf_s("%39s%*[^\n]", nag_enum_arg, (unsigned)_countof(nag_enum_arg));
#else
  scanf("%39s%*[^\n]", nag_enum_arg);
#endif
  pstrat = (Nag_SparseSym_Piv) nag_enum_name_to_value(nag_enum_arg);
```

```
  /* Allocate memory */
  num = 2 * nnz;
  ipiv = NAG_ALLOC(n, Integer);
  istr = NAG_ALLOC(n + 1, Integer);
  irow = NAG_ALLOC(num, Integer);
  icol = NAG_ALLOC(num, Integer);
  a = NAG_ALLOC(num, double);

  if (!ipiv || !istr || !irow || !icol || !a) {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }

  /* Read the matrix a */

  for (i = 1; i <= nnz; ++i)
#ifdef _WIN32
    scanf_s("%lf%" NAG_IFMT "%" NAG_IFMT "%*[^\n]", &a[i - 1], &irow[i - 1],
            &icol[i - 1]);
#else
    scanf("%lf%" NAG_IFMT "%" NAG_IFMT "%*[^\n]", &a[i - 1], &irow[i - 1],
          &icol[i - 1]);
#endif

  /* Calculate incomplete Cholesky factorization */

  /* nag_sparse_sym_chol_fac (f11jac).
   * Incomplete Cholesky factorization (symmetric)
   */
  nag_sparse_sym_chol_fac(n, nnz, &a, &num, &irow, &icol, lfill, dtol, mic,
                          dscale, pstrat, ipiv, istr, &nnzc, &npivm, &comm,
                          &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_sparse_sym_chol_fac (f11jac).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }

  /* Output original matrix */

  printf(" Original Matrix \n");
  printf(" n     = %6" NAG_IFMT "\n", n);
  printf(" nnz   = %6" NAG_IFMT "\n\n", nnz);
  for (i = 1; i <= nnz; ++i)
    printf(" %8" NAG_IFMT "%16.4e%8" NAG_IFMT "%8" NAG_IFMT "\n", i, a[i - 1],
           irow[i - 1], icol[i - 1]);
  printf("\n");

  /* Output details of the factorization */
  printf(" Factorization\n n = %6" NAG_IFMT " \n nnz = %6" NAG_IFMT "\n", n,
         nnzc);
  printf(" npivm = %6" NAG_IFMT "\n\n", npivm);
  for (i = nnz + 1; i <= nnz + nnzc; ++i)
    printf(" %8" NAG_IFMT "%16.4e%8" NAG_IFMT "%8" NAG_IFMT "\n", i, a[i - 1],
           irow[i - 1], icol[i - 1]);

  printf("\n        i     ipiv(i) \n");
  for (i = 1; i <= n; ++i)
    printf(" %8" NAG_IFMT "%8" NAG_IFMT "\n", i, ipiv[i - 1]);

END:
  NAG_FREE(irow);
  NAG_FREE(icol);
  NAG_FREE(a);
  NAG_FREE(istr);
  NAG_FREE(ipiv);
  return exit_status;
}
```

10.2 Program Data

```
nag_sparse_sym_chol_fac (f11jac) Example Program Data
 7                               n
 16                              nnz
 0 0.0                           lfill, dtol
 Nag_SparseSym_UnModFact 0.0     mic, dscale
 Nag_SparseSym_MarkPiv           pstrat
  4.   1    1
  1.   2    1
  5.   2    2
  2.   3    3
  2.   4    2
  3.   4    4
 -1.   5    1
  1.   5    4
  4.   5    5
  1.   6    2
 -2.   6    5
  3.   6    6
  2.   7    1
 -1.   7    2
 -2.   7    3
  5.   7    7        a[i-1], irow[i-1], icol[i-1], i=1,...,nnz
```

10.3 Program Results

```
nag_sparse_sym_chol_fac (f11jac) Example Program Results

 Original Matrix
 n     =      7
 nnz   =     16

       1      4.0000e+00       1       1
       2      1.0000e+00       2       1
       3      5.0000e+00       2       2
       4      2.0000e+00       3       3
       5      2.0000e+00       4       2
       6      3.0000e+00       4       4
       7     -1.0000e+00       5       1
       8      1.0000e+00       5       4
       9      4.0000e+00       5       5
      10      1.0000e+00       6       2
      11     -2.0000e+00       6       5
      12      3.0000e+00       6       6
      13      2.0000e+00       7       1
      14     -1.0000e+00       7       2
      15     -2.0000e+00       7       3
      16      5.0000e+00       7       7

 Factorization
 n =      7
 nnz =     16
 npivm =      0

      17      5.0000e-01       1       1
      18      3.3333e-01       2       2
      19      3.3333e-01       3       2
      20      2.7273e-01       3       3
      21     -5.4545e-01       4       3
      22      5.2381e-01       4       4
      23     -2.7273e-01       5       3
      24      2.6829e-01       5       5
      25      6.6667e-01       6       2
      26      5.2381e-01       6       4
      27      2.6829e-01       6       5
      28      3.4788e-01       6       6
      29     -1.0000e+00       7       1
      30      5.3659e-01       7       5
      31     -5.3455e-01       7       6
```

```
    32      9.0461e-01       7        7

     i      ipiv(i)
     1        3
     2        4
     3        5
     4        6
     5        1
     6        2
     7        7
```
