NAG Toolbox for MATLAB

f01bl

1 Purpose

f01bl calculates the rank and pseudo-inverse of an m by n real matrix, $m \geq n$, using a QR factorization with column interchanges.

2 Syntax

```
[a, aijmax, irank, inc, ifail] = f01bl(m, t, a, 'n', n)
```

3 Description

Householder's factorization with column interchanges is used in the decomposition $F = QU$, where F is A with its columns permuted, Q is the first r columns of an m by m orthogonal matrix and U is an r by n upper-trapezoidal matrix of rank r. The pseudo-inverse of F is given by X where

$$X = U^{\mathrm{T}}\left(UU^{\mathrm{T}}\right)^{-1}Q^{\mathrm{T}}.$$

If the matrix is found to be of maximum rank, $r = n$, U is a nonsingular n by n upper-triangular matrix and the pseudo-inverse of F simplifies to $X = U^{-1}Q^{\mathrm{T}}$. The transpose of the pseudo-inverse of A is overwritten on A.

4 References

Peters G and Wilkinson J H 1970 The least-squares problem and pseudo-inverses *Comput. J.* **13** 309–316

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

5 Parameters

5.1 Compulsory Input Parameters

1: **m – int32 scalar**

m and n, the number of rows and columns in the matrix A.

Constraint: $\mathbf{m} \geq \mathbf{n}$.

2: **t – double scalar**

The tolerance used to decide when elements can be regarded as zero (see Section 8).

3: **a(lda,n) – double array**

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

The m by n rectangular matrix A.

5.2 Optional Input Parameters

1: **n – int32 scalar**

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

m and n, the number of rows and columns in the matrix A.

Constraint: $\mathbf{m} \geq \mathbf{n}$.

5.3 Input Parameters Omitted from the MATLAB Interface

lda, d, u, ldu, du

5.4 Output Parameters

1: **a(lda,n) – double array**

The transpose of the pseudo-inverse of A.

2: **aijmax(n) – double array**

aijmax(i) contains the element of largest modulus in the reduced matrix at the ith stage. If $r < n$, then only the first $r + 1$ elements of **aijmax** have values assigned to them; the remaining elements are unused. The ratio **aijmax**$(1)/$**aijmax**(r) usually gives an indication of the condition number of the original matrix (see Section 8).

3: **irank – int32 scalar**

r, the rank of A as determined using the tolerance **t**.

4: **inc(n) – int32 array**

The record of the column interchanges in the Householder factorization.

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 $= 1$

Inverse not found, due to an incorrect determination of **irank** (see Section 8).

ifail $= 2$

Invalid tolerance, due to

(i) **t** is negative, **irank** $= -1$;

(ii) **t** too large, **irank** $= 0$;

(iii) **t** too small, **irank** > 0.

ifail $= 3$

On entry, $\mathbf{m} < \mathbf{n}$.

7 Accuracy

For most matrices the pseudo-inverse is the best possible having regard to the condition of A and the choice of **t**. Note that only the singular value decomposition method can be relied upon to give maximum accuracy for the precision of computation used and correct determination of the condition of a matrix (see Wilkinson and Reinsch 1971).

The computed factors Q and U satisfy the relation $QU = F + E$ where

$$\|E\|_2 < c\epsilon\|A\|_2 + \eta\sqrt{(m-r)(n-r)}$$

in which c is a modest function of m and n, η is the value of **t**, and ϵ is the ***machine precision***.

8 Further Comments

The time taken by f01bl is approximately proportional to mnr.

The most difficult practical problem is the determination of the rank of the matrix (see pages 314–315 of Peters and Wilkinson 1970); only the singular value decomposition method gives a reliable indication of rank deficiency (see pages 134–151 of Wilkinson and Reinsch 1971 and f08kb). In f01bl a tolerance, **t**, is used to recognize 'zero' elements in the remaining matrix at each step in the factorization. The value of **t** should be set at n times the bound on possible errors in individual elements of the original matrix. If the elements of A vary widely in their orders of magnitude, of course this presents severe difficulties. Sound decisions can only be made by somebody who appreciates the underlying physical problem.

If the condition number of A is 10^p we expect to get p figures wrong in the pseudo-inverse. An estimate of the condition number is usually given by **aijmax**$(1)/$**aijmax**(r).

9 Example

```
m = int32(6);
t = 2.99772935794301e-15;
a = [7, -2, 4, 9, 1.8;
     3, 8, -4, 6, 1.3;
     9, 6, 1, 5, 2.1;
     -8, 7, 5, 2, 0.6;
     4, -1, 2, 8, 1.3;
     1, 6, 3, -5, 0.5];
[aOut, aijmax, irank, inc, ifail] = f01bl(m, t, a)
```

```
aOut =
    0.0178   -0.0216    0.0520    0.0237    0.0072
   -0.0118    0.0434   -0.0813    0.0357   -0.0014
    0.0472    0.0294    0.0139   -0.0138    0.0077
   -0.0566    0.0291    0.0474    0.0305    0.0050
   -0.0037   -0.0138    0.0166    0.0357    0.0035
    0.0384    0.0343    0.0576   -0.0571    0.0073
aijmax =
    9.0000
    9.3101
    8.7461
    5.6832
    0.0000
irank =
           4
inc =
           4
           2
           4
           4
           0
ifail =
           0
```