F11JEF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

F11JEF 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

```
 SUBROUTINE F11JEF(METHOD, PRECON, N, NNZ, A, IROW, ICOL, OMEGA, B,
1                  TOL, MAXITN, X, RNORM, ITN, WORK, LWORK, IWORK,
2                  IFAIL)
 INTEGER           N, NNZ, IROW(NNZ), ICOL(NNZ), MAXITN, ITN,
1                  IWORK(N+1), LWORK, IFAIL
 real              A(NNZ), OMEGA, B(N), TOL, X(N), RNORM,
1                  WORK(LWORK)
 CHARACTER*(*)     METHOD
 CHARACTER*1       PRECON
```

3 Description

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

$$Ax = b,$$

using a preconditioned conjugate gradient method [1], or a preconditioned Lanczos method based on the algorithm SYMMLQ [2]. 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 [1].

The routine allows the following choices for the preconditioner:

no preconditioning;

Jacobi preconditioning [3];

symmetric successive-over-relaxation (SSOR) preconditioning [3].

For incomplete Cholesky (IC) preconditioning see F11JCF.

The matrix A is represented in symmetric coordinate storage (SCS) format (see Section 2.1.2 of the Chapter Introduction) in the arrays A, IROW and ICOL. The array A holds the non-zero entries in the lower triangular part of the matrix, while IROW and ICOL hold the corresponding row and column indices.

4 References

[1] 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

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

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

5 Parameters

1: METHOD — CHARACTER*(*) *Input*

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

'CG' conjugate gradient method;
'SYMMLQ' Lanczos method (SYMMLQ).

Constraint: METHOD = 'CG' or 'SYMMLQ'.

2: PRECON — CHARACTER*1 *Input*

On entry: specifies the type of preconditioning to be used. The possible choices are:

'N' no preconditioning;
'J' Jacobi;
'S' symmetric successive-over-relaxation (SSOR).

Constraint: PRECON = 'N', 'J' or 'S'.

3: N — INTEGER *Input*

On entry: n, the order of the matrix A.

Constraint: N $\geq$ 1.

4: NNZ — INTEGER *Input*

On entry: the number of non-zero elements in the lower triangular part of the matrix A.

Constraint: 1 $\leq$ NNZ $\leq$ N $\times$ (N+1)/2.

5: A(NNZ) — ***real*** array *Input*

On entry: the non-zero 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 routine F11ZBF may be used to order the elements in this way.

6: IROW(NNZ) — INTEGER array *Input*
7: ICOL(NNZ) — INTEGER array *Input*

On entry: the row and column indices of the non-zero elements supplied in A.

Constraints: IROW and ICOL must satisfy the following constraints (which may be imposed by a call to F11ZBF):

1 $\leq$ IROW(i) $\leq$ N and 1 $\leq$ ICOL(i) $\leq$ IROW(i), for $i = 1, 2, \ldots$,NNZ.
IROW($i-1$) < IROW(i), or
IROW($i-1$) = IROW(i) and ICOL($i-1$) < ICOL(i), for $i = 2, 3, \ldots$,NNZ.

8: OMEGA — ***real*** *Input*

On entry: if PRECON = 'S', OMEGA is the relaxation parameter ω to be used in the SSOR method. Otherwise OMEGA need not be initialized.

Constraint: 0.0 $\leq$ OMEGA $\leq$ 2.0.

9: B(N) — ***real*** array *Input*

On entry: the right-hand side vector b.

10: TOL — ***real*** *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:

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

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

Constraint: TOL < 1.0.

11: MAXITN — INTEGER *Input*

On entry: the maximum number of iterations allowed.

Constraint: MAXITN ≥ 1.

12: X(N) — ***real*** array *Input/Output*

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

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

13: RNORM — ***real*** *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: WORK(LWORK) — ***real*** array *Workspace*

16: LWORK — INTEGER *Input*

On entry: the dimension of the array WORK as declared in the (sub)program from which F11JEF is called.

Constraints:

if METHOD = 'CG' then LWORK $\ge 6 \times \mathrm{N} + \nu + 120$;
if METHOD = 'SYMMLQ' then LWORK $\ge 7 \times \mathrm{N} + \nu + 120$;

where $\nu = \mathrm{N}$ for PRECON = 'J' or 'S', and 0 otherwise.

