

## NAG Library Function Document

### nag\_dspgvx (f08tbc)

#### 1 Purpose

nag\_dspgvx (f08tbc) computes selected eigenvalues and, optionally, eigenvectors of a real generalized symmetric-definite eigenproblem, of the form

$$Az = \lambda Bz, \quad ABz = \lambda z \quad \text{or} \quad BAz = \lambda z,$$

where  $A$  and  $B$  are symmetric, stored in packed storage, and  $B$  is also positive definite. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

#### 2 Specification

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

void nag_dspgvx (Nag_OrderType order, Integer itype, Nag_JobType job,
                 Nag_RangeType range, Nag_UploType uplo, Integer n, double ap[],
                 double bp[], double vl, double vu, Integer il, Integer iu,
                 double abstol, Integer *m, double w[], double z[], Integer pdz,
                 Integer jfail[], NagError *fail)
```

#### 3 Description

nag\_dspgvx (f08tbc) first performs a Cholesky factorization of the matrix  $B$  as  $B = U^T U$ , when **uplo** = Nag\_Upper or  $B = LL^T$ , when **uplo** = Nag\_Lower. The generalized problem is then reduced to a standard symmetric eigenvalue problem

$$Cx = \lambda x,$$

which is solved for the desired eigenvalues and eigenvectors; the eigenvectors are then backtransformed to give the eigenvectors of the original problem.

For the problem  $Az = \lambda Bz$ , the eigenvectors are normalized so that the matrix of eigenvectors,  $Z$ , satisfies

$$Z^T A Z = \Lambda \quad \text{and} \quad Z^T B Z = I,$$

where  $\Lambda$  is the diagonal matrix whose diagonal elements are the eigenvalues. For the problem  $ABz = \lambda z$  we correspondingly have

$$Z^{-1} A Z^{-T} = \Lambda \quad \text{and} \quad Z^T B Z = I,$$

and for  $BAz = \lambda z$  we have

$$Z^T A Z = \Lambda \quad \text{and} \quad Z^T B^{-1} Z = I.$$

## 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>

Demmel J W and Kahan W (1990) Accurate singular values of bidiagonal matrices *SIAM J. Sci. Statist. Comput.* **11** 873–912

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 2.3.1.3 in How to Use the NAG Library and its Documentation for a more detailed explanation of the use of this argument.  
*Constraint:* **order** = Nag\_RowMajor or Nag\_ColMajor.
- 2: **itype** – Integer *Input*  
*On entry:* specifies the problem type to be solved.  
**itype** = 1  
 $Az = \lambda Bz.$   
**itype** = 2  
 $ABz = \lambda z.$   
**itype** = 3  
 $BAz = \lambda z.$   
*Constraint:* **itype** = 1, 2 or 3.
- 3: **job** – Nag\_JobType *Input*  
*On entry:* indicates whether eigenvectors are computed.  
**job** = Nag\_EigVals  
Only eigenvalues are computed.  
**job** = Nag\_DoBoth  
Eigenvalues and eigenvectors are computed.  
*Constraint:* **job** = Nag\_EigVals or Nag\_DoBoth.
- 4: **range** – Nag\_RangeType *Input*  
*On entry:* if **range** = Nag\_AllValues, all eigenvalues will be found.  
If **range** = Nag\_Interval, all eigenvalues in the half-open interval  $(\mathbf{vl}, \mathbf{vu}]$  will be found.  
If **range** = Nag\_Indices, the **ilth** to **iuth** eigenvalues will be found.  
*Constraint:* **range** = Nag\_AllValues, Nag\_Interval or Nag\_Indices.
- 5: **uplo** – Nag\_UploType *Input*  
*On entry:* if **uplo** = Nag\_Upper, the upper triangles of *A* and *B* are stored.  
If **uplo** = Nag\_Lower, the lower triangles of *A* and *B* are stored.  
*Constraint:* **uplo** = Nag\_Upper or Nag\_Lower.

- 6: **n** – Integer *Input*  
*On entry:*  $n$ , the order of the matrices  $A$  and  $B$ .  
*Constraint:*  $n \geq 0$ .
- 7: **ap**[*dim*] – double *Input/Output*  
**Note:** the dimension, *dim*, of the array **ap** must be at least  $\max(1, n \times (n + 1)/2)$ .  
*On entry:* the upper or lower triangle of the  $n$  by  $n$  symmetric matrix  $A$ , packed by rows or columns.  
The storage of elements  $A_{ij}$  depends on the **order** and **uplo** arguments as follows:
  - if **order** = Nag\_ColMajor and **uplo** = Nag\_Upper,  
 $A_{ij}$  is stored in **ap**[( $j - 1$ )  $\times$   $j/2 + i - 1$ ], for  $i \leq j$ ;
  - if **order** = Nag\_ColMajor and **uplo** = Nag\_Lower,  
 $A_{ij}$  is stored in **ap**[( $2n - j$ )  $\times$  ( $j - 1$ )/2 +  $i - 1$ ], for  $i \geq j$ ;
