NAG Toolbox for MATLAB

f05aa

1 Purpose

f05aa applies the Schmidt orthogonalisation process to n vectors in m-dimensional space, $n \leq m$.

2 Syntax

```
[a, cc, icol, ifail] = f05aa(a, m, n1, 'n2', n2)
```

3 Description

f05aa applies the Schmidt orthogonalisation process to n linearly independent vectors in m-dimensional space, $n \leq m$. The effect of this process is to replace the original n vectors by n orthonormal vectors which have the property that the rth vector is linearly dependent on the first r of the original vectors, and that the sum of squares of the elements of the rth vector is equal to 1, for $r = 1, 2, \ldots, n$. Inner-products are accumulated using ***additional precision***.

4 References

None.

5 Parameters

5.1 Compulsory Input Parameters

1: **a(lda,n2) – double array**

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

Columns **n1** to **n2** contain the vectors to be orthogonalised. The vectors are stored by columns in elements 1 to m.

2: **m – int32 scalar**

m, the number of elements in each vector.

3: **n1 – int32 scalar**

the indices of the first and last columns of A to be orthogonalised.

Constraint: **n1** $\leq$ **n2**.

5.2 Optional Input Parameters

1: **n2 – int32 scalar**

Default: The dimension of the array **a**.

the indices of the first and last columns of A to be orthogonalised.

Constraint: **n1** $\leq$ **n2**.

5.3 Input Parameters Omitted from the MATLAB Interface

lda, s

5.4 Output Parameters

1: **a(lda,n2) – double array**

These vectors are overwritten by the orthonormal vectors.

2: **cc – double scalar**

Is used to indicate linear dependence of the original vectors. The nearer **cc** is to 1.0, the more likely vector **icol** is dependent on vectors **n1** to **icol** − 1. See Section 8.

3: **icol – int32 scalar**

The column number corresponding to **cc**. See Section 8.

4: **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

On entry, **n1** > **n2**.

7 Accuracy

Innerproducts are accumulated using ***additional precision*** arithmetic and full machine accuracy should be obtained except when **cc** > 0.99999. (See Section 8.)

8 Further Comments

The time taken by f05aa is approximately proportional to nm^2, where $n = \mathbf{n2} - \mathbf{n1} + 1$.

Parameters **cc** and **icol** have been included to give some indication of whether or not the vectors are nearly linearly independent, and their values should always be tested on exit from the function. **cc** will be in the range $[0.0, 1.0]$ and the closer **cc** is to 1.0, the more likely the vector **icol** is to be linearly dependent on vectors **n1** to **icol** − 1. Theoretically, when the vectors are linearly dependent, **cc** should be exactly 1.0. In practice, because of rounding errors, it may be difficult to decide whether or not a value of **cc** close to 1.0 indicates linear dependence. As a general guide a value of **cc** > 0.99999 usually indicates linear dependence, but examples exist which give **cc** > 0.99999 for linearly independent vectors. If one of the original vectors is zero or if, possibly due to rounding errors, an exactly zero vector is produced by the Gram–Schmidt process, then **cc** is set exactly to 1.0 and the vector is not, of course, normalized. If more than one such vector occurs then **icol** references the last of these vectors.

If you are who concerned about testing for near linear dependence in a set of vectors you may wish to consider using function f08kb.

9 Example

```
a = [1, -2, 3, 1;
     -2, 1, -2, -1;
     3, -2, 1, 5;
     4, 1, 5, 3];
m = int32(4);
n1 = int32(2);
[aOut, cc, icol, ifail] = f05aa(a, m, n1)
```

```
aOut =
    1.0000   -0.6325    0.3310   -0.5404
   -2.0000    0.3162   -0.2483    0.2119
    3.0000   -0.6325   -0.0000    0.7735
    4.0000    0.3162    0.9104    0.2543
cc =
    0.5822
icol =
           4
ifail =
           0
```