

NAG Library Function Document

nag_zgesvd (f08kpc)

1 Purpose

nag_zgesvd (f08kpc) computes the singular value decomposition (SVD) of a complex m by n matrix A , optionally computing the left and/or right singular vectors.

2 Specification

```
#include <nag.h>
#include <nagf08.h>

void nag_zgesvd (Nag_OrderType order, Nag_ComputeUType jobu,
                Nag_ComputeVTType jobvt, Integer m, Integer n, Complex a[], Integer pda,
                double s[], Complex u[], Integer pdu, Complex vt[], Integer pdvt,
                double rwork[], NagError *fail)
```

3 Description

The SVD is written as

$$A = U\Sigma V^H,$$

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 unitary matrix, and V is an n by n unitary 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^H , 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 Arguments

1: **order** – Nag_OrderType *Input*

On entry: the **order** argument specifies the two-dimensional storage scheme being used, i.e., row-major ordering or column-major ordering. C language defined storage is specified by **order** = Nag_RowMajor. See Section 3.2.1.3 in the Essential Introduction for a more detailed explanation of the use of this argument.

Constraint: **order** = Nag_RowMajor or Nag_ColMajor.

2: **jobu** – Nag_ComputeUType *Input*

On entry: specifies options for computing all or part of the matrix U .

jobu = Nag_AllU

All m columns of U are returned in array **u**.

jobu = Nag_SingularVecsU

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

jobu = Nag_Overwrite

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

jobu = Nag_NotU

No columns of U (no left singular vectors) are computed.

Constraint: **jobu** = Nag_AllU, Nag_SingularVecsU, Nag_Overwrite or Nag_NotU.

3: **jobvt** – Nag_ComputeVTType *Input*

On entry: specifies options for computing all or part of the matrix V^H .

jobvt = Nag_AllVT

All n rows of V^H are returned in the array **vt**.

jobvt = Nag_SingularVecsVT

The first $\min(m, n)$ rows of V^H (the right singular vectors) are returned in the array **vt**.

jobvt = Nag_OverwriteVT

The first $\min(m, n)$ rows of V^H (the right singular vectors) are overwritten on the array **a**.

jobvt = Nag_NotVT

No rows of V^H (no right singular vectors) are computed.

Constraints:

jobvt = Nag_AllVT, Nag_SingularVecsVT, Nag_OverwriteVT or Nag_NotVT;

If **jobu** = Nag_Overwrite, **jobvt** cannot be Nag_OverwriteVT.

4: **m** – Integer *Input*

On entry: m , the number of rows of the matrix A .

Constraint: $m \geq 0$.

5: **n** – Integer *Input*

On entry: n , the number of columns of the matrix A .

Constraint: $n \geq 0$.

6: **a**[*dim*] – Complex *Input/Output*

Note: the dimension, *dim*, of the array **a** must be at least

$\max(1, \mathbf{pda} \times \mathbf{n})$ when **order** = Nag_ColMajor;

$\max(1, \mathbf{m} \times \mathbf{pda})$ when **order** = Nag_RowMajor.

The (i, j) th element of the matrix A is stored in

a[($j - 1$) \times **pda** + $i - 1$] when **order** = Nag_ColMajor;

a[($i - 1$) \times **pda** + $j - 1$] when **order** = Nag_RowMajor.

On entry: the m by n matrix A .

On exit: if **jobu** = Nag_Overwrite, **a** is overwritten with the first $\min(m, n)$ columns of U (the left singular vectors, stored column-wise).

If **jobvt** = Nag_OverwriteVT, **a** is overwritten with the first $\min(m, n)$ rows of V^H (the right singular vectors, stored row-wise).

If **jobu** \neq Nag_Overwrite and **jobvt** \neq Nag_OverwriteVT, the contents of **a** are destroyed.

