F08AEF (SGEQRF/DGEQRF) - 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

F08AEF (SGEQRF/DGEQRF) computes the QR factorization of a real m by n matrix.

2 Specification

SUBROUTINE FO8AEF(M, N, A, LDA, TAU, WORK, LWORK, INFO) ENTRY sgeqrf(M, N, A, LDA, TAU, WORK, LWORK, INFO) INTEGER M, N, LDA, LWORK, INFO real A(LDA,*), TAU(*), WORK(LWORK)

The ENTRY statement enables the routine to be called by its LAPACK name.

3 Description

This routine forms the QR factorization of an arbitrary rectangular real m by n matrix. No pivoting is performed.

If $m \geq n$, the factorization is given by:

$$A = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$$

where R is an n by n upper triangular matrix and Q is an m by m orthogonal matrix. It is sometimes more convenient to write the factorization as

$$A = (Q_1 Q_2) \begin{pmatrix} R \\ 0 \end{pmatrix}$$

which reduces to

$$A = Q_1 R$$
,

where Q_1 consists of the first n columns of Q_1 and Q_2 the remaining m-n columns.

If m < n, R is trapezoidal, and the factorization can be written

$$A = Q(R_1 R_2),$$

where R_1 is upper triangular and R_2 is rectangular.

The matrix Q is not formed explicitly but is represented as a product of $\min(m, n)$ elementary reflectors (see the Chapter Introduction for details). Routines are provided to work with Q in this representation (see Section 8).

Note also that for any k < n, the information returned in the first k columns of the array A represents a QR factorization of the first k columns of the original matrix A.

4 References

[1] Golub G H and van Loan C F (1996) *Matrix Computations* Johns Hopkins University Press (3rd Edition), Baltimore

5 Parameters

1: M — INTEGER

On entry: m, the number of rows of the matrix A.

Constraint: $M \geq 0$.

2: N — INTEGER Input

On entry: n, the number of columns of the matrix A.

Constraint: $N \geq 0$.

3: A(LDA,*) - real array

Input/Output

Note: the second dimension of the array A must be at least max(1,N).

On entry: the m by n matrix A.

On exit: if $m \geq n$, the elements below the diagonal are overwritten by details of the orthogonal matrix Q and the upper triangle is overwritten by the corresponding elements of the n by n upper triangular matrix R.

If m < n, the strictly lower triangular part is overwritten by details of the orthogonal matrix Q and the remaining elements are overwritten by the corresponding elements of the m by n upper trapezoidal matrix R.

4: LDA — INTEGER Input

On entry: the first dimension of the array A as declared in the (sub)program from which F08AEF (SGEQRF/DGEQRF) is called.

Constraint: LDA $\geq \max(1,M)$.

5: TAU(*) - real array

Output

Note: the dimension of the array TAU must be at least max(1,min(M,N)).

On exit: further details of the orthogonal matrix Q.

6: WORK(LWORK) — real array

Workspace

On exit: if INFO = 0, WORK(1) contains the minimum value of LWORK required for optimum performance.

7: LWORK — INTEGER

Input

On entry: the dimension of the array WORK as declared in the (sub)program from which F08AEF (SGEQRF/DGEQRF) is called.

Suggested value: for optimum performance LWORK should be at least N \times nb, where nb is the **blocksize**.

Constraint: LWORK $\geq \max(1,N)$.

8: INFO — INTEGER

Output

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

6 Error Indicators and Warnings

INFO < 0

If INFO = -i, the *i*th parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

7 Accuracy

The computed factorization is the exact factorization of a nearby matrix A + E, where

$$||E||_2 = O(\epsilon)||A||_2$$

and ϵ is the *machine precision*.

8 Further Comments

The total number of floating-point operations is approximately $\frac{2}{3}n^2(3m-n)$ if $m \ge n$ or $\frac{2}{3}m^2(3n-m)$ if m < n.

To form the orthogonal matrix Q this routine may be followed by a call to F08AFF (SORGQR/DORGQR):

but note that the second dimension of the array A must be at least M, which may be larger than was required by F08AEF.

When $m \ge n$, it is often only the first n columns of Q that are required, and they may be formed by the call:

```
CALL SORGQR (M,N,N,A,LDA,TAU,WORK,LWORK,INFO)
```

To apply Q to an arbitrary real rectangular matrix C, this routine may be followed by a call to F08AGF (SORMQR/DORMQR). For example,

forms $C = Q^T C$, where C is m by p.

