

## NAG Library Routine Document

### F08ZEF (DGGQRF)

**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

F08ZEF (DGGQRF) computes a generalized  $QR$  factorization of a real matrix pair  $(A, B)$ , where  $A$  is an  $n$  by  $m$  matrix and  $B$  is an  $n$  by  $p$  matrix.

#### 2 Specification

```
SUBROUTINE F08ZEF (N, M, P, A, LDA, TAUA, B, LDB, TAUB, WORK, LWORK, INFO)
INTEGER          N, M, P, LDA, LDB, LWORK, INFO
REAL (KIND=nag_wp) A(LDA,*), TAUA(min(N,M)), B(LDB,*), TAUB(min(N,P)), &
                WORK(max(1,LWORK))
```

The routine may be called by its LAPACK name *dggqrf*.

#### 3 Description

F08ZEF (DGGQRF) forms the generalized  $QR$  factorization of an  $n$  by  $m$  matrix  $A$  and an  $n$  by  $p$  matrix  $B$

$$A = QR, \quad B = QTZ,$$

where  $Q$  is an  $n$  by  $n$  orthogonal matrix,  $Z$  is a  $p$  by  $p$  orthogonal matrix and  $R$  and  $T$  are of the form

$$R = \begin{cases} \begin{matrix} m \\ n-m \end{matrix} \begin{pmatrix} R_{11} \\ 0 \end{pmatrix}, & \text{if } n \geq m; \\ n \begin{pmatrix} R_{11} & R_{12} \end{pmatrix}, & \text{if } n < m, \end{cases}$$

with  $R_{11}$  upper triangular,

$$T = \begin{cases} n \begin{pmatrix} p-n & n \\ 0 & T_{12} \end{pmatrix}, & \text{if } n \leq p, \\ n-p \begin{pmatrix} p \\ T_{11} \\ T_{21} \end{pmatrix}, & \text{if } n > p, \end{cases}$$

with  $T_{12}$  or  $T_{21}$  upper triangular.

In particular, if  $B$  is square and nonsingular, the generalized  $QR$  factorization of  $A$  and  $B$  implicitly gives the  $QR$  factorization of  $B^{-1}A$  as

$$B^{-1}A = Z^T(T^{-1}R).$$

## 4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia <http://www.netlib.org/lapack/lug>

Anderson E, Bai Z and Dongarra J (1992) Generalized  $QR$  factorization and its applications *Linear Algebra Appl.* (Volume 162–164) 243–271

Hammarling S (1987) The numerical solution of the general Gauss-Markov linear model *Mathematics in Signal Processing* (eds T S Durrani, J B Abbiss, J E Hudson, R N Madan, J G McWhirter and T A Moore) 441–456 Oxford University Press

Paige C C (1990) Some aspects of generalized  $QR$  factorizations . *In Reliable Numerical Computation* (eds M G Cox and S Hammarling) 73–91 Oxford University Press

## 5 Parameters

- 1: N – INTEGER *Input*  
*On entry:*  $n$ , the number of rows of the matrices  $A$  and  $B$ .  
*Constraint:*  $N \geq 0$ .
- 2: M – INTEGER *Input*  
*On entry:*  $m$ , the number of columns of the matrix  $A$ .  
*Constraint:*  $M \geq 0$ .
- 3: P – INTEGER *Input*  
*On entry:*  $p$ , the number of columns of the matrix  $B$ .  
*Constraint:*  $P \geq 0$ .
- 4: A(LDA,\*) – REAL (KIND=nag\_wp) array *Input/Output*  
**Note:** the second dimension of the array  $A$  must be at least  $\max(1, M)$ .  
*On entry:* the  $n$  by  $m$  matrix  $A$ .  
*On exit:* the elements on and above the diagonal of the array contain the  $\min(n, m)$  by  $m$  upper trapezoidal matrix  $R$  ( $R$  is upper triangular if  $n \geq m$ ); the elements below the diagonal, with the array TAU, represent the orthogonal matrix  $Q$  as a product of  $\min(n, m)$  elementary reflectors (see Section 3.3.6 in the F08 Chapter Introduction).
- 5: LDA – INTEGER *Input*  
*On entry:* the first dimension of the array  $A$  as declared in the (sub)program from which F08ZEF (DGGQRF) is called.  
*Constraint:*  $LDA \geq \max(1, N)$ .
- 6: TAU(min(N, M)) – REAL (KIND=nag\_wp) array *Output*  
*On exit:* the scalar factors of the elementary reflectors which represent the orthogonal matrix  $Q$ .
- 7: B(LDB,\*) – REAL (KIND=nag\_wp) array *Input/Output*  
**Note:** the second dimension of the array  $B$  must be at least  $\max(1, P)$ .  
*On entry:* the  $n$  by  $p$  matrix  $B$ .  
*On exit:* if  $n \leq p$ , the upper triangle of the subarray  $B(1 : n, p - n + 1 : p)$  contains the  $n$  by  $n$  upper triangular matrix  $T_{12}$ .

