nag_sparse_sym_chol_sol (f11jcc)

1. Purpose

nag_sparse_sym_chol_sol (f11jcc) solves a real sparse symmetric system of linear equations, represented in symmetric coordinate storage format, using a conjugate gradient or Lanczos method, with incomplete Cholesky preconditioning.

2. Specification

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

void nag_sparse_sym_chol_sol(Nag_SparseSym_Method method, Integer n,
             Integer nnz, double a[], Integer la, Integer irow[],
             Integer icol[], Integer ipiv[], Integer istr[], double b[],
             double tol, Integer maxitn, double x[], double *rnorm,
             Integer *itn, Nag_Sparse_Comm *comm, NagError *fail)
```

3. Description

This routine solves a real sparse symmetric linear system of equations:

$$Ax = b,$$

using a preconditioned conjugate gradient method (Meijerink and van der Vorst (1977)), or a preconditioned Lanczos method based on the algorithm SYMMLQ (Paige and Saunders (1975)). The conjugate gradient method is more efficient if A is positive-definite, but may fail to converge for indefinite matrices. In this case the Lanczos method should be used instead. For further details see Barrett *et al.* (1994).

nag_sparse_sym_chol_sol uses the incomplete Cholesky factorization determined by nag_sparse_sym_chol_fac (f11jac) as the preconditioning matrix. A call to nag_sparse_sym_chol_sol must always be preceeded by a call to nag_sparse_sym_chol_fac (f11jac). Alternative preconditioners for the same storage scheme are available by calling nag_sparse_sym_sol (f11jec).

The matrix A, and the preconditioning matrix M, are represented in symmetric coordinate storage (SCS) format (see Section 2.1.2. of the Chapter Introduction) in the arrays **a**, **irow** and **icol**, as returned from nag_sparse_sym_chol_fac (f11jac). The array **a** holds the non-zero entries in the lower triangular parts of these matrices, while **irow** and **icol** hold the corresponding row and column indices.

4. Parameters

method

Input: specifies the iterative method to be used. The possible choices are:

if **method** = **Nag_SparseSym_CG** then the conjugate gradient method is used;

if **method** = **Nag_SparseSym_Lanczos** then the Lanczos method, SYMMLQ is used.

Constraint: **method** = **Nag_SparseSym_CG** or **Nag_SparseSym_Lanczos**.

n

Input: the order of the matrix A. This **must** be the same value as was supplied in the preceding call to nag_sparse_sym_chol_fac (f11jac).
Constraint: $\mathbf{n} \geq 1$.

nnz

Input: the number of non-zero elements in the lower triangular part of the matrix A. This **must** be the same value as was supplied in the preceding call to nag_sparse_sym_chol_fac (f11jac).

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

a[la]

Input: the values returned in array **a** by a previous call to nag_sparse_sym_chol_fac (f11jac).

la

Input: the dimension of the arrays **a**, **irow** and **icol**, this **must** be the same value as returned by a previous call to nag_sparse_sym_chol_fac (f11jac).

Constraint: **la** $\geq 2 \times$ **nnz**.

irow[la]

icol[la]

ipiv[n]

istr[n+1]

Input: the values returned in the arrays **irow**, **icol**, **ipiv** and **istr** by a previous call to nag_sparse_sym_chol_fac (f11jac).

b[n]

Input: the right-hand side vector b.

tol

Input: the required tolerance. Let x_k denote the approximate solution at iteration k, and r_k the corresponding residual. The algorithm is considered to have converged at iteration k if:

$$\|r_k\|_\infty \leq \tau \times (\|b\|_\infty + \|A\|_\infty \|x_k\|_\infty).$$

If **tol** ≤ 0.0, $\tau = \max(\sqrt{\epsilon}, \sqrt{\mathbf{n}}\,\epsilon)$ is used, where ϵ is the ***machine precision***. Otherwise $\tau = \max(\mathbf{tol}, 10\epsilon, \sqrt{\mathbf{n}}\,\epsilon)$ is used.
Constraint: **tol** < 1.0.

maxitn

Input: the maximum number of iterations allowed.

Constraint: **maxitn** ≥ 1.

x[n]

Input: an initial approximation to the solution vector x.