To compute a QR factorization with column pivoting, use F08BEF (SGEQPF/DGEQPF).

The complex analogue of this routine is F08ASF (CGEQRF/ZGEQRF).

9 Example

To solve the linear least-squares problem minimize $||Ax_i - b_i||_2$ for i = 1, 2 where b_1 and b_2 are the columns of the matrix B,

$$A = \begin{pmatrix} -0.57 & -1.28 & -0.39 & 0.25 \\ -1.93 & 1.08 & -0.31 & -2.14 \\ 2.30 & 0.24 & 0.40 & -0.35 \\ -1.93 & 0.64 & -0.66 & 0.08 \\ 0.15 & 0.30 & 0.15 & -2.13 \\ -0.02 & 1.03 & -1.43 & 0.50 \end{pmatrix} \text{ and } B = \begin{pmatrix} -3.15 & 2.19 \\ -0.11 & -3.64 \\ 1.99 & 0.57 \\ -2.70 & 8.23 \\ 0.26 & -6.35 \\ 4.50 & -1.48 \end{pmatrix}.$$

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.

- * FO8AEF Example Program Text
- * Mark 16 Release. NAG Copyright 1992.
- * .. Parameters ..

INTEGER NIN, NOUT
PARAMETER (NIN=5,NOUT=6)

```
INTEGER
                 MMAX, NMAX, LDA, LDB, NRHMAX, LWORK
PARAMETER
                  (MMAX=8, NMAX=8, LDA=MMAX, LDB=MMAX, NRHMAX=NMAX,
                  LWORK=64*NMAX)
                  ONE
real
PARAMETER
                  (\mathtt{ONE=1.0}e0)
 .. Local Scalars ..
INTEGER
                 I, IFAIL, INFO, J, M, N, NRHS
.. Local Arrays ..
                 A(LDA,NMAX), B(LDB,NRHMAX), TAU(NMAX),
real
                  WORK (LWORK)
 .. External Subroutines ..
EXTERNAL sgeqrf, sormqr, strsm, X04CAF
 .. Executable Statements ...
WRITE (NOUT,*) 'FO8AEF Example Program Results'
Skip heading in data file
READ (NIN,*)
READ (NIN,*) M, N, NRHS
IF (M.LE.MMAX .AND. N.LE.NMAX .AND. M.GE.N .AND. NRHS.LE.NRHMAX)
    THF.N
    Read A and B from data file
    READ (NIN,*) ((A(I,J),J=1,N),I=1,M)
    READ (NIN,*) ((B(I,J),J=1,NRHS),I=1,M)
    Compute the QR factorization of A
    CALL sgeqrf(	exttt{M}, 	exttt{N}, 	exttt{A}, 	exttt{LDA}, 	exttt{TAU}, 	exttt{WORK}, 	exttt{LWORK}, 	exttt{INFO})
    Compute C = (Q**T)*B, storing the result in B
    CALL sormqr('Left', 'Transpose', M, NRHS, N, A, LDA, TAU, B, LDB, WORK,
                 LWORK, INFO)
    Compute least-squares solution by backsubstitution in R*X = C
    CALL strsm('Left', 'Upper', 'No transpose', 'Non-Unit', N, NRHS, ONE,
                A,LDA,B,LDB)
+
    Print least-squares solution(s)
    WRITE (NOUT,*)
    IFAIL = 0
    CALL XO4CAF('General',' ',N,NRHS,B,LDB,
                 'Least-squares solution(s)', IFAIL)
END IF
STOP
END
```

9.2 Program Data

```
FO8AEF Example Program Data
6 4 2 :Values of M, N and NRHS
-0.57 -1.28 -0.39 0.25
-1.93 1.08 -0.31 -2.14
2.30 0.24 0.40 -0.35
```

```
-1.93 0.64 -0.66 0.08
0.15 0.30 0.15 -2.13
-0.02 1.03 -1.43 0.50 :End of matrix A
-3.15 2.19
-0.11 -3.64
     0.57
1.99
-2.70 8.23
0.26 -6.35
                  :End of matrix B
4.50 -1.48
```

9.3Program Results

FO8AEF Example Program Results

Least-squares solution(s)

	-	
	1	2
1	1.5146	-1.5838
2	1.8621	0.5536
3	-1.4467	1.3491
4	0.0396	2.9600