17: IWORK(N+1) — INTEGER array *Workspace*

18: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Errors and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors detected by the routine:

IFAIL = 1

On entry, METHOD $\ne$ 'CG' or 'SYMMLQ',
or PRECON $\ne$ 'N', 'J' or 'S',
or N < 1,
or NNZ < 1,

or NNZ > N × (N+1)/2,

or OMEGA lies outside the interval $[0.0, 2.0]$,

or TOL $\geq$ 1.0,

or MAXITN $<$ 1,

or LWORK too small.

IFAIL = 2

On entry, the arrays IROW and ICOL fail to satisfy the following constraints:

$1 \leq$ IROW$(i) \leq$ N and $1 \leq$ ICOL$(i) \leq$ IROW(i), for $i = 1, 2, \ldots,$NNZ.
IROW$(i-1) <$ IROW(i), or
IROW$(i-1) =$ IROW(i) and ICOL$(i-1) <$ ICOL(i), for $i = 2, 3, \ldots,$NNZ.

Therefore a non-zero element has been supplied which does not lie in the lower triangular part of A, is out of order, or has duplicate row and column indices. Call F11ZBF to reorder and sum or remove duplicates.

IFAIL = 3

On entry, the matrix A has a zero diagonal element. Jacobi and SSOR preconditioners are not appropriate for this problem.

IFAIL = 4

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

IFAIL = 5

Required accuracy not obtained in MAXITN iterations.

IFAIL = 6

The preconditioner appears not to be positive-definite.

IFAIL = 7

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

IFAIL = 8

A serious error has occurred in an internal call to F11GAF, F11GBF or F11GCF. Check all subroutine calls and array sizes. Seek expert help.

7 Accuracy

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

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

The value of the final residual norm is returned in RNORM.

8 Further Comments

The time taken by F11JEF 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 $\bar{A} = M^{-1}A$.

9 Example

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

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     F11JEF Example Program Text
*     Mark 19 Revised. NAG Copyright 1999.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, LA, LWORK
      PARAMETER        (NMAX=1000,LA=10000,LWORK=7*NMAX+120)
*     .. Local Scalars ..
      real             OMEGA, RNORM, TOL
      INTEGER          I, IFAIL, ITN, MAXITN, N, NNZ
      CHARACTER        PRECON
      CHARACTER*6      METHOD
*     .. Local Arrays ..
      real             A(LA), B(NMAX), WORK(LWORK), X(NMAX)
      INTEGER          ICOL(LA), IROW(LA), IWORK(NMAX+1)
*     .. External Subroutines ..
      EXTERNAL         F11JEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F11JEF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
*
*     Read algorithmic parameters
*
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
         READ (NIN,*) NNZ
         READ (NIN,*) METHOD, PRECON
         READ (NIN,*) OMEGA
         READ (NIN,*) TOL, MAXITN
*
*     Read the matrix A
*
         DO 20 I = 1, NNZ
            READ (NIN,*) A(I), IROW(I), ICOL(I)
   20    CONTINUE
*
*     Read right-hand side vector b and initial approximate solution x
*
         READ (NIN,*) (B(I),I=1,N)
         READ (NIN,*) (X(I),I=1,N)
*
*     Solve Ax = b using F11JEF
*
         IFAIL = 0
         CALL F11JEF(METHOD,PRECON,N,NNZ,A,IROW,ICOL,OMEGA,B,TOL,MAXITN,
     +               X,RNORM,ITN,WORK,LWORK,IWORK,IFAIL)
*
```

```
         WRITE (NOUT,99999) 'Converged in', ITN, ' iterations'
         WRITE (NOUT,99998) 'Final residual norm =', RNORM
*
*     Output x
*
         DO 40 I = 1, N
            WRITE (NOUT,99997) X(I)
   40    CONTINUE
      END IF
      STOP
*
99999 FORMAT (1X,A,I10,A)
99998 FORMAT (1X,A,1P,e16.3)
99997 FORMAT (1X,1P,e16.4)
      END
```

9.2 Program Data

```
F11JEF Example Program Data
  7                  N
  16                 NNZ
 'CG' 'SSOR'          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), IROW(I), ICOL(I), I=1,...,NNZ
 15.  18.  -8.  21.
 11.  10.  29.        B(I), I=1,...,N
  0.   0.   0.   0.
  0.   0.   0.        X(I), I=1,...,N
```

9.3 Program Results

```
F11JEF 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
```