If  $n > p$ , the elements on and above the  $(n - p)$ th subdiagonal contain the  $n$  by  $p$  upper trapezoidal matrix  $T$ ; the remaining elements, with the array TAUB, represent the orthogonal matrix  $Z$  as a product of elementary reflectors (see Section 3.3.6 in the F08 Chapter Introduction).

- 8: LDB – INTEGER *Input*  
*On entry:* the first dimension of the array B as declared in the (sub)program from which F08ZEF (DGGQRF) is called.  
*Constraint:*  $LDB \geq \max(1, N)$ .
- 9: TAUB( $\min(N, P)$ ) – REAL (KIND=nag\_wp) array *Output*  
*On exit:* the scalar factors of the elementary reflectors which represent the orthogonal matrix  $Z$ .
- 10: WORK( $\max(1, LWORK)$ ) – REAL (KIND=nag\_wp) array *Workspace*  
*On exit:* if INFO = 0, WORK(1) contains the minimum value of LWORK required for optimal performance.
- 11: LWORK – INTEGER *Input*  
*On entry:* the dimension of the array WORK as declared in the (sub)program from which F08ZEF (DGGQRF) is called.  
 If LWORK = -1, a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array, and no error message related to LWORK is issued.  
*Suggested value:* for optimal performance,  $LWORK \geq \max(N, M, P) \times \max(nb1, nb2, nb3)$ , where  $nb1$  is the optimal **block size** for the  $QR$  factorization of an  $n$  by  $m$  matrix,  $nb2$  is the optimal **block size** for the  $RQ$  factorization of an  $n$  by  $p$  matrix, and  $nb3$  is the optimal **block size** for a call of F08AGF (DORMQR).  
*Constraint:*  $LWORK \geq \max(1, N, M, P)$  or LWORK = -1.
- 12: INFO – INTEGER *Output*  
*On exit:* INFO = 0 unless the routine detects an error (see Section 6).

## 6 Error Indicators and Warnings

Errors or warnings detected by the routine:

INFO < 0

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

## 7 Accuracy

The computed generalized  $QR$  factorization is the exact factorization for nearby matrices  $(A + E)$  and  $(B + F)$ , where

$$\|E\|_2 = O\epsilon\|A\|_2 \quad \text{and} \quad \|F\|_2 = O\epsilon\|B\|_2,$$

and  $\epsilon$  is the *machine precision*.

## 8 Further Comments

The orthogonal matrices  $Q$  and  $Z$  may be formed explicitly by calls to F08AFF (DORGQR) and F08CJF (DORGRQ) respectively. F08AGF (DORMQR) may be used to multiply  $Q$  by another matrix and F08CKF (DORMRQ) may be used to multiply  $Z$  by another matrix.

The complex analogue of this routine is F08ZSF (ZGGQRF).

## 9 Example

This example solves the general Gauss–Markov linear model problem

$$\min_x \|y\|_2 \quad \text{subject to} \quad d = Ax + By$$

where

$$A = \begin{pmatrix} -0.57 & -1.28 & -0.39 \\ -1.93 & 1.08 & -0.31 \\ 2.30 & 0.24 & -0.40 \\ -0.02 & 1.03 & -1.43 \end{pmatrix}, \quad B = \begin{pmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 1.0 & 0 & 0 \\ 0 & 0 & 2.0 & 0 \\ 0 & 0 & 0 & 5.0 \end{pmatrix} \quad \text{and} \quad d = \begin{pmatrix} 1.32 \\ -4.00 \\ 5.52 \\ 3.24 \end{pmatrix}.$$

The solution is obtained by first computing a generalized  $QR$  factorization of the matrix pair  $(A, B)$ . The example illustrates the general solution process, although the above data corresponds to a simple weighted least squares problem.

Note that the block size (NB) of 64 assumed in this example is not realistic for such a small problem, but should be suitable for large problems.

