NAG Toolbox for MATLAB

f04am

1 Purpose

f04am calculates the accurate least-squares solution of a set of m linear equations in n unknowns, $m \geq n$ and rank $= n$, with multiple right-hand sides, $AX = B$, using a QR factorization and iterative refinement.

2 Syntax

```
[x, qr, alpha, ipiv, ifail] = f04am(a, b, m, eps, 'n', n, 'ir', ir)
```

3 Description

To compute the least-squares solution to a set of m linear equations in n unknowns $(m \geq n)$ $AX = B$, f04am first computes a QR factorization of A with column pivoting, $AP = QR$, where R is upper triangular, Q is an m by m orthogonal matrix, and P is a permutation matrix. Q^{T} is applied to the m by r right-hand side matrix B to give $C = Q^{\mathrm{T}}B$, and the n by r solution matrix X is calculated, to a first approximation, by back-substitution in $RX = C$. The residual matrix $S = B - AX$ is calculated using ***additional precision***, and a correction D to X is computed as the least-squares solution to $AD = S$. X is replaced by $X + D$ and this iterative refinement of the solution is repeated until full machine accuracy has been obtained.

4 References

Wilkinson J H and Reinsch C 1971 *Handbook for Automatic Computation II, Linear Algebra* Springer–Verlag

5 Parameters

5.1 Compulsory Input Parameters

1: **a(lda,n) – double array**

lda, the first dimension of the array, must be at least **m**.

The m by n matrix A.

2: **b(ldb,ir) – double array**

ldb, the first dimension of the array, must be at least **m**.

The m by r right-hand side matrix B.

3: **m – int32 scalar**

m, the number of rows of the matrix A, i.e., the number of equations.

Constraint: **m** ≥ 1.

4: **eps – double scalar**

Must be set to the value of the ***machine precision***.

5.2 Optional Input Parameters

1: **n – int32 scalar**

Default: The dimension of the arrays **a**, **qr**, **alpha**, **ipiv**. (An error is raised if these dimensions are not equal.)

n, the number of columns of the matrix A, i.e., the number of unknowns.

Constraint: $0 \leq \mathbf{n} \leq \mathbf{m}$.

2: **ir – int32 scalar**

Default: The dimension of the arrays **b**, **x**. (An error is raised if these dimensions are not equal.)

r, the number of right-hand sides.

5.3 Input Parameters Omitted from the MATLAB Interface

lda, ldx, ldb, ldqr, e, y, z, r

5.4 Output Parameters

1: **x(ldx,ir) – double array**

The n by r solution matrix X.

2: **qr(ldqr,n) – double array**

Details of the QR factorization.

3: **alpha(n) – double array**

The diagonal elements of the upper triangular matrix R.

4: **ipiv(n) – int32 array**

Details of the column interchanges.

5: **ifail – int32 scalar**

0 unless the function detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail $= 1$

The rank of A is less than n; the problem does not have a unique solution.

ifail $= 2$

The iterative refinement fails to converge, i.e., the matrix A is too ill-conditioned.

7 Accuracy

Although the correction process is continued until the solution has converged to full machine accuracy, all the figures in the final solution may not be correct since the correction D to X is itself the solution to a linear least-squares problem. For a detailed error analysis see page 116 of Wilkinson and Reinsch 1971.

8 Further Comments

The time taken by f04am is approximately proportional to $n^2(3m - n)$, provided r is small compared with n.

9 Example

```
a = [1.1, 0.9;
     1.2, 1;
     1, 1];
b = [2.2;
     2.3;
     2.1];
m = int32(3);
eps = 1.111307226797642e-16;
[x, qr, alpha, ipiv, ifail] = f04am(a, b, m, eps)
```

```
x =
    1.3010
    0.7935
qr =
    3.0105   -1.6697
    1.2000   -0.1727
    1.0000    0.1464
alpha =
   -1.9105
    0.1484
ipiv =
           1
           2
ifail =
           0
```