

NAG Library Routine Document

F08KAF (DGELSS)

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

F08KAF (DGELSS) computes the minimum norm solution to a real linear least-squares problem

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

2 Specification

```
SUBROUTINE F08KAF(M, N, NRHS, A, LDA, B, LDB, S, RCOND, RANK, WORK,
1                      LWORK, INFO)
    INTEGER          M, N, NRHS, LDA, LDB, RANK, LWORK, INFO
    double precision A(LDA,*), B(LDB,*), S(*), RCOND, WORK(max(1,LWORK))
```

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

3 Description

F08KAF (DGELSS) uses the singular value decomposition (SVD) of A , where 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; they are stored as the columns of the m by r right-hand side matrix B and the n by r solution matrix X .

The effective rank of A is determined by treating as zero those singular values which are less than RCOND times the largest singular value.

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: the first $\min(m, n)$ rows of A are overwritten with its right singular vectors, stored row-wise.
- 5: LDA – INTEGER *Input*
On entry: the first dimension of the array A as declared in the (sub)program from which F08KAF (DGELSS) 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: B is overwritten by the n by r solution matrix X . If $m \geq n$ and $RANK = n$, the residual sum of squares for the solution in the i th column is given by the sum of squares of elements $n + 1, \dots, m$ in that column.
- 7: LDB – INTEGER *Input*
On entry: the first dimension of the array B as declared in the (sub)program from which F08KAF (DGELSS) is called.
Constraint: $LDB \geq \max(1, \max(M, N))$.
- 8: S(*) – **double precision** array *Output*
Note: the dimension of the array S must be at least $\max(1, \min(M, N))$.
On exit: the singular values of A in decreasing order.
- 9: RCOND – **double precision** *Input*
On entry: used to determine the effective rank of A . Singular values $S(i) \leq RCOND \times S(1)$ are treated as zero. If $RCOND < 0$, **machine precision** is used instead.
- 10: RANK – INTEGER *Output*
On exit: the effective rank of A , i.e., the number of singular values which are greater than $RCOND \times S(1)$.
- 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 F08KAF (DGELSS) 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 should generally be larger. Consider increasing LWORK by at least $nb \times \min(M, N)$, where nb is the optimal **block size**.
Constraint: $LWORK \geq 1$, and also
 $LWORK \geq 3 \times \min(M, N) + \max(2 \times \min(M, N), \max(M, N), NRHS)$.

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.

INFO > 0

The algorithm for computing the SVD failed to converge; if INFO = i , i off-diagonal elements of an intermediate bidiagonal form did not converge to zero.

7 Accuracy

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

8 Further Comments

The complex analogue of this routine is F08KNF (ZGELSS).

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

```
*      F08KAF 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*(MMAX+NMAX))
*      .. Local Scalars ..
      DOUBLE PRECISION RCOND, RNORM
      INTEGER          I, INFO, J, M, N, RANK
*      .. Local Arrays ..
      DOUBLE PRECISION A(LDA,NMAX), B(MMAX), S(NMAX), WORK(LWORK)
*      .. External Functions ..
      DOUBLE PRECISION DNRM2
```

```

      EXTERNAL          DNRM2
*      .. External Subroutines ..
      EXTERNAL          DGELSS
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F08KAF 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)
*
*      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 DGELSS(M,N,1,A,LDA,B,M,S,RCOND,RANK,WORK,LWORK,INFO)
*
      IF (INFO.EQ.0) THEN
*
*      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
*
*      Print singular values of A
*
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Singular values of A'
      WRITE (NOUT,99999) (S(I),I=1,N)
*
*      Compute and print estimate of the square root of the
*      residual sum of squares
*
      IF (RANK.EQ.N) THEN
          RNORM = DNRM2(M-N,B(N+1),1)
          WRITE (NOUT,*)
          WRITE (NOUT,*)
          +      'Square root of the residual sum of squares'
          WRITE (NOUT,99998) RNORM
      END IF
      ELSE
          WRITE (NOUT,*) 'The SVD algorithm failed to converge'
      END IF
      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

F08KAF 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

F08KAF Example Program Results

```

Least squares solution
 0.6344    0.9699   -1.4403    3.3678    3.3992

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

Singular values of A
 3.9997    2.9962    2.0001    0.9988    0.0025
```