### 9.1 Program Text

```

Program f08zefe

!      F08ZEF Example Program Text

!      Mark 24 Release. NAG Copyright 2012.

!      .. Use Statements ..
!      Use nag_library, Only: dgemv, dggqrf, dnrn2, dormqr, dormrq, dtrtrs,      &
!                               nag_wp
!      .. Implicit None Statement ..
!      Implicit None
!      .. Parameters ..
!      Real (Kind=nag_wp), Parameter      :: one = 1.0E0_nag_wp
!      Real (Kind=nag_wp), Parameter      :: zero = 0.0E0_nag_wp
!      Integer, Parameter                  :: nb = 64, nin = 5, nout = 6
!      .. Local Scalars ..
!      Real (Kind=nag_wp)                  :: rnorm
!      Integer                              :: i, info, lda, ldb, lwork, m, n, p
!      .. Local Arrays ..
!      Real (Kind=nag_wp), Allocatable     :: a(:, :), b(:, :), d(:), taua(:),      &
!                               taub(:), work(:), y(:)
!      .. Intrinsic Procedures ..
!      Intrinsic                          :: max, min
!      .. Executable Statements ..
!      Write (nout,*) 'F08ZEF Example Program Results'
!      Write (nout,*)
!      Skip heading in data file
!      Read (nin,*)
!      Read (nin,*) n, m, p
!      lda = n
!      ldb = n
!      lwork = nb*(m+p)
!      Allocate (a(lda,m),b(ldb,p),d(n),taua(m),taub(m+p),work(lwork),y(p))

!      Read A, B and D from data file
!      Read (nin,*)(a(i,1:m),i=1,n)
!      Read (nin,*)(b(i,1:p),i=1,n)
!      Read (nin,*) d(1:n)

!      Compute the generalized QR factorization of (A,B) as
!      A = Q*(R),   B = Q*(T11 T12)*Z
!      (O)         (O T22)
!      The NAG name equivalent of dggqrf is f08zef
!      Call dggqrf(n,m,p,a,lda,taua,b,ldb,taub,work,lwork,info)

```

```

!      Compute c = (c1) = (Q**T)*d, storing the result in D
!                  (c2)
!      The NAG name equivalent of dormqr is f08agf
!      Call dormqr('Left','Transpose',n,l,m,a,lda,taua,d,n,work,lwork,info)

!      Putting Z*y = w = (w1), set w1 = 0, storing the result in Y1
!                  (w2)
y(1:m+p-n) = zero

If (n>m) Then

!      Copy c2 into Y2
y(m+p-n+1:p) = d(m+1:n)

!      Solve T22*w2 = c2 for w2, storing result in Y2
!      The NAG name equivalent of dtrtrs is f07tef
!      Call dtrtrs('Upper','No transpose','Non-unit',n-m,1,b(m+1,m+p-n+1), &
!                ldb,y(m+p-n+1),n-m,info)

!      If (info>0) Then
!          Write (nout,*) &
!              'The upper triangular factor, T22, of B is singular, '
!          Write (nout,*) 'the least squares solution could not be computed'
!          Go To 100
!      End If

!      Compute estimate of the square root of the residual sum of squares
!      norm(y) = norm(w2)

!      The NAG name equivalent of dnorm2 is f06ejf
!      rnorm = dnorm2(n-m,y(m+p-n+1),1)

!      Form c1 - T12*w2 in D
!      The NAG name equivalent of dgemv is f06paf
!      Call dgemv('No transpose',m,n-m,-one,b(1,m+p-n+1),ldb,y(m+p-n+1),1, &
!                one,d,1)
!      End If

!      Solve R*x = c1 - T12*w2 for x
!      The NAG name equivalent of dtrtrs is f07tef
!      Call dtrtrs('Upper','No transpose','Non-unit',m,1,a,lda,d,m,info)

!      If (info>0) Then
!          Write (nout,*) 'The upper triangular factor, R, of A is singular, '
!          Write (nout,*) 'the least squares solution could not be computed'
!      Else

!      Compute y = (Z**T)*w
!      The NAG name equivalent of dormrq is f08ckf
!      Call dormrq('Left','Transpose',p,1,min(n,p),b(max(1, &
!                n-p+1),1),ldb,taub,y,p,work,lwork,info)

!      Print least squares solution x

!      Write (nout,*) 'Generalized least squares solution'
!      Write (nout,99999) d(1:m)

!      Print residual vector y

!      Write (nout,*)
!      Write (nout,*) 'Residual vector'
!      Write (nout,99998) y(1:p)

!      Print estimate of the square root of the residual sum of squares

!      Write (nout,*)
!      Write (nout,*) 'Square root of the residual sum of squares'
!      Write (nout,99998) rnorm
!      End If

```

```
100 Continue
99999 Format (1X,7F11.4)
99998 Format (3X,1P,7E11.2)
      End Program f08zefe
```

## 9.2 Program Data

F08ZEF Example Program Data

```
  4      3      4          :Values of N, M and P
-0.57 -1.28 -0.39
-1.93  1.08 -0.31
  2.30  0.24 -0.40
-0.02  1.03 -1.43          :End of matrix A

  0.50  0.00  0.00  0.00
  0.00  1.00  0.00  0.00
  0.00  0.00  2.00  0.00
  0.00  0.00  0.00  5.00 :End of matrix B

  1.32
 -4.00
  5.52
  3.24          :End of vector d
```

## 9.3 Program Results

F08ZEF Example Program Results

Generalized least squares solution  
 1.9889 -1.0058 -2.9911

Residual vector  
 -6.37E-04 -2.45E-03 -4.72E-03 7.70E-03

Square root of the residual sum of squares  
 9.38E-03

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