

NAG Library Routine Document

F08BAF (DGELSY)

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

F08BAF (DGELSY) computes the minimum norm solution to a real linear least-squares problem

$$\min_x \|b - Ax\|_2$$

using a complete orthogonal factorization of A . A is an m by n matrix which may be rank-deficient. Several right-hand side vectors b and solution vectors x can be handled in a single call.

2 Specification

```
SUBROUTINE F08BAF(M, N, NRHS, A, LDA, B, LDB, JPVT, RCOND, RANK, WORK,
1                LWORK, INFO)
    INTEGER      M, N, NRHS, LDA, LDB, JPVT(*), RANK, LWORK, INFO
    double precision A(LDA,*), B(LDB,*), RCOND, WORK(max(1,LWORK))
```

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

3 Description

The right-hand side vectors are stored as the columns of the m by r matrix B and the solution vectors in the n by r matrix X .

F08BAF (DGELSY) first computes a QR factorization with column pivoting

$$AP = Q \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{pmatrix},$$

with R_{11} defined as the largest leading sub-matrix whose estimated condition number is less than $1/\text{RCOND}$. The order of R_{11} , RANK , is the effective rank of A .

Then, R_{22} is considered to be negligible, and R_{12} is annihilated by orthogonal transformations from the right, arriving at the complete orthogonal factorization

$$AP = Q \begin{pmatrix} T_{11} & 0 \\ 0 & 0 \end{pmatrix} Z.$$

The minimum norm solution is then

$$X = PZ^T \begin{pmatrix} T_{11}^{-1} Q_1^T b \\ 0 \end{pmatrix}$$

where Q_1 consists of the first RANK columns of Q .

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>

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

5 Parameters

- 1: M – INTEGER *Input*
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: NRHS – INTEGER *Input*
On entry: r , the number of right-hand sides, i.e., the number of columns of the matrices B and X .
Constraint: $NRHS \geq 0$.

- 4: A(LDA,*) – **double precision** 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: A has been overwritten by details of its complete orthogonal factorization.

- 5: LDA – INTEGER *Input*
On entry: the first dimension of the array A as declared in the (sub)program from which F08BAF (DGELSY) is called.
Constraint: $LDA \geq \max(1, M)$.

- 6: B(LDB,*) – **double precision** array *Input/Output*
Note: the second dimension of the array B must be at least $\max(1, NRHS)$.
On entry: the m by r right-hand side matrix B .
On exit: the n by r solution matrix X .

- 7: LDB – INTEGER *Input*
On entry: the first dimension of the array B as declared in the (sub)program from which F08BAF (DGELSY) is called.
Constraint: $LDB \geq \max(1, M, N)$.

- 8: JPVT(*) – INTEGER array *Input/Output*
Note: the dimension of the array JPVT must be at least $\max(1, N)$.
On entry: if $JPVT(i) \neq 0$, the i th column of A is permuted to the front of AP , otherwise column i is a free column.
On exit: if $JPVT(i) = k$, then the i th column of AP was the k th column of A .

- 9: RCOND – **double precision** *Input*
On entry: used to determine the effective rank of A , which is defined as the order of the largest leading triangular sub-matrix R_{11} in the QR factorization of A , whose estimated condition number is $< 1/RCOND$.

- 10: RANK – INTEGER *Output*
On exit: the effective rank of A , i.e., the order of the sub-matrix R_{11} . This is the same as the order of the sub-matrix T_{11} in the complete orthogonal factorization of A .

- 11: WORK(max(1,LWORK)) – **double precision** array *Workspace*
On exit: if INFO = 0, WORK(1) contains the minimum value of LWORK required for optimal performance.
- 12: LWORK – INTEGER *Input*
On entry: the dimension of the array WORK as declared in the (sub)program from which F08BAF (DGELSY) 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,

$$\text{LWORK} \geq \max(k + 2 \times N + nb \times (N + 1), 2 \times k + nb \times \text{NRHS}),$$
 where $k = \min(M, N)$ and nb is the optimal **block size**.
Constraint: $\text{LWORK} \geq \max(k + 3 \times N + 1, 2 \times k + \text{NRHS})$, where $k = \min(M, N)$ or $\text{LWORK} = -1$.
- 13: 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

See Section 4.5 of Anderson *et al.* (1999) for details of error bounds.

