NAG Library Function Document

nag_sparse_sym_sol (f11jec)

1 Purpose

nag_sparse_sym_sol (f11jec) solves a real sparse symmetric system of linear equations, represented in symmetric coordinate storage format, using a conjugate gradient or Lanczos method, without preconditioning, with Jacobi or with SSOR preconditioning.

2 Specification

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

```
void nag_sparse_sym_sol (Nag_SparseSym_Method method,
     Nag_SparseSym_PrecType precon, Integer n, Integer nnz, const double a[],
     const Integer irow[], const Integer icol[], double omega,
     const double b[], double tol, Integer maxitn, double x[], double *rnorm,
     Integer *itn, Nag_Sparse_Comm *comm, NagError *fail)
```

3 Description

nag_sparse_sym_sol (f11jec) solves a real sparse symmetric linear system of equations:

$$Ax = b,$$

using a preconditioned conjugate gradient method (see Barrett *et al.* (1994)), 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).

The function allows the following choices for the preconditioner:

no preconditioning;

Jacobi preconditioning (see Young (1971);

symmetric successive-over-relaxation (SSOR) preconditioning (see Young (1971)).

For incomplete Cholesky (IC) preconditioning see nag_sparse_sym_chol_sol (f11jcc).

The matrix A is represented in symmetric coordinate storage (SCS) format (see the f11 Chapter Introduction) in the arrays **a**, **irow** and **icol**. The array **a** holds the nonzero entries in the lower triangular part of the matrix, while **irow** and **icol** hold the corresponding row and column indices.

4 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

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

Young D (1971) *Iterative Solution of Large Linear Systems* Academic Press, New York

5 Arguments

1: **method** – Nag_SparseSym_Method *Input*

On entry: specifies the iterative method to be used.

method = Nag_SparseSym_CG
The conjugate gradient method is used.

method = Nag_SparseSym_Lanczos
The Lanczos method (SYMMLQ) is used.

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

2: **precon** – Nag_SparseSym_PrecType *Input*

On entry: specifies the type of preconditioning to be used.

precon = Nag_SparseSym_NoPrec
No preconditioning is used.

precon = Nag_SparseSym_SSORPrec
Symmetric successive-over-relaxation is used.

precon = Nag_SparseSym_JacPrec
Jacobi preconditioning is used.

Constraint: **precon** = Nag_SparseSym_NoPrec, Nag_SparseSym_SSORPrec or Nag_SparseSym_JacPrec.

3: **n** – Integer *Input*

On entry: the order of the matrix A.

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

4: **nnz** – Integer *Input*

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

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

5: **a**[**nnz**] – const double *Input*

On entry: the nonzero elements of 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.

6: **irow**[**nnz**] – const Integer *Input*
7: **icol**[**nnz**] – const Integer *Input*

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 $1 \leq \mathbf{icol}[i] \leq \mathbf{irow}[i]$, 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 $i = 1, 2, \ldots, \mathbf{nnz} - 1$.

8: **omega** – double *Input*

On entry: if **precon** = Nag_SparseSym_SSORPrec, **omega** is the relaxation argument ω to be used in the SSOR method. Otherwise **omega** need not be initialized.

Constraint: $0.0 \leq \mathbf{omega} \leq 2.0$.

9: **b**[**n**] – const double *Input*

On entry: the right-hand side vector b.

10: **tol** – double *Input*

On entry: 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:

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

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

Constraint: $\mathbf{tol} < 1.0$.

11: **maxitn** – Integer *Input*

On entry: the maximum number of iterations allowed.

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

12: **x**[**n**] – double *Input/Output*

On entry: an initial approximation of the solution vector x.

On exit: an improved approximation to the solution vector x.

13: **rnorm** – double * *Output*

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

14: **itn** – Integer * *Output*

On exit: the number of iterations carried out.

15: **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.

16: **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_ACC_LIMIT

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

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_BAD_PARAM

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

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

NE_COEFF_NOT_POS_DEF

The matrix of coefficients appears not to be positive definite (conjugate gradient method only).

NE_INT_2

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

NE_INT_ARG_LT

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

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_NOT_REQ_ACC

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

NE_PRECOND_NOT_POS_DEF

The preconditioner appears not to be positive definite.

NE_REAL

On entry, **omega** $= \langle value \rangle$.
Constraint: $0.0 \leq$ **omega** ≤ 2.0.

NE_REAL_ARG_GE

On entry, **tol** must not be greater than or equal to 1.0: **tol** $= \langle value \rangle$.

