NAG Library Routine Document

F11JDF

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

F11JDF solves a system of linear equations involving the preconditioning matrix corresponding to SSOR applied to a real sparse symmetric matrix, represented in symmetric coordinate storage format.

2 Specification

3 Description

F11JDF solves a system of equations

$$Mx = y$$

involving the preconditioning matrix

$$M = \frac{1}{\omega(2-\omega)}(D+\omega L)D^{-1}(D+\omega L)^{\mathrm{T}}$$

corresponding to symmetric successive-over-relaxation (SSOR) (see Young (1971)) on a linear system Ax = b, where A is a sparse symmetric matrix stored in symmetric coordinate storage (SCS) format (see Section 2.1.2 in the F11 Chapter Introduction).

In the definition of M given above D is the diagonal part of A, L is the strictly lower triangular part of A, and ω is a user-defined relaxation parameter.

It is envisaged that a common use of F11JDF will be to carry out the preconditioning step required in the application of F11GEF to sparse linear systems. For an illustration of this use of F11JDF see the example program given in Section 10.1. F11JDF is also used for this purpose by the Black Box routine F11JEF.

4 References

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

5 Parameters

1: N – INTEGER Input

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

Constraint: $N \ge 1$.

2: NNZ – INTEGER Input

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

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

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3: A(NNZ) – REAL (KIND=nag wp) array

Input

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 routine F11ZBF may be used to order the elements in this way.

4: IROW(NNZ) – INTEGER array

Input

5: ICOL(NNZ) – INTEGER array

Input

On entry: the row and column indices of the nonzero elements supplied in array A.

Constraints:

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

$$1 \leq \text{IROW}(i) \leq \text{N}$$
 and $1 \leq \text{ICOL}(i) \leq \text{IROW}(i)$, for $i = 1, 2, \dots, \text{NNZ}$; $\text{IROW}(i-1) < \text{IROW}(i)$ or $\text{IROW}(i-1) = \text{IROW}(i)$ and $\text{ICOL}(i-1) < \text{ICOL}(i)$, for $i = 2, 3, \dots, \text{NNZ}$.

6: RDIAG(N) – REAL (KIND=nag_wp) array

Input

On entry: the elements of the diagonal matrix D^{-1} , where D is the diagonal part of A.

7: OMEGA – REAL (KIND=nag_wp)

Input

On entry: the relaxation parameter ω .

Constraint: 0.0 < OMEGA < 2.0.

8: CHECK - CHARACTER(1)

Input

On entry: specifies whether or not the input data should be checked.

CHECK = 'C'

Checks are carried out on the values of N, NNZ, IROW, ICOL and OMEGA.

CHECK = 'N'

None of these checks are carried out.

See also Section 9.2.

Constraint: CHECK = 'C' or 'N'.

9: $Y(N) - REAL (KIND=nag_wp) array$

Input

On entry: the right-hand side vector y.

10: $X(N) - REAL (KIND=nag_wp) array$

Output

On exit: the solution vector x.

11: IWORK(N + 1) - INTEGER array

Workspace

12: IFAIL - INTEGER

Input/Output

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this parameter, the recommended value is 0. When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.

On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

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6 Error Indicators 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 or warnings detected by the routine:

IFAIL = 1

On entry, CHECK \neq 'C' or 'N'.

IFAIL = 2

On entry, N < 1, or NNZ < 1, or NNZ > N \times (N + 1)/2, or OMEGA lies outside the interval (0.0, 2.0),

IFAIL = 3

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

```
1 \leq \text{IROW}(i) \leq \text{N} and 1 \leq \text{ICOL}(i) \leq \text{IROW}(i), for i = 1, 2, \dots, \text{NNZ}; \text{IROW}(i-1) < \text{IROW}(i) or \text{IROW}(i-1) = \text{IROW}(i) and \text{ICOL}(i-1) < \text{ICOL}(i), for i = 2, 3, \dots, \text{NNZ}.
```

Therefore a nonzero 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.

$$IFAIL = -99$$

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.8 in the Essential Introduction for further information.

$$IFAIL = -399$$

Your licence key may have expired or may not have been installed correctly.

