NAG Toolbox

nag_eigen_real_triang_svd (f02wu)

1 Purpose

nag_eigen_real_triang_svd (f02wu) returns all, or part, of the singular value decomposition of a real upper triangular matrix.

2 Syntax

```
[a, b, q, sv, work, ifail] = nag_eigen_real_triang_svd(a, b, wantq, wantp, 'n',
n, 'ncolb', ncolb)
```

```
[a, b, q, sv, work, ifail] = f02wu(a, b, wantq, wantp, 'n', n, 'ncolb', ncolb)
```

3 Description

The n by n upper triangular matrix R is factorized as

$$R = QSP^{\mathrm{T}},$$

where Q and P are n by n orthogonal matrices and S is an n by n diagonal matrix with non-negative diagonal elements, $\sigma_1, \sigma_2, \ldots, \sigma_n$, ordered such that

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0.$$

The columns of Q are the left-hand singular vectors of R, the diagonal elements of S are the singular values of R and the columns of P are the right-hand singular vectors of R.

Either or both of Q and P^{T} may be requested and the matrix C given by

$$C = Q^{\mathrm{T}}B,$$

where B is an n by $ncolb$ given matrix, may also be requested.

The function obtains the singular value decomposition by first reducing R to bidiagonal form by means of Givens plane rotations and then using the QR algorithm to obtain the singular value decomposition of the bidiagonal form.

Good background descriptions to the singular value decomposition are given in Chan (1982), Dongarra *et al.* (1979), Golub and Van Loan (1996), Hammarling (1985) and Wilkinson (1978).

Note that if K is any orthogonal diagonal matrix so that

$$KK^{\mathrm{T}} = I$$

(that is the diagonal elements of K are $+1$ or -1) then

$$A = (QK)S(PK)^{\mathrm{T}}$$

is also a singular value decomposition of A.

4 References

Chan T F (1982) An improved algorithm for computing the singular value decomposition *ACM Trans. Math. Software* **8** 72–83

Dongarra J J, Moler C B, Bunch J R and Stewart G W (1979) *LINPACK Users' Guide* SIAM, Philadelphia

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

Hammarling S (1985) The singular value decomposition in multivariate statistics *SIGNUM Newsl.* **20(3)** 2–25

Wilkinson J H (1978) Singular Value Decomposition – Basic Aspects *Numerical Software – Needs and Availability* (ed D A H Jacobs) Academic Press

5 Parameters

5.1 Compulsory Input Parameters

1: **a**(lda, :) – REAL (KIND=nag_wp) array

The first dimension of the array **a** must be at least $\max(1, \mathbf{n})$.

The second dimension of the array **a** must be at least $\max(1, \mathbf{n})$.

The leading n by n upper triangular part of the array **a** must contain the upper triangular matrix R.

2: **b**(ldb, :) – REAL (KIND=nag_wp) array

The first dimension, ldb, of the array **b** must satisfy

if $\mathbf{ncolb} > 0$, $ldb \geq \max(1, \mathbf{n})$;
otherwise $ldb \geq 1$.

The second dimension of the array **b** must be at least $\max(1, \mathbf{ncolb})$.

With $\mathbf{ncolb} > 0$, the leading n by $ncolb$ part of the array **b** must contain the matrix to be transformed.

3: **wantq** – LOGICAL

Must be *true* if the matrix Q is required.

If $\mathbf{wantq} = \mathit{false}$, the array **q** is not referenced.

4: **wantp** – LOGICAL

Must be *true* if the matrix P^{T} is required, in which case P^{T} is overwritten on the array **a**, otherwise **wantp** must be *false*.

5.2 Optional Input Parameters

1: **n** – INTEGER

Default: the first dimension of the array **a** and the second dimension of the array **a**.

n, the order of the matrix R.

If $\mathbf{n} = 0$, an immediate return is effected.

Constraint: $\mathbf{n} \geq 0$.

2: **ncolb** – INTEGER

Default: the second dimension of the array **b**.

$ncolb$, the number of columns of the matrix B.

If $\mathbf{ncolb} = 0$, the array **b** is not referenced.

Constraint: $\mathbf{ncolb} \geq 0$.

5.3 Output Parameters

1: **a**$(lda,:)$ – REAL (KIND=nag_wp) array

The first dimension of the array **a** will be $\max(1,\mathbf{n})$.

The second dimension of the array **a** will be $\max(1,\mathbf{n})$.

If **wantp** $= true$, the n by n part of **a** will contain the n by n orthogonal matrix P^{T}, otherwise the n by n upper triangular part of **a** is used as internal workspace, but the strictly lower triangular part of **a** is not referenced.

2: **b**$(ldb,:)$ – REAL (KIND=nag_wp) array

The first dimension, ldb, of the array **b** will be

if **ncolb** > 0, $ldb = \max(1,\mathbf{n})$;
otherwise $ldb = 1$.

The second dimension of the array **b** will be $\max(1,\mathbf{ncolb})$.

The leading n by $ncolb$ part of the array **b** stores the matrix $Q^{\mathrm{T}}B$.

3: **q**$(ldq,:)$ – REAL (KIND=nag_wp) array

The first dimension, ldq, of the array **q** will be

if **wantq** $= true$, $ldq = \max(1,\mathbf{n})$;
otherwise $ldq = 1$.