Output: an improved approximation to the solution vector x.

rnorm

Output: the final value of the residual norm $\|r_k\|_\infty$, where k is the output value of **itn**.

itn

Output: the number of iterations carried out.

comm

Input/Output: a pointer to a structure of type **Nag_Sparse_Comm** whose members are used by the iterative solver.

fail

The NAG error parameter, see the Essential Introduction to the NAG C Library.

5. Error Indications and Warnings

NE_BAD_PARAM

On entry, parameter **method** had an illegal value.

NE_INT_ARG_LT

On entry, **n** must not be less than 1: **n** = ⟨*value*⟩.
On entry, **maxitn** must not be less than 1: **maxitn** = ⟨*value*⟩.

NE_INT_2

On entry, **nnz** = ⟨*value*⟩, **n** = ⟨*value*⟩.
Constraint: $1 \leq$ **nnz** $\leq$ **n** $\times$ (**n**+1)/2.

NE_REAL_ARG_GE

On entry, **tol** must not be greater than or equal to 1.0: **tol** = ⟨*value*⟩.

NE_2_INT_ARG_LT

On entry, **la** = ⟨*value*⟩ while **nnz** = ⟨*value*⟩.
These parameters must satisfy **la** $\geq 2 \times$ **nnz**.

NE_INVALID_SCS

The SCS representation of the matrix A is invalid. Check that the call to nag_sparse_sym_chol_sol has been preceded by a valid call to nag_sparse_sym_chol_fac (f11jac), and that the arrays **a**, **irow** and **icol** have not been corrupted between the two calls.

NE_INVALID_SCS_PRECOND

The SCS representation of the preconditioning matrix M is invalid. Check that the call to nag_sparse_sym_chol_sol has been preceded by a valid call to nag_sparse_sym_chol_fac (f11jac), and that the arrays **a**, **irow**, **icol**, **ipiv** and **istr** have not been corrupted between the two calls.

NE_PRECOND_NOT_POS_DEF

The preconditioner appears not to be positive-definite.

NE_COEFF_NOT_POS_DEF

The matrix of coefficients appears not to be positive-definite.

NE_ACC_LIMIT

The required accuracy could not be obtained. However, a reasonable accuracy has been obtained and further iterations cannot improve the result.

NE_NOT_REQ_ACC

The required accuracy has not been obtained in **maxitn** iterations.

NE_ALLOC_FAIL

Memory allocation failed.

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 consult NAG for assistance.

6. Further Comments

The time taken by nag_sparse_sym_chol_sol for each iteration is roughly proportional to the value of **nnzc** returned from the preceding call to nag_sparse_sym_chol_fac (f11jac). One iteration with the Lanczos method (SYMMLQ) requires a slightly larger number of operations than one iteration with the conjugate gradient method.

The number of iterations required to achieve a prescribed accuracy cannot be easily determined a priori, as it can depend dramatically on the conditioning and spectrum of the preconditioned matrix of the coefficients $\bar{A} = M^{-1}A$.

Some illustrations of the application of nag_sparse_sym_chol_sol 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).

6.1. Accuracy

On successful termination, the final residual $r_k = b - Ax_k$, where $k =$ **itn**, satisfies the termination criterion

$$\|r_k\|_\infty \leq \tau \times (\|b\|_\infty + \|A\|_\infty \|x_k\|_\infty).$$

The value of the final residual norm is returned in **rnorm**.

6.2. References

Barrett R, Berry M, Chan T F, Demmel J, Donato J, Dongarra J, Eijkhout V, Pozo R, Romine C and van der Vorst H (1994) *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods* SIAM, Philadelphia.

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.

Paige C C and Saunders M A (1975) Solution of sparse indefinite systems of linear equations *SIAM J. Numer. Anal.* **12** 617–629.

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*, NAG Ltd, Oxford.

7. See Also

nag_sparse_sym_chol_fac (f11jac)
nag_sparse_sym_sol (f11jec)
nag_sparse_sym_sort (f11zbc)

8. Example

This example program solves a symmetric positive-definite system of equations using the conjugate gradient method, with incomplete Cholesky preconditioning.

8.1. Program Text