- 7: **pda** – Integer *Input*
- On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **a**.
- Constraints:*
- if **order** = Nag_ColMajor, **pda** \geq max(1, **m**);
if **order** = Nag_RowMajor, **pda** \geq max(1, **n**).
- 8: **s**[*dim*] – double *Output*
- Note:** the dimension, *dim*, of the array **s** must be at least max(1, min(**m**, **n**)).
- On exit:* the singular values of *A*, sorted so that $\mathbf{s}[i - 1] \geq \mathbf{s}[i]$.
- 9: **u**[*dim*] – Complex *Output*
- Note:** the dimension, *dim*, of the array **u** must be at least
- max(1, **pdu** \times **m**) when **jobu** = Nag_AllU;
max(1, **pdu** \times min(**m**, **n**)) when **jobu** = Nag_SingularVecsU and **order** = Nag_ColMajor;
max(1, **m** \times **pdu**) when **jobu** = Nag_SingularVecsU and **order** = Nag_RowMajor;
1 otherwise.
- The (*i*, *j*)th element of the matrix *U* is stored in
- u**[(*j* - 1) \times **pdu** + *i* - 1] when **order** = Nag_ColMajor;
u[(*i* - 1) \times **pdu** + *j* - 1] when **order** = Nag_RowMajor.
- On exit:* if **jobu** = Nag_AllU, **u** contains the *m* by *m* unitary matrix *U*.
- If **jobu** = Nag_SingularVecsU, **u** contains the first min(*m*, *n*) columns of *U* (the left singular vectors, stored column-wise).
- If **jobu** = Nag_NotU or Nag_Overwrite, **u** is not referenced.
- 10: **pdu** – Integer *Input*
- On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **u**.
- Constraints:*
- if **order** = Nag_ColMajor,
 if **jobu** = Nag_AllU, **pdu** \geq max(1, **m**);
 if **jobu** = Nag_SingularVecsU, **pdu** \geq max(1, **m**);
 otherwise **pdu** \geq 1.;
if **order** = Nag_RowMajor,
 if **jobu** = Nag_AllU, **pdu** \geq max(1, **m**);
 if **jobu** = Nag_SingularVecsU, **pdu** \geq max(1, min(**m**, **n**));
 otherwise **pdu** \geq 1..
- 11: **vt**[*dim*] – Complex *Output*
- Note:** the dimension, *dim*, of the array **vt** must be at least
- max(1, **pdt** \times **n**) when **jobvt** = Nag_AllVT;
max(1, **pdt** \times **n**) when **jobvt** = Nag_SingularVecsVT and **order** = Nag_ColMajor;
max(1, min(**m**, **n**) \times **pdt**) when **jobvt** = Nag_SingularVecsVT and **order** = Nag_RowMajor;
1 otherwise.
- The (*i*, *j*)th element of the matrix is stored in
- vt**[(*j* - 1) \times **pdt** + *i* - 1] when **order** = Nag_ColMajor;
vt[(*i* - 1) \times **pdt** + *j* - 1] when **order** = Nag_RowMajor.

On exit: if **jobvt** = Nag_AllVT, **vt** contains the n by n unitary matrix V^H .

If **jobvt** = Nag_SingularVecsVT, **vt** contains the first $\min(m, n)$ rows of V^H (the right singular vectors, stored row-wise).

If **jobvt** = Nag_NotVT or Nag_OverwriteVT, **vt** is not referenced.

12: **pdvt** – Integer *Input*

On entry: the stride separating row or column elements (depending on the value of **order**) in the array **vt**.

Constraints:

```

if order = Nag_ColMajor,
    if jobvt = Nag_AllVT, pdvt  $\geq$   $\max(1, n)$ ;
    if jobvt = Nag_SingularVecsVT, pdvt  $\geq$   $\max(1, \min(m, n))$ ;
    otherwise pdvt  $\geq$  1.;
if order = Nag_RowMajor,
    if jobvt = Nag_AllVT, pdvt  $\geq$   $\max(1, n)$ ;
    if jobvt = Nag_SingularVecsVT, pdvt  $\geq$   $\max(1, n)$ ;
    otherwise pdvt  $\geq$  1..

```

13: **rwork**[$\min(m, n)$] – double *Output*

On exit: if **fail.code** = NE_CONVERGENCE, **RWORK**(1 : $\min(m, n) - 1$) (using the notation described in Section 3.2.1.4 in the Essential Introduction) contains the unconverged superdiagonal elements of an upper bidiagonal matrix B whose diagonal is in S (not necessarily sorted). B satisfies $A = UBV^T$, so it has the same singular values as A , and singular vectors related by U and V^T .

14: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_BAD_PARAM

On entry, argument $\langle value \rangle$ had an illegal value.

NE_CONVERGENCE

If nag_zgesvd (f08kpc) did not converge, **fail.errnum** specifies how many superdiagonals of an intermediate bidiagonal form did not converge to zero.

