NAG Toolbox

nag_lapack_dgesvd (f08kb)

1 Purpose

nag_lapack_dgesvd (f08kb) computes the singular value decomposition (SVD) of a real m by n matrix A, optionally computing the left and/or right singular vectors.

2 Syntax

```
[a, s, u, vt, work, info] = nag_lapack_dgesvd(jobu, jobvt, a, 'm', m, 'n', n)
[a, s, u, vt, work, info] = f08kb(jobu, jobvt, a, 'm', m, 'n', n)
```

Note: the interface to this routine has changed since earlier releases of the toolbox:

At Mark 23: **work** was made an output parameter.

3 Description

The SVD is written as

$$A = U\Sigma V^{\mathrm{T}},$$

where Σ is an m by n matrix which is zero except for its $\min(m,n)$ diagonal elements, U is an m by m orthogonal matrix, and V is an n by n orthogonal matrix. The diagonal elements of Σ are the singular values of A; they are real and non-negative, and are returned in descending order. The first $\min(m,n)$ columns of U and V are the left and right singular vectors of A.

Note that the function returns V^{T}, not V.

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 http://www.netlib.org/lapack/lug

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

5 Parameters

5.1 Compulsory Input Parameters

1: **jobu** – CHARACTER(1)

Specifies options for computing all or part of the matrix U.

jobu = 'A'
: All m columns of U are returned in array **u**.

jobu = 'S'
: The first $\min(m,n)$ columns of U (the left singular vectors) are returned in the array **u**.

jobu = 'O'
: The first $\min(m,n)$ columns of U (the left singular vectors) are overwritten on the array **a**.

jobu = 'N'
No columns of U (no left singular vectors) are computed.

Constraint: **jobu** = 'A', 'S', 'O' or 'N'.

2: **jobvt** – CHARACTER(1)

Specifies options for computing all or part of the matrix V^{T}.

jobvt = 'A'
All n rows of V^{T} are returned in the array **vt**.

jobvt = 'S'
The first $\min(m,n)$ rows of V^{T} (the right singular vectors) are returned in the array **vt**.

jobvt = 'O'
The first $\min(m,n)$ rows of V^{T} (the right singular vectors) are overwritten on the array **a**.

jobvt = 'N'
No rows of V^{T} (no right singular vectors) are computed.

Constraints:

jobvt = 'A', 'S', 'O' or 'N';
jobvt and **jobu** cannot both be 'O'.

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

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

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

The m by n matrix A.

5.2 Optional Input Parameters

1: **m** – INTEGER

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

m, the number of rows of the matrix A.

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

2: **n** – INTEGER

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

n, the number of columns of the matrix A.

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

5.3 Output Parameters

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

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

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

If **jobu** = 'O', **a** is overwritten with the first $\min(m,n)$ columns of U (the left singular vectors, stored column-wise).

If **jobvt** = 'O', **a** is overwritten with the first $\min(m,n)$ rows of V^{T} (the right singular vectors, stored row-wise).

If **jobu** $\neq$ 'O' and **jobvt** $\neq$ 'O', the contents of **a** are destroyed.

2: **s**(:) – REAL (KIND=nag_wp) array

The dimension of the array **s** will be $\max(1, \min(\mathbf{m}, \mathbf{n}))$

The singular values of A, sorted so that $\mathbf{s}(i) \geq \mathbf{s}(i+1)$.

3: **u**$(ldu, :)$ – REAL (KIND=nag_wp) array

The first dimension, ldu, of the array **u** will be

if **jobu** = 'A' or 'S', $ldu = \max(1, \mathbf{m})$;
otherwise $ldu = 1$.

The second dimension of the array **u** will be $\max(1, \mathbf{m})$ if **jobu** = 'A', $\max(1, \min(\mathbf{m}, \mathbf{n}))$ if **jobu** = 'S' and 1 otherwise.

If **jobu** = 'A', **u** contains the m by m orthogonal matrix U.

If **jobu** = 'S', **u** contains the first $\min(m, n)$ columns of U (the left singular vectors, stored column-wise).

If **jobu** = 'N' or 'O', **u** is not referenced.