8 Further Comments

The complex analogue of this routine is F08BNF (ZGELSY).

9 Example

This example solves the linear least-squares problem

$$\min_x \|b - Ax\|_2$$

for the solution, x , of minimum norm, where

$$A = \begin{pmatrix} -0.09 & 0.14 & -0.46 & 0.68 & 1.29 \\ -1.56 & 0.20 & 0.29 & 1.09 & 0.51 \\ -1.48 & -0.43 & 0.89 & -0.71 & -0.96 \\ -1.09 & 0.84 & 0.77 & 2.11 & -1.27 \\ 0.08 & 0.55 & -1.13 & 0.14 & 1.74 \\ -1.59 & -0.72 & 1.06 & 1.24 & 0.34 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 7.4 \\ 4.2 \\ -8.3 \\ 1.8 \\ 8.6 \\ 2.1 \end{pmatrix}.$$

A tolerance of 0.01 is used to determine the effective rank of A .

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

```

*      F08BAF Example Program Text
*      Mark 21 Release. NAG Copyright 2004.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MMAX, NB, NMAX
      PARAMETER        (MMAX=16,NB=64,NMAX=8)
      INTEGER          LDA, LWORK
      PARAMETER        (LDA=MMAX,LWORK=3*NMAX+NB*(NMAX+1))
*      .. Local Scalars ..
      DOUBLE PRECISION RCOND
      INTEGER          I, INFO, J, M, N, RANK
*      .. Local Arrays ..
      DOUBLE PRECISION A(LDA,NMAX), B(MMAX), WORK(LWORK)
      INTEGER          JPVT(NMAX)
*      .. External Subroutines ..
      EXTERNAL         DGELSY, F06DBF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F08BAF Example Program Results'
      WRITE (NOUT,*)
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) M, N
      IF (M.LE.MMAX .AND. N.LE.NMAX .AND. M.GE.N) THEN
*
*          Read A and B from data file
*
*          READ (NIN,*) ((A(I,J),J=1,N),I=1,M)
*          READ (NIN,*) (B(I),I=1,M)
*
*          Initialize JPVT to be zero so that all columns are free
*
*          CALL F06DBF(N,O,JPVT,1)
*
*          Choose RCOND to reflect the relative accuracy of the input data
*
*          RCOND = 0.01D0
*
*          Solve the least squares problem min( norm2(b - Ax) ) for the x
*          of minimum norm.
*
*          CALL DGELSY(M,N,1,A,LDA,B,M,JPVT,RCOND,RANK,WORK,LWORK,INFO)
*
*          Print solution
*
*          WRITE (NOUT,*) 'Least squares solution'
*          WRITE (NOUT,99999) (B(I),I=1,N)
*
*          Print the effective rank of A
*
*          WRITE (NOUT,*)
*          WRITE (NOUT,*) 'Tolerance used to estimate the rank of A'
*          WRITE (NOUT,99998) RCOND
*          WRITE (NOUT,*) 'Estimated rank of A'
*          WRITE (NOUT,99997) RANK
      ELSE
*          WRITE (NOUT,*) 'MMAX and/or NMAX too small, and/or M.LT.N'
      END IF
*
99999 FORMAT (1X,7F11.4)
99998 FORMAT (3X,1P,E11.2)
99997 FORMAT (1X,I6)
      END

```

9.2 Program Data

F08BAF Example Program Data

```

6          5                               :Values of M and N
-0.09    0.14   -0.46    0.68    1.29
-1.56    0.20    0.29    1.09    0.51
-1.48   -0.43    0.89   -0.71   -0.96
-1.09    0.84    0.77    2.11   -1.27
  0.08    0.55   -1.13    0.14    1.74
-1.59   -0.72    1.06    1.24    0.34 :End of matrix A

 7.4
 4.2
-8.3
 1.8
 8.6
 2.1                               :End of vector b
```

9.3 Program Results

F08BAF Example Program Results

```

Least squares solution
 0.6344    0.9699   -1.4402    3.3678    3.3992

Tolerance used to estimate the rank of A
 1.00E-02
Estimated rank of A
 4
```