NE_ENUM_INT_2

On entry, **jobu** = $\langle value \rangle$, **pdu** = $\langle value \rangle$ and **m** = $\langle value \rangle$.
 Constraint: if **jobu** = Nag_AllU, **pdu** \geq $\max(1, m)$;
 if **jobu** = Nag_SingularVecsU, **pdu** \geq $\max(1, m)$;
 otherwise **pdu** \geq 1.

NE_ENUM_INT_3

On entry, **jobu** = $\langle value \rangle$, **pdu** = $\langle value \rangle$, **m** = $\langle value \rangle$ and **n** = $\langle value \rangle$.
 Constraint: if **jobu** = Nag_AllU, **pdu** \geq $\max(1, \mathbf{m})$;
 if **jobu** = Nag_SingularVecsU, **pdu** \geq $\max(1, \min(\mathbf{m}, \mathbf{n}))$;
 otherwise **pdu** \geq 1.

On entry, **jobvt** = $\langle value \rangle$, **pdvt** = $\langle value \rangle$, **m** = $\langle value \rangle$ and **n** = $\langle value \rangle$.
 Constraint: if **jobvt** = Nag_AllVT, **pdvt** \geq $\max(1, \mathbf{n})$;
 if **jobvt** = Nag_SingularVecsVT, **pdvt** \geq $\max(1, \min(\mathbf{m}, \mathbf{n}))$;
 otherwise **pdvt** \geq 1.

On entry, **jobvt** = $\langle value \rangle$, **pdvt** = $\langle value \rangle$, **m** = $\langle value \rangle$ and **n** = $\langle value \rangle$.
 Constraint: if **jobvt** = Nag_AllVT, **pdvt** \geq $\max(1, \mathbf{n})$;
 if **jobvt** = Nag_SingularVecsVT, **pdvt** \geq $\max(1, \mathbf{n})$;
 otherwise **pdvt** \geq 1.

NE_INT

On entry, **m** = $\langle value \rangle$.
 Constraint: **m** \geq 0.

On entry, **n** = $\langle value \rangle$.
 Constraint: **n** \geq 0.

On entry, **pda** = $\langle value \rangle$.
 Constraint: **pda** $>$ 0.

On entry, **pdu** = $\langle value \rangle$.
 Constraint: **pdu** $>$ 0.

On entry, **pdvt** = $\langle value \rangle$.
 Constraint: **pdvt** $>$ 0.

NE_INT_2

On entry, **pda** = $\langle value \rangle$ and **m** = $\langle value \rangle$.
 Constraint: **pda** \geq $\max(1, \mathbf{m})$.

On entry, **pda** = $\langle value \rangle$ and **n** = $\langle value \rangle$.
 Constraint: **pda** \geq $\max(1, \mathbf{n})$.

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

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 Parallelism and Performance

nag_zgesvd (f08kpc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_zgesvd (f08kpc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the Users' Note for your implementation for any additional implementation-specific information.

9 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 real analogue of this function is nag_dgesvd (f08kbc).

10 Example

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

$$A = \begin{pmatrix} 0.96 - 0.81i & -0.03 + 0.96i & -0.91 + 2.06i & -0.05 + 0.41i \\ -0.98 + 1.98i & -1.20 + 0.19i & -0.66 + 0.42i & -0.81 + 0.56i \\ 0.62 - 0.46i & 1.01 + 0.02i & 0.63 - 0.17i & -1.11 + 0.60i \\ -0.37 + 0.38i & 0.19 - 0.54i & -0.98 - 0.36i & 0.22 - 0.20i \\ 0.83 + 0.51i & 0.20 + 0.01i & -0.17 - 0.46i & 1.47 + 1.59i \\ 1.08 - 0.28i & 0.20 - 0.12i & -0.07 + 1.23i & 0.26 + 0.26i \end{pmatrix},$$

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

The example program for nag_zgesdd (f08krc) illustrates finding a singular value decomposition for the case $m \leq n$.