4: **vt**$(ldvt, :)$ – REAL (KIND=nag_wp) array

The first dimension, $ldvt$, of the array **vt** will be

if **jobvt** = 'A', $ldvt = \max(1, \mathbf{n})$;
if **jobvt** = 'S', $ldvt = \max(1, \min(\mathbf{m}, \mathbf{n}))$;
otherwise $ldvt = 1$.

The second dimension of the array **vt** will be $\max(1, \mathbf{n})$ if **jobvt** = 'A' or 'S' and 1 otherwise.

If **jobvt** = 'A', **vt** contains the n by n orthogonal matrix V^{T}.

If **jobvt** = 'S', **vt** contains the first $\min(m, n)$ rows of V^{T} (the right singular vectors, stored row-wise).

If **jobvt** = 'N' or 'O', **vt** is not referenced.

5: **work**$(\mathbf{max}(\mathbf{1}, lwork))$ – REAL (KIND=nag_wp) array

If **info** $= 0$, **work**(1) returns the optimal $lwork$.

If **info** > 0, **work**$(2 : \min(\mathbf{m}, \mathbf{n}))$ contains the unconverged superdiagonal elements of an upper bidiagonal matrix B whose diagonal is in **s** (not necessarily sorted). B satisfies $A = UBV^{\mathrm{T}}$, so it has the same singular values as A, and singular vectors related by U and V^{T}.

6: **info** – INTEGER

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

6 Error Indicators and Warnings

info < 0

If **info** $= -i$, argument i had an illegal value. An explanatory message is output, and execution of the program is terminated.

info > 0

If nag_lapack_dgesvd (f08kb) did not converge, **info** specifies how many superdiagonals of an intermediate bidiagonal form did not converge to zero.

7 Accuracy

The computed singular value decomposition is nearly the exact singular value decomposition for a nearby matrix $(A+E)$, where

$$\|E\|_2 = O(\epsilon)\|A\|_2,$$

and ϵ is the ***machine precision***. In addition, the computed singular vectors are nearly orthogonal to working precision. See Section 4.9 of Anderson *et al.* (1999) for further details.

8 Further Comments

The total number of floating-point operations is approximately proportional to mn^2 when $m > n$ and m^2n otherwise.

The singular values are returned in descending order.

The complex analogue of this function is nag_lapack_zgesvd (f08kp).

9 Example

This example finds the singular values and left and right singular vectors of the 6 by 4 matrix

$$A = \begin{pmatrix} 2.27 & -1.54 & 1.15 & -1.94 \\ 0.28 & -1.67 & 0.94 & -0.78 \\ -0.48 & -3.09 & 0.99 & -0.21 \\ 1.07 & 1.22 & 0.79 & 0.63 \\ -2.35 & 2.93 & -1.45 & 2.30 \\ 0.62 & -7.39 & 1.03 & -2.57 \end{pmatrix},$$

together with approximate error bounds for the computed singular values and vectors.

The example program for nag_lapack_dgesdd (f08kd) illustrates finding a singular value decomposition for the case $m \leq n$.

9.1 Program Text

```
     function f08kb_example

fprintf('f08kb example results\n\n');

% SVD of A to obtain Least-sqares solution of Ax=b, where
a = [ 2.27, -1.54,  1.15, -1.94;
      0.28, -1.67,  0.94, -0.78;
     -0.48, -3.09,  0.99, -0.21;
      1.07,  1.22,  0.79,  0.63;
     -2.35,  2.93, -1.45,  2.30;
      0.62, -7.39,  1.03, -2.57];
[m,n] = size(a);
b     = ones(m,1);

% SVD of A
jobu =  'Singular vectors part of U';
jobvt = 'Singular vectors part of VT';
[~, s, u, vt, work, info] = f08kb( ...
                                   jobu, jobvt, a);

disp('Singular values of A');
disp(s');

% Use SVD to compute least-squares solution: VS^(-1)U'b
y = u'*b;
y = y./s;
x = vt'*y;
```

```
disp('Least squares solution:');
disp(x');
disp('Norm of Residual:');
disp(norm(b - a*x));
```

9.2 Program Results

```
     f08kb example results

Singular values of A
    9.9966    3.6831    1.3569    0.5000

Least squares solution:
   -0.0563   -0.1700    0.8202    0.5545

Norm of Residual:
    1.7472
```