```
/* nag_sparse_sym_chol_sol (f11jcc) Example Program.
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 *
 */
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nag_string.h>
#include <nagf11.h>

main()
{
  double dtol;
  double *a=0, *b=0;
  double *x=0;
  double rnorm, dscale;
  double tol;

  Integer *icol=0;
  Integer *ipiv=0, nnzc, *irow=0, *istr=0;
  Integer i;
  Integer n;
  Integer lfill, npivm;
  Integer maxitn;
  Integer itn;
  Integer nnz;
  Integer num;

  Nag_SparseSym_Method method;
  Nag_SparseSym_Piv pstrat;
  Nag_SparseSym_Fact mic;
  Nag_Sparse_Comm comm;

  char char_enum[20];

  Vprintf("f11jcc Example Program Results\n");

  /*  Skip heading in data file  */
  Vscanf(" %*[^\n]");

  /*  Read algorithmic parameters */
  Vscanf("%ld%*[^\n]",&n);
  Vscanf("%ld%*[^\n]",&nnz);
  Vscanf("%ld%lf%*[^\n]",&lfill, &dtol);
  Vscanf("%s%*[^\n]",char_enum);
  if (!strcmp(char_enum, "CG"))
    method = Nag_SparseSym_CG;
  else if (!strcmp(char_enum, "Lanczos"))
    method = Nag_SparseSym_Lanczos;
  else
    {
      Vprintf("Unrecognised string for method enum representation.\n");
      exit (EXIT_FAILURE);
    }
```

```
Vscanf("%s%lf%*[^\n]",char_enum, &dscale);
if (!strcmp(char_enum, "ModFact"))
  mic = Nag_SparseSym_ModFact;
else if (!strcmp(char_enum, "UnModFact"))
  mic = Nag_SparseSym_UnModFact;
else
  {
    Vprintf("Unrecognised string for mic enum representation.\n");
    exit (EXIT_FAILURE);
  }

Vscanf("%s%*[^\n]",char_enum);
if (!strcmp(char_enum, "NoPiv"))
  pstrat = Nag_SparseSym_NoPiv;
else if (!strcmp(char_enum, "MarkPiv"))
  pstrat = Nag_SparseSym_MarkPiv;
else if (!strcmp(char_enum, "UserPiv"))
  pstrat = Nag_SparseSym_UserPiv;
else
  {
    Vprintf("Unrecognised string for pstrat enum representation.\n");
    exit (EXIT_FAILURE);
  }

Vscanf("%lf%ld%*[^\n]",&tol, &maxitn);

/*  Read the matrix a */

num = 2 * nnz;
irow = NAG_ALLOC(num,Integer);
icol = NAG_ALLOC(num,Integer);
a = NAG_ALLOC(num,double);
b = NAG_ALLOC(n,double);
x = NAG_ALLOC(n,double);
istr = NAG_ALLOC(n+1,Integer);
ipiv = NAG_ALLOC(num,Integer);

if (!irow || !icol || !a || !x || !istr ||!ipiv)
  {
    Vprintf("Allocation failure\n");
    exit (EXIT_FAILURE);
  }

for (i = 1; i <= nnz; ++i)
  Vscanf("%lf%ld%ld%*[^\n]",&a[i-1], &irow[i-1], &icol[i-1]);

/*  Read right-hand side vector b and initial approximate solution x */

for (i = 1; i <= n; ++i)
  Vscanf("%lf",&b[i-1]);
Vscanf(" %*[^\n]");

for (i = 1; i <= n; ++i)
  Vscanf("%lf",&x[i-1]);
Vscanf("%*[^\n]");

/*  Calculate incomplete Cholesky factorization */

f11jac(n, nnz, &a, &num, &irow, &icol, lfill, dtol, mic,
       dscale, pstrat, ipiv, istr, &nnzc, &npivm, &comm, NAGERR_DEFAULT);

/*  Solve Ax = b */

f11jcc(method, n, nnz, a, num, irow, icol, ipiv, istr, b,
       tol, maxitn, x, &rnorm, &itn, &comm, NAGERR_DEFAULT);

Vprintf(" %s%10ld%s\n","Converged in",itn," iterations");
Vprintf(" %s%16.3e\n","Final residual norm =",rnorm);
```

```
  /*  Output x */

  for (i = 1; i <= n; ++i)
    Vprintf(" %16.4e\n",x[i-1]);

  NAG_FREE(irow);
  NAG_FREE(icol);
  NAG_FREE(a);
  NAG_FREE(b);
  NAG_FREE(x);
  NAG_FREE(ipiv);
  NAG_FREE(istr);
  exit (EXIT_SUCCESS);
}
```

8.2. Program Data

```
f11jcc Example Program Data
  7                     n
  16                    nnz
  1 0.0                 lfill, dtol
  CG                    method
  UnModFact 0.0         mic  dscale
  MarkPiv               pstrat
  1.0e-6 100            tol, maxitn
  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
 15.  18.  -8.  21.
 11.  10.  29.          b[i-1], i=1,...,n
  0.   0.   0.   0.
  0.   0.   0.          x[i-1], i=1,...,n
```

8.3. Program Results

```
f11jcc Example Program Results
 Converged in         1 iterations
 Final residual norm =       7.105e-15
       1.0000e+00
       2.0000e+00
       3.0000e+00
       4.0000e+00
       5.0000e+00
       6.0000e+00
       7.0000e+00
```