NAG Fortran Library Routine Document

F11MGF

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

F11MGF computes an estimate of the reciprocal of the condition number of a sparse matrix given an LU factorization of the matrix computed by F11MEF.

2 Specification

```
SUBROUTINE F11MGF (NORM, N, IL, LVAL, IU, UVAL, ANORM, RCOND, IFAIL)
INTEGER             N, IL(*), IU(*), IFAIL
double precision    LVAL(*), UVAL(*), ANORM, RCOND
CHARACTER*1         NORM
```

3 Description

F11MGF estimates the condition number of a real sparse matrix A, in either the 1-norm or the ∞-norm:

$$\kappa_1(A) = \|A\|_1 \left\|A^{-1}\right\|_1 \quad \text{or} \quad \kappa_\infty(A) = \|A\|_\infty \left\|A^{-1}\right\|_\infty.$$

Note that $\kappa_\infty(A) = \kappa_1\left(A^T\right)$.

Because the condition number is infinite if A is singular, the routine actually returns an estimate of the **reciprocal** of the condition number.

The routine should be preceded by a call to F11MLF to compute $\|A\|_1$ or $\|A\|_\infty$, and a call to F11MEF to compute the LU factorization of A. The routine then estimates $\left\|A^{-1}\right\|_1$ or $\left\|A^{-1}\right\|_\infty$ and computes the reciprocal of the condition number.

4 References

None.

5 Parameters

1: NORM – CHARACTER*1 *Input*

On entry: indicates whether $\kappa_1(A)$ or $\kappa_\infty(A)$ is to be estimated as follows:

if NORM = '1' or 'O', $\kappa_1(A)$ is estimated;
if NORM = 'I', $\kappa_\infty(A)$ is estimated.

Constraint: NORM = '1', 'O' or 'I'.

2: N – INTEGER *Input*

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

Constraint: $\text{N} \geq 0$.

3: IL($*$) – INTEGER array *Input*

On entry: records the sparsity pattern of matrix L as computed by F11MEF.

4: LVAL($*$) – ***double precision*** array *Input*

On entry: records the non-zero values of matrix L and some non-zero values of matrix U as computed by F11MEF.

5: IU($*$) – INTEGER array *Input*

On entry: records the sparsity pattern of matrix U as computed by F11MEF.

6: UVAL($*$) – ***double precision*** array *Input*

On entry: records some non-zero values of matrix U as computed by F11MEF.

7: ANORM – ***double precision*** *Input*

On entry: if NORM = '1' or 'O', the 1-norm of the matrix A; if NORM = 'I', the ∞-norm of the matrix A. ANORM may be computed by calling F11MLF with the same value for the parameter NORM.

Constraint: $\mathrm{ANORM} \geq 0.0$.

8: RCOND – ***double precision*** *Output*

On exit: an estimate of the reciprocal of the condition number of A. RCOND is set to zero if exact singularity is detected or the estimate underflows. If RCOND is less than ***machine precision***, A is singular to working precision.

9: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

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

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, for users 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.**

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, NORM $\neq$ '1', 'O' or 'I',
or N < 0,
or ANORM < 0.0.

IFAIL = 301

Unable to allocate required internal workspace.

7 Accuracy

The computed estimate RCOND is never less than the true value ρ, and in practice is nearly always less than 10ρ, although examples can be constructed where RCOND is much larger.

8 Further Comments

A call to F11MGF involves solving a number of systems of linear equations of the form $Ax = b$ or $A^T x = b$.

9 Example

To estimate the condition number in the 1-norm of the matrix A, where

$$A = \begin{pmatrix} 2.00 & 1.00 & 0 & 0 & 0 \\ 0 & 0 & 1.00 & -1.00 & 0 \\ 4.00 & 0 & 1.00 & 0 & 1.00 \\ 0 & 0 & 0 & 1.00 & 2.00 \\ 0 & -2.00 & 0 & 0 & 3.00 \end{pmatrix}.$$

Here A is nonsymmetric and must first be factorized by F11MEF. The true condition number in the 1-norm is 20.25.

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.

```
*     F11MGF Example Program Text
*     Mark 21 Release. NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          LA, NMAX
      PARAMETER        (LA=10000,NMAX=1000)
      DOUBLE PRECISION ONE
      PARAMETER        (ONE=1.D0)
*     .. Local Scalars ..
      DOUBLE PRECISION ANORM, FLOP, RCOND, THRESH
      INTEGER          I, IFAIL, N, NNZ, NNZL, NNZU, NZLMX, NZLUMX,
     +                 NZUMX
      CHARACTER        NORM, SPEC
*     .. Local Arrays ..
      DOUBLE PRECISION A(LA), LVAL(8*LA), UVAL(8*LA)
      INTEGER          ICOLZP(NMAX+1), IL(7*NMAX+8*LA+4), IPRM(7*NMAX),
     +                 IROWIX(LA), IU(2*NMAX+8*LA+1)
*     .. External Subroutines ..
      EXTERNAL         F11MDF, F11MEF, F11MGF, F11MLF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F11MGF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
*
*     Read order of matrix
*
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*        Read the matrix A
*
         DO 20 I = 1, N + 1
            READ (NIN,*) ICOLZP(I)
   20    CONTINUE
         NNZ = ICOLZP(N+1) - 1
         DO 40 I = 1, NNZ
            READ (NIN,*) A(I), IROWIX(I)
   40    CONTINUE

*
*        Calculate COLAMD permutation
*
         SPEC = 'M'
```

```
         IFAIL = 0
         CALL F11MDF(SPEC,N,ICOLZP,IROWIX,IPRM,IFAIL)
*
*        Factorise
*
         THRESH = ONE
         IFAIL = 0
         NZLMX = 8*NNZ
         NZLUMX = 8*NNZ
         NZUMX = 8*NNZ
         CALL F11MEF(N,IROWIX,A,IPRM,THRESH,NZLMX,NZLUMX,NZUMX,IL,
     +               LVAL,IU,UVAL,NNZL,NNZU,FLOP,IFAIL)
*
*        Calculate norm
*
         NORM = '1'
         IFAIL = 0
         CALL F11MLF(NORM,ANORM,N,ICOLZP,IROWIX,A,IFAIL)
*
*        Calculate condition number
*
         IFAIL = 0
         CALL F11MGF(NORM,N,IL,LVAL,IU,UVAL,ANORM,RCOND,IFAIL)
*
*         Output result
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Norm  ,Condition number'
         WRITE (NOUT,'(F7.3,A1,F7.3)') ANORM, ',', 1/RCOND

*
      END IF
      END
```

9.2 Program Data

```
F11MGF Example Program Data
  5  N
 1
 3
 5
 7
 9
 12   ICOLZP(I) I=1,..,N+1
  2.   1
  4.   3
  1.   1
 -2.   5
  1.   2
  1.   3
 -1.   2
  1.   4
  1.   3
  2.   4
  3.   5    A(I), IROWIX(I) I=1,NNZ
```

9.3 Program Results

```
 F11MGF Example Program Results

 Norm  ,Condition number
  6.000, 20.250
```