See Section 3.7 in the Essential Introduction for further information.

$$IFAIL = -999$$

Dynamic memory allocation failed.

See Section 3.6 in the Essential Introduction for further information.

7 Accuracy

The computed solution x is the exact solution of a perturbed system of equations $(M + \delta M)x = y$, where

$$|\delta M| \le c(n)\epsilon |D + \omega L| |D^{-1}| |(D + \omega L)^{\mathsf{T}}|,$$

c(n) is a modest linear function of n, and ϵ is the machine precision.

8 Parallelism and Performance

Not applicable.

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9 Further Comments

9.1 Timing

The time taken for a call to F11JDF is proportional to NNZ.

9.2 Use of CHECK

It is expected that a common use of F11JDF will be to carry out the preconditioning step required in the application of F11GEF to sparse symmetric linear systems. In this situation F11JDF is likely to be called many times with the same matrix M. In the interests of both reliability and efficiency, you are recommended to set CHECK = 'C' for the first of such calls, and to set CHECK = 'N' for all subsequent calls.

10 Example

This example solves a sparse symmetric linear system of equations

$$Ax = b$$
,

using the conjugate-gradient (CG) method with SSOR preconditioning.

The CG algorithm itself is implemented by the reverse communication routine F11GEF, which returns repeatedly to the calling program with various values of the parameter IREVCM. This parameter indicates the action to be taken by the calling program.

If IREVCM = 1, a matrix-vector product v = Au is required. This is implemented by a call to F11XEF.

If IREVCM = 2, a solution of the preconditioning equation Mv = u is required. This is achieved by a call to F11JDF.

If IREVCM = 4, F11GEF has completed its tasks. Either the iteration has terminated, or an error condition has arisen.

For further details see the routine document for F11GEF.

10.1 Program Text

```
Program f11jdfe
1
     F11JDF Example Program Text
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!
!
      .. Use Statements ..
     Use nag_library, Only: f11gdf, f11gef, f11gff, f11jdf, f11xef, nag_wp
      .. Implicit None Statement ..
!
     Implicit None
      .. Parameters ..
                                       :: nin = 5, nout = 6
     Integer, Parameter
      .. Local Scalars ..
                                       :: anorm, omega, sigerr, sigmax,
     Real (Kind=nag_wp)
                                                                                 &
                                           sigtol, stplhs, stprhs, tol
     Integer
                                        :: i, ifail, ifail1, irevcm, iterm,
                                                                                 &
                                           itn, its, liwork, lwneed, lwork,
                                          maxitn, maxits, monit, n, nnz
     Character (1)
                                        :: ckjdf, ckxef, norm, precon, sigcmp,
                                           weight
      Character (6)
                                        :: method
!
      .. Local Arrays ..
     Real (Kind=nag_wp), Allocatable :: a(:), b(:), rdiag(:), wgt(:),
                                         work(:), x(:)
      Integer, Allocatable
                                        :: icol(:), irow(:), iwork(:)
!
      .. Executable Statements ..
     Write (nout,*) 'F11JDF Example Program Results'
     Skip heading in data file
```