10.1 Program Text

```

/* nag_zgesvd (f08kpc) Example Program.
 *
 * Copyright 2011 Numerical Algorithms Group.
 *
 * Mark 23, 2011.
 */

#include <stdio.h>
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf08.h>
#include <nagf16.h>
#include <nagx02.h>
#include <nagx04.h>
#include <naga02.h>

int main(void)
{
    /* Scalars */
    Complex      alpha, beta;
    double       eps, norm, serrbd;
    Integer      exit_status = 0, i, j, m, n, pda, pdd, pdu, pdvt;

    /* Arrays */
    Complex      *a = 0, *d = 0, *u = 0, *vt = 0;
    double       *rcondv = 0, *rcondv = 0, *s = 0, *uerrbd = 0, *verrbd = 0;
    double       *rwork = 0;

    /* Nag Types */
    NagError     fail;
    Nag_OrderType order;

#ifdef NAG_COLUMN_MAJOR
#define A(I, J) a[(J - 1) * pda + I - 1]
    order = Nag_ColMajor;

```

```

#else
#define A(I, J) a[(I - 1) * pda + J - 1]
    order = Nag_RowMajor;
#endifif

    INIT_FAIL(fail);

    printf("nag_zgesvd (f08kpc) Example Program Results\n\n");

    /* Skip heading in data file */
    scanf("%*[\n]");
    scanf("%ld%ld%*[\n]", &m, &n);
    if (m < 0 || n < 0)
    {
        printf("Invalid m or n\n");
        exit_status = 1;
        goto END;
    }

    /* Allocate memory: these assume that A is overwritten by U, and
    * all of VT is required.
    */
    if (!(a      = NAG_ALLOC(m * n, Complex)) ||
        !(d      = NAG_ALLOC(m * n, Complex)) ||
        !(u      = NAG_ALLOC(1, Complex)) ||
        !(vt     = NAG_ALLOC(MIN(m, n) * n, Complex)) ||
        !(rcondu = NAG_ALLOC(MIN(m, n), double)) ||
        !(rcondv = NAG_ALLOC(MIN(m, n), double)) ||
        !(s      = NAG_ALLOC(MIN(m, n), double)) ||
        !(uerrbd = NAG_ALLOC(MIN(m, n), double)) ||
        !(verrbd = NAG_ALLOC(MIN(m, n), double)) ||
        !(rwork  = NAG_ALLOC(MIN(m, n), double)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

#ifdef NAG_COLUMN_MAJOR
    pda = m;
#else
    pda = n;
#endifif
    pdu = 1;
    pdvt = n;
    pdd = pda;

    /* Read the m by n matrix A from data file. */
    for (i = 1; i <= m; ++i)
        for (j = 1; j <= n; ++j)
            scanf(" ( %lf , %lf )", &A(i, j).re, &A(i, j).im);
    scanf("%*[\n]");

    /* Copy A to D: nag_zge_copy (f16tfc),
    * Complex valued general matrix copy.
    */
    nag_zge_copy(order, Nag_NoTrans, m, n, a, pda, d, pdd, &fail);

    /* nag_gen_complx_mat_print_comp (x04dbc): Print matrix A */
    fflush(stdout);
    nag_gen_complx_mat_print_comp(order, Nag_GeneralMatrix, Nag_NonUnitDiag, m,
                                  n, a, pda, Nag_BracketForm, "%7.4f", "Matrix A",
                                  Nag_IntegerLabels, 0, Nag_IntegerLabels, 0, 80,
                                  0, 0, &fail);

    printf("\n");
    if (fail.code != NE_NOERROR)
    {
        printf("Error from nag_gen_complx_mat_print_comp (x04dbc).\n%s\n",
              fail.message);
        exit_status = 1;
        goto END;
    }