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:

$1 \leq$ **irow**$[i] \leq$ **n** and $1 \leq$ **icol**$[i] \leq$ **irow**$[i]$, for $i = 0, 1, \ldots,$ **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** $- 1$.

Call nag_sparse_sym_sort (f11zbc) to reorder and sum or remove duplicates.

NE_ZERO_DIAGONAL_ELEM

The matrix A has a zero diagonal element. Jacobi and SSOR preconditioners are not appropriate for this problem.

7 Accuracy

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

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

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

8 Parallelism and Performance

nag_sparse_sym_sol (f11jec) is not threaded in any implementation.

9 Further Comments

The time taken by nag_sparse_sym_sol (f11jec) for each iteration is roughly proportional to **nnz**. 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 $\bar{A} = M^{-1}A$.

10 Example

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

10.1 Program Text

```
/* nag_sparse_sym_sol (f11jec) 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 *a = 0, *b = 0, *x = 0;
  double omega;
  double rnorm;
  double tol;
  Integer exit_status = 0;
  Integer *icol, *irow;
  Integer i, n, maxitn, itn, nnz;
  char nag_enum_arg[40];
  Nag_SparseSym_Method method;
  Nag_SparseSym_PrecType precon;
  Nag_Sparse_Comm comm;
  NagError fail;

  INIT_FAIL(fail);

  printf("nag_sparse_sym_sol (f11jec) Example Program Results\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]", &n);
#else
  scanf("%" NAG_IFMT "%*[^\n]", &n);
#endif
#ifdef _WIN32
  scanf_s("%" NAG_IFMT "%*[^\n]", &nnz);
#else
```

```
  scanf("%" NAG_IFMT "%*[^\n]", &nnz);
#endif

#ifdef _WIN32
  scanf_s("%39s", nag_enum_arg, (unsigned)_countof(nag_enum_arg));
#else
  scanf("%39s", nag_enum_arg);
#endif
  /* nag_enum_name_to_value (x04nac).
   * Converts NAG enum member name to value
   */
  method = (Nag_SparseSym_Method) 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
  precon = (Nag_SparseSym_PrecType) nag_enum_name_to_value(nag_enum_arg);

#ifdef _WIN32
  scanf_s("%lf%*[^\n]", &omega);
#else
  scanf("%lf%*[^\n]", &omega);
#endif
#ifdef _WIN32
  scanf_s("%lf%" NAG_IFMT "%*[^\n]", &tol, &maxitn);
#else
  scanf("%lf%" NAG_IFMT "%*[^\n]", &tol, &maxitn);
#endif

  /* Allocate memory */
  x = NAG_ALLOC(n, double);
  b = NAG_ALLOC(n, double);
  a = NAG_ALLOC(nnz, double);
  irow = NAG_ALLOC(nnz, Integer);
  icol = NAG_ALLOC(nnz, Integer);
  if (!irow || !icol || !a || !x || !b) {
    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

  /* Read right-hand side vector b and initial approximate solution x */
  for (i = 1; i <= n; ++i)
#ifdef _WIN32
    scanf_s("%lf", &b[i - 1]);
#else
    scanf("%lf", &b[i - 1]);
#endif
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif

  for (i = 1; i <= n; ++i)
#ifdef _WIN32
    scanf_s("%lf", &x[i - 1]);
#else
    scanf("%lf", &x[i - 1]);
#endif
```

```
#ifdef _WIN32
  scanf_s(" %*[^\n]");
#else
  scanf(" %*[^\n]");
#endif

  /* Solve Ax = b  */
  /* nag_sparse_sym_sol (f11jec).
   * Solver with Jacobi, SSOR, or no preconditioning
   * (symmetric)
   */
  nag_sparse_sym_sol(method, precon, n, nnz, a, irow, icol, omega, b, tol,
                     maxitn, x, &rnorm, &itn, &comm, &fail);

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

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

END:
  NAG_FREE(irow);
  NAG_FREE(icol);
  NAG_FREE(a);
  NAG_FREE(x);
  NAG_FREE(b);

  return exit_status;
}
```

10.2 Program Data

```
nag_sparse_sym_sol (f11jec) Example Program Data
  7                                           n
  16                                          nnz
  Nag_SparseSym_CG Nag_SparseSym_SSORPrec  method, precon
  1.1                                         omega
  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
```

10.3 Program Results

```
nag_sparse_sym_sol (f11jec) Example Program Results
 Converged in         6 iterations
 Final residual norm =       5.026e-06
       1.0000e-00
       2.0000e+00
       3.0000e+00
       4.0000e+00
       5.0000e+00
       6.0000e+00
       7.0000e+00
```