NAG Fortran Library Routine Document F04.IMF

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

F04JMF solves a real linear equality-constrained least-squares problem.

2 Specification

```
SUBROUTINE F04JMF(M, N, P, A, LDA, B, LDB, C, D, X, WORK, LWORK, IFAIL) INTEGER M, N, P, LDA, LDB, LWORK, IFAIL real A(LDA,*), B(LDB,*), C(*), D(*), X(*), WORK(*)
```

3 Description

This routine solves the real linear equality-constrained least-squares (LSE) problem

$$\underset{x}{\operatorname{minimize}} \|c - Ax\|_2 \quad \text{subject to} \quad Bx = d$$

where A is an m by n matrix, B is a p by n matrix, c is an m element vector and d is a p element vector. It is assumed that $p \le n \le m + p$, $\operatorname{rank}(B) = p$ and $\operatorname{rank}(E) = n$, where $E = \begin{pmatrix} A \\ B \end{pmatrix}$. These conditions ensure that the LSE problem has a unique solution, which is obtained using a generalized RQ factorization of the matrices B and A.

F04JMF is based on the LAPACK routine SGGLSE/DGGLSE, see Anderson et al. (1999).

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

Anderson E, Bai Z and Dongarra J (1991) Generalized *QR* factorization and its applications *LAPACK Working Note No. 31* University of Tennessee, Knoxville

Eldèn L (1980) Perturbation theory for the least-squares problem with linear equality constraints SIAM J. Numer. Anal. 17 338–350

5 Parameters

1: M – INTEGER Input

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

Constraint: M > 0.

2: N – INTEGER Input

On entry: n, the number of columns of the matrices A and B.

Constraint: $N \ge 0$.

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3: P – INTEGER Input

On entry: p, the number of rows of the matrix B.

Constraint: $0 \le P \le N \le M + P$.

4: 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: A is overwritten.

5: LDA – INTEGER

Input

On entry: the first dimension of the array A as declared in the (sub)program from which F04JMF is called.

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

6: B(LDB,*) - real array

Input/Output

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

On entry: the p by n matrix B.

On exit: B is overwritten.

7: LDB – INTEGER

Input

On entry: the first dimension of the array B as declared in the (sub)program from which F04JMF is called.

Constraint: LDB $\geq \max(1, P)$.

8: C(*) - real array

Input/Output

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

On entry: the right-hand side vector c for the least-squares part of the LSE problem.

On exit: the residual sum of squares for the solution vector x is given by the sum of squares of elements $C(N-P+1), C(N-P+2), \ldots, C(M)$, provided m+p>n; the remaining elements are overwritten.

9: D(*) - real array

Input/Output

Note: the dimension of the array D must be at least max(1, P).

On entry: the right-hand side vector d for the equality constraints.

On exit: D is overwritten.

10: X(*) - real array

Output

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

On exit: the solution vector x of the LSE problem.

11: WORK(*) - *real* array

Workspace

Note: the dimension of the array WORK must be at least max(1, LWORK).

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

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12: LWORK – INTEGER

Input

On entry: the dimension of the array WORK as declared in the subprogram from which F04JMF is called unless LWORK =-1, in which case a workspace query is assumed and the routine only calculates the optimal dimension of WORK (using the formula given below).

Suggested value: for optimum performance LWORK should be at least $P + \min(M, N) + \max(M, N) \times nb$, where nb is the **blocksize**.

Constraint: LWORK $\geq \max(1, M + N + P)$ or LWORK = -1.