```

```

    }

/* nag_zgesvd (f08kpc)
 * Compute the singular values and left and right singular vectors
 * of A ( $A = U*S*(V^*H)$ ,  $m.ge.n$ )
 */
nag_zgesvd(order, Nag_Overwrite, Nag_AllVT, m, n, a, pda, s, u, pdu, vt, pdvt,
           rwork, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_zgesvd (f08kpc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Reconstruct A from its decomposition and subtract from original A:
 * first,  $A \leftarrow U(A)*S$ , then  $D \leftarrow D - U*S*V^*H$  using
 * nag_zgemm (f16zac).
 */
for(i = 1; i <= m; i++)
    for(j = 1; j <= MIN(m,n); j++)
        A(i, j).re *= s[j-1], A(i, j).im *= s[j-1];

alpha = nag_complex(-1.0,0.0);
beta = nag_complex(1.0,0.0);
nag_zgemm(order, Nag_NoTrans, Nag_NoTrans, m, n, n, alpha, a, pda, vt, pdvt,
          beta, d, pdd, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_zgemm (f16zac).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Find norm of difference matrix D and print warning if it is too large:
 * nag_zge_norm (f16uac) using one-norm.
 */
nag_zge_norm(order, Nag_OneNorm, m, n, d, pdd, &norm, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_zge_norm (f16uac).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Get the machine precision, using nag_machine_precision (x02ajc) */
eps = nag_machine_precision;
if (norm > pow(eps,0.8))
{
    printf("Norm of  $A-(U*S*V^*H)$  is much greater than 0.\n"
           " Schur factorization has failed.\n");
    exit_status = 1;
    goto END;
}

/* Print singular values and error estimates on values and vectors. */
printf("\nSingular values\n");
for (i = 0; i < n; ++i) printf("%10.4f%s", s[i], i%8 == 7?"\n":"" );
printf("\n\n");

/* Approximate error bound for the computed singular values.
 * Note that for the 2-norm,  $s[0] = \text{norm}(A)$ .
 */
serrbd = eps * s[0];

/* Call nag_ddisna (f08flc) to estimate reciprocal condition numbers for the
 * singular vectors.
 */
nag_ddisna(Nag_LeftSingVecs, m, n, s, rcondu, &fail);
nag_ddisna(Nag_RightSingVecs, m, n, s, rcondv, &fail);

/* Compute the error estimates for the singular vectors */
for (i = 0; i < n; ++i)

```



```

    {
        uerrbd[i] = serrbd / rcondu[i];
        verrbd[i] = serrbd / rcondv[i];
    }
    printf("Error estimate for the singular values\n%11.1e\n", serrbd);

    printf("\nError estimates for the left singular vectors\n");
    for (i = 0; i < n; ++i) printf(" %10.1e%s", uerrbd[i], i%6 == 5?"\n":""");

    printf("\n\nError estimates for the right singular vectors\n");
    for (i = 0; i < n; ++i) printf(" %10.1e%s", verrbd[i], i%6 == 5?"\n":""");
    printf("\n\n");

END:
    NAG_FREE(a);
    NAG_FREE(d);
    NAG_FREE(u);
    NAG_FREE(vt);
    NAG_FREE(rcondu);
    NAG_FREE(rcondv);
    NAG_FREE(s);
    NAG_FREE(uerrbd);
    NAG_FREE(verrbd);
    NAG_FREE(rwork);

    return exit_status;
}
#endif A

```

10.2 Program Data

nag_zgesvd (f08kpc) Example Program Data

```

    6                4                :Values of M and N

( 0.96,-0.81) (-0.03, 0.96) (-0.91, 2.06) (-0.05, 0.41)
(-0.98, 1.98) (-1.20, 0.19) (-0.66, 0.42) (-0.81, 0.56)
( 0.62,-0.46) ( 1.01, 0.02) ( 0.63,-0.17) (-1.11, 0.60)
(-0.37, 0.38) ( 0.19,-0.54) (-0.98,-0.36) ( 0.22,-0.20)
( 0.83, 0.51) ( 0.20, 0.01) (-0.17,-0.46) ( 1.47, 1.59)
( 1.08,-0.28) ( 0.20,-0.12) (-0.07, 1.23) ( 0.26, 0.26) :End of matrix A

```

10.3 Program Results

nag_zgesvd (f08kpc) Example Program Results

```

Matrix A
          1          2          3          4
1 ( 0.9600,-0.8100) (-0.0300, 0.9600) (-0.9100, 2.0600) (-0.0500, 0.4100)
2 (-0.9800, 1.9800) (-1.2000, 0.1900) (-0.6600, 0.4200) (-0.8100, 0.5600)
3 ( 0.6200,-0.4600) ( 1.0100, 0.0200) ( 0.6300,-0.1700) (-1.1100, 0.6000)
4 (-0.3700, 0.3800) ( 0.1900,-0.5400) (-0.9800,-0.3600) ( 0.2200,-0.2000)
5 ( 0.8300, 0.5100) ( 0.2000, 0.0100) (-0.1700,-0.4600) ( 1.4700, 1.5900)
6 ( 1.0800,-0.2800) ( 0.2000,-0.1200) (-0.0700, 1.2300) ( 0.2600, 0.2600)

```

```

Singular values
3.9994    3.0003    1.9944    0.9995

```

```

Error estimate for the singular values
4.4e-16

```

```

Error estimates for the left singular vectors
4.4e-16    4.4e-16    4.5e-16    4.5e-16

```

```

Error estimates for the right singular vectors
4.4e-16    4.4e-16    4.5e-16    4.5e-16

```