The second dimension of the array **q** will be $\max(1,\mathbf{n})$ if **wantq** $= true$ and 1 otherwise.

With **wantq** $= true$, the leading n by n part of the array **q** will contain the orthogonal matrix Q. Otherwise the array **q** is not referenced.

4: **sv**$(\mathbf{n})$ – REAL (KIND=nag_wp) array

The array **sv** will contain the n diagonal elements of the matrix S.

5: **work**$(:)$ – REAL (KIND=nag_wp) array

The dimension of the array **work** will be $\max(1,2\times(\mathbf{n}-1))$ if **ncolb** $= 0$ and **wantq** $= false$ and **wantp** $= false$, $\max(1,3\times(\mathbf{n}-1))$ if (**ncolb** $= 0$ and **wantq** $= false$ and **wantp** $= true$) or (**wantp** $= false$ and (**ncolb** > 0 or **wantq** $= true$)) and $\max(1,5\times(\mathbf{n}-1))$ otherwise

work$(\mathbf{n})$ contains the total number of iterations taken by the QR algorithm.

The rest of the array is used as internal workspace.

6: **ifail** – INTEGER

ifail $= 0$ unless the function detects an error (see Section 5).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail $= -1$

On entry, **n** < 0,
or $lda < \mathbf{n}$,
or **ncolb** < 0,
or $ldb < \mathbf{n}$ and **ncolb** > 0,
or $ldq < \mathbf{n}$ and **wantq** $= true$.

ifail > 0 (*warning*)

The QR algorithm has failed to converge in $50 \times \mathbf{n}$ iterations. In this case $\mathbf{sv}(1), \mathbf{sv}(2), \ldots, \mathbf{sv}(\mathbf{ifail})$ may not have been found correctly and the remaining singular values may not be the smallest. The matrix R will nevertheless have been factorized as $R = QEP^{\mathrm{T}}$, where E is a bidiagonal matrix with $\mathbf{sv}(1), \mathbf{sv}(2), \ldots, \mathbf{sv}(n)$ as the diagonal elements and $\mathbf{work}(1), \mathbf{work}(2), \ldots, \mathbf{work}(n-1)$ as the superdiagonal elements.

This failure is not likely to occur.

ifail $= -99$

An unexpected error has been triggered by this routine. Please contact NAG.

ifail $= -399$

Your licence key may have expired or may not have been installed correctly.

ifail $= -999$

Dynamic memory allocation failed.

7 Accuracy

The computed factors Q, S and P satisfy the relation

$$QSP^{\mathrm{T}} = R + E,$$

where

$$\|E\| \leq c\epsilon\|A\|,$$

ϵ is the ***machine precision***, c is a modest function of n and $\|.\|$ denotes the spectral (two) norm. Note that $\|A\| = \mathbf{sv}(1)$.

A similar result holds for the computed matrix $Q^{\mathrm{T}}B$.

The computed matrix Q satisfies the relation

$$Q = T + F,$$

where T is exactly orthogonal and

$$\|F\| \leq d\epsilon,$$

where d is a modest function of n. A similar result holds for P.

8 Further Comments

For given values of **ncolb**, **wantq** and **wantp**, the number of floating-point operations required is approximately proportional to n^3.

>Following the use of nag_eigen_real_triang_svd (f02wu) the rank of R may be estimated as follows:

```
tol = eps;
 irank = 1;
 while (irank <= numel(sv) && sv(irank) >= tol*sv(1) )
   irank = irank + 1;
 end
```

returns the value k in `irank`, where k is the smallest integer for which $\mathbf{sv}(k) < tol \times \mathbf{sv}(1)$, where tol is typically the ***machine precision***, so that `irank` is an estimate of the rank of S and thus also of R.

9 Example

This example finds the singular value decomposition of the 3 by 3 upper triangular matrix

$$A = \begin{pmatrix} -4 & -2 & -3 \\ 0 & -3 & -2 \\ 0 & 0 & -4 \end{pmatrix},$$

together with the vector $Q^{\mathrm{T}}b$ for the vector

$$b = \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix}.$$

9.1 Program Text

```
function f02wu_example

fprintf('f02wu example results\n\n');

% SVD of upper triangular A
a = [-4, -2, -3;
      0, -3, -2;
      0,  0, -4];

b = [-1; -1; -1];
wantq = true;
wantp = true;
[a, b, q, sv, work, ifail] = f02wu( ...
                                    a, b, wantq, wantp);

fprintf('Singular value decomposition of A\n\n');

disp('Singular values');
disp(sv');
disp('Left-hand singular vectors, by column');
disp(q);
disp('Right-hand singular vectors, by column');
disp(a');
disp('Vector Q''*B');
disp(b');
```

9.2 Program Results

```
f02wu example results

Singular value decomposition of A

Singular values
    6.5616    3.0000    2.4384

Left-hand singular vectors, by column
   -0.7699    0.5883   -0.2471
   -0.4324   -0.1961    0.8801
   -0.4694   -0.7845   -0.4054

Right-hand singular vectors, by column
    0.4694   -0.7845    0.4054
    0.4324   -0.1961   -0.8801
    0.7699    0.5883    0.2471

Vector Q'*B
    1.6716    0.3922   -0.2276
```