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```
Read (nin,*)
     Read algorithmic parameters
     Read (nin,*) n
     Read (nin,*) nnz
      liwork = n + 1
      lwork = 6*n + 120
     Allocate (a(nnz),b(n),rdiag(n),wgt(n),work(lwork),x(n),icol(nnz), &
        irow(nnz),iwork(liwork))
     Read (nin,*) method
     Read (nin,*) precon, sigcmp, norm, iterm
     Read (nin,*) tol, maxitn
     Read (nin,*) anorm, sigmax
     Read (nin,*) sigtol, maxits
     Read (nin,*) omega
     Read the matrix A
     Do i = 1, nnz
       Read (nin,*) a(i), irow(i), icol(i)
     End Do
     Read right-hand side vector b and initial approximate solution x
!
     Read (nin,*) b(1:n)
     Read (nin,*) x(1:n)
     Call F11GDF to initialize solver
     weight = 'N'
     monit = 0
      ifail: behaviour on error exit
              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
      ifail = 0
     Call f11gdf(method,precon,sigcmp,norm,weight,iterm,n,tol,maxitn,anorm, &
       sigmax, sigtol, maxits, monit, lwneed, work, lwork, ifail)
     Calculate reciprocal diagonal matrix elements.
      iwork(1:n) = 0
     Do i = 1, nnz
       If (irow(i)==icol(i)) Then
          iwork(irow(i)) = iwork(irow(i)) + 1
          If (a(i)/=0.0E0_nag_wp) Then
           rdiag(irow(i)) = 1.0E0_nag_wp/a(i)
          Else
           Write (nout,*) 'Matrix has a zero diagonal element'
           Go To 100
          End If
       End If
     End Do
     Do i = 1, n
       If (iwork(i)==0) Then
         Write (nout,*) 'Matrix has a missing diagonal element'
         Go To 100
       End If
       If (iwork(i) \ge 2) Then
         Write (nout,*) 'Matrix has a multiple diagonal element'
         Go To 100
       End If
     End Do
     Call F11GEF to solve the linear system
      irevcm = 0
     ckxef = 'C'
```

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```
ckjdf = 'C'
      ifail = 1
loop: Do
        Call f11gef(irevcm,x,b,wgt,work,lwork,ifail)
        If (irevcm/=4) Then
          ifail1 = -1
          Select Case (irevcm)
          Case (1)
!
            Compute matrix vector product
            Call f11xef(n,nnz,a,irow,icol,ckxef,x,b,ifail1)
            ckxef = 'N'
          Case (2)
            SSOR preconditioning
            Call f11jdf(n,nnz,a,irow,icol,rdiag,omega,ckjdf,x,b,iwork,ifail1)
            ckjdf = 'N'
          End Select
          If (ifail1/=0) irevcm = 6
        Else If (ifail/=0) Then
          Write (nout, 99996) ifail
          Go To 100
        Else
         Exit loop
        End If
     End Do loop
     Termination
     Call f11gff(itn,stplhs,stprhs,anorm,sigmax,its,sigerr,work,lwork,ifail)
     Write (nout,99999) 'Converged in', itn, ' iterations'
     Write (nout, 99998) 'Final residual norm =', stplhs
     Output x
     Write (nout, 99997) x(1:n)
100
     Continue
99999 Format (1X,A,I10,A)
99998 Format (1X,A,1P,E16.3)
99997 Format (1X,1P,E16.4)
99996 Format (1X/1X,' ** F11GEF returned with IFAIL = ',I5)
   End Program flljdfe
10.2 Program Data
F11JDF Example Program Data
 7
16
                      NNZ
 'CG'
                      METHOD
 'P' 'N' 'I' 1
                      PRECON, SIGCMP, NORM, ITERM
1.0D-6 100
                      TOL, MAXITN
0.0D0 0.0D0
                      ANORM, SIGMAX
0.0D0 10
                      SIGTOL, MAXITS
1.0D0
                      OMEGA
 4.
            1
```

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1.

5.

2.

2.

3.

-1.

1.

4.

2

2

3

4

4

5

5

5

1

2

3

2

4

1

4

5

```
1.
-2.
      6
           5
           6
3.
      6
2.
      7
           1
      7
           2
-1.
-2.
5.
      7
           7
                     A(I), IROW(I), ICOL(I), I=1,...,NNZ
15.
     18.
          -8.
                     B(I), I=1,...,N
11.
     10.
           29.
0.
     0.
           0.
                 0.
                     X(I), I=1,\ldots,N
 0.
      0.
          0.
```

10.3 Program Results

```
F11JDF Example Program Results
Converged in 6 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
```

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