13: 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, M < 0, or N < 0, or P < 0, or P < N, or P < N, or P < N - M, or P < N
```

7 Accuracy

For an error analysis, see Anderson et al. (1991) and Eldèn (1980).

8 Further Comments

When $m \ge n = p$, the total number of floating-point operations is approximately $\frac{2}{3}n^2(6m+n)$; if $p \ll n$, the number reduces to approximately $\frac{2}{3}n^2(3m-n)$.

E04NCF/E04NCA may also be used to solve LSE problems. It differs from F04JMF in that it uses an iterative (rather than direct) method, and that it allows general upper and lower bounds to be specified for the variables x and the linear constraints Bx.

9 Example

To solve the least-squares problem

$$\underset{x}{\text{minimize}} \|c - Ax\|_2 \quad \text{subject to} \quad x_1 = x_3 \quad \text{and} \quad x_2 = x_4$$

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where

$$c = \begin{pmatrix} -3.15 \\ -0.11 \\ 1.99 \\ -2.70 \\ 0.26 \\ 4.50 \end{pmatrix}$$

and

$$A = \begin{pmatrix} -0.57 & -1.28 & -0.39 & 0.25 \\ -1.93 & 1.08 & -0.31 & -2.14 \\ 2.30 & 0.24 & 0.40 & -0.35 \\ -1.93 & 0.64 & -0.66 & 0.08 \\ 0.15 & 0.30 & 0.15 & -2.13 \\ -0.02 & 1.03 & -1.43 & 0.50 \end{pmatrix}$$

the equality constraints are formulated by setting

$$B = \begin{pmatrix} 1.0 & 0.0 & -1.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & -1.0 \end{pmatrix}$$

and

$$d = \begin{pmatrix} 0.0 \\ 0.0 \end{pmatrix}.$$

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.

```
FO4JMF Example Program Text.
Mark 17 Release. NAG Copyright 1995.
.. Parameters ..
INTEGER
                  NIN, NOUT
                  (NIN=5,NOUT=6)
PARAMETER
                 MMAX, NMAX, PMAX, LDA, LDB, LWORK
INTEGER
PARAMETER
                  (MMAX=10,NMAX=10,PMAX=10,LDA=MMAX,LDB=PMAX,
                  LWORK=PMAX+NMAX+64*(MMAX+NMAX))
.. Local Scalars ..
real
                  RSS
INTEGER
                  I, IFAIL, J, M, N, P
.. Local Arrays ..
                  A(LDA,NMAX), B(LDB,NMAX), C(MMAX), D(PMAX), WORK(LWORK), X(NMAX)
real
.. External Functions ..
                  sdot
real
EXTERNAL
                  sdot
.. External Subroutines ..
EXTERNAL
                FO4JMF
.. Executable Statements ..
WRITE (NOUT,*) 'F04JMF Example Program Results'
Skip heading in data Ûle
READ (NIN, *)
READ (NIN,*) M, N, P
IF (M.LE.MMAX .AND. N.LE.NMAX .AND. P.LE.PMAX) THEN
   Read A, B, C and D from data Ûle
   READ (NIN,*) ((A(I,J),J=1,N),I=1,M)
   READ (NIN,*) ((B(I,J),J=1,N),I=1,P)
   READ (NIN, \star) (C(I), I=1, M)
   READ (NIN, \star) (D(I), I=1,P)
   Solve the equality-constrained least-squares problem
```

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```
*
    minimize ||C - A*X|| (in the 2-norm) subject to B*X = D

*
    IFAIL = 0

*
    CALL F04JMF(M,N,P,A,LDA,B,LDB,C,D,X,WORK,LWORK,IFAIL)

*
    Print least-squares solution

*
    WRITE (NOUT,*)
    WRITE (NOUT,*) 'Constrained least-squares solution'
    WRITE (NOUT,99999) (X(I),I=1,N)

*
    Compute the residual sum of squares

*
    WRITE (NOUT,*)
    RSS = sdot(M-N+P,C(N-P+1),1,C(N-P+1),1)
    WRITE (NOUT,99998) 'Residual sum of squares = ', RSS
    END IF
    STOP

*
99999 FORMAT (1X,8F9.4)
99998 FORMAT (1X,A,1P,e10.2)
    FND
```

9.2 Program Data

```
FO4JMF Example Program Data
6 4 2
-0.57 -1.28 -0.39 0.25
                           :Values of M, N and P
       1.08 -0.31 -2.14
-1.93
 2.30 0.24 0.40 -0.35
      0.64 -0.66 0.08
0.30 0.15 -2.13
-1.93
 0.15
       1.03 -1.43 0.50 :End of matrix A
-0.02
 1.00 0.00 -1.00 0.00
       1.00 0.00 -1.00 :End of matrix B
 0.00
-3.15
-0.11
 1.99
-2.70
 0.26
 4.50
                           :End of C
 0.00
 0.00
                           :End of D
```

9.3 Program Results

```
F04JMF Example Program Results

Constrained least-squares solution
   0.4857   0.9956   0.4857   0.9956

Residual sum of squares = 2.95E+01
```

[NP3546/20A] F04JMF.5 (last)