  - if **order** = Nag\_RowMajor and **uplo** = Nag\_Upper,  
 $A_{ij}$  is stored in **ap**[( $2n - i$ )  $\times$  ( $i - 1$ )/2 +  $j - 1$ ], for  $i \leq j$ ;
  - if **order** = Nag\_RowMajor and **uplo** = Nag\_Lower,  
 $A_{ij}$  is stored in **ap**[( $i - 1$ )  $\times$   $i/2 + j - 1$ ], for  $i \geq j$ .*On exit:* the contents of **ap** are destroyed.
- 8: **bp**[*dim*] – double *Input/Output*  
**Note:** the dimension, *dim*, of the array **bp** must be at least  $\max(1, n \times (n + 1)/2)$ .  
*On entry:* the upper or lower triangle of the  $n$  by  $n$  symmetric matrix  $B$ , packed by rows or columns.  
The storage of elements  $B_{ij}$  depends on the **order** and **uplo** arguments as follows:
  - if **order** = Nag\_ColMajor and **uplo** = Nag\_Upper,  
 $B_{ij}$  is stored in **bp**[( $j - 1$ )  $\times$   $j/2 + i - 1$ ], for  $i \leq j$ ;
  - if **order** = Nag\_ColMajor and **uplo** = Nag\_Lower,  
 $B_{ij}$  is stored in **bp**[( $2n - j$ )  $\times$  ( $j - 1$ )/2 +  $i - 1$ ], for  $i \geq j$ ;
  - if **order** = Nag\_RowMajor and **uplo** = Nag\_Upper,  
 $B_{ij}$  is stored in **bp**[( $2n - i$ )  $\times$  ( $i - 1$ )/2 +  $j - 1$ ], for  $i \leq j$ ;
  - if **order** = Nag\_RowMajor and **uplo** = Nag\_Lower,  
 $B_{ij}$  is stored in **bp**[( $i - 1$ )  $\times$   $i/2 + j - 1$ ], for  $i \geq j$ .*On exit:* the triangular factor  $U$  or  $L$  from the Cholesky factorization  $B = U^T U$  or  $B = LL^T$ , in the same storage format as  $B$ .
- 9: **vl** – double *Input*  
10: **vu** – double *Input*  
*On entry:* if **range** = Nag\_Interval, the lower and upper bounds of the interval to be searched for eigenvalues.  
If **range** = Nag\_AllValues or Nag\_Indices, **vl** and **vu** are not referenced.  
*Constraint:* if **range** = Nag\_Interval,  $vl < vu$ .
- 11: **il** – Integer *Input*  
12: **iu** – Integer *Input*  
*On entry:* if **range** = Nag\_Indices, the indices (in ascending order) of the smallest and largest eigenvalues to be returned.  
If **range** = Nag\_AllValues or Nag\_Interval, **il** and **iu** are not referenced.

Constraints:

if **range** = Nag\_Indices and **n** = 0, **il** = 1 and **iu** = 0;  
 if **range** = Nag\_Indices and **n** > 0,  $1 \leq \mathbf{il} \leq \mathbf{iu} \leq \mathbf{n}$ .

13: **abstol** – double Input

*On entry:* the absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval  $[a, b]$  of width less than or equal to

$$\mathbf{abstol} + \epsilon \max(|a|, |b|),$$

where  $\epsilon$  is the *machine precision*. If **abstol** is less than or equal to zero, then  $\epsilon \|T\|_1$  will be used in its place, where  $T$  is the tridiagonal matrix obtained by reducing  $C$  to tridiagonal form. Eigenvalues will be computed most accurately when **abstol** is set to twice the underflow threshold  $2 \times \text{nag\_real\_safe\_small\_number}()$ , not zero. If this function returns with **fail.code** = NE\_CONVERGENCE, indicating that some eigenvectors did not converge, try setting **abstol** to  $2 \times \text{nag\_real\_safe\_small\_number}()$ . See Demmel and Kahan (1990).

14: **m** – Integer \* Output

*On exit:* the total number of eigenvalues found.  $0 \leq \mathbf{m} \leq \mathbf{n}$ .

If **range** = Nag\_AllValues, **m** = **n**.

If **range** = Nag\_Indices, **m** = **iu** – **il** + 1.

15: **w[n]** – double Output

*On exit:* the first **m** elements contain the selected eigenvalues in ascending order.

16: **z[dim]** – double Output

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

$\max(1, \mathbf{pdz} \times \mathbf{n})$  when **job** = Nag\_DoBoth;  
 1 otherwise.

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

$\mathbf{z}[(j-1) \times \mathbf{pdz} + i - 1]$  when **order** = Nag\_ColMajor;  
 $\mathbf{z}[(i-1) \times \mathbf{pdz} + j - 1]$  when **order** = Nag\_RowMajor.

*On exit:* if **job** = Nag\_DoBoth, then

if **fail.code** = NE\_NOERROR, the first **m** columns of  $Z$  contain the orthonormal eigenvectors of the matrix  $A$  corresponding to the selected eigenvalues, with the  $i$ th column of  $Z$  holding the eigenvector associated with  $\mathbf{w}[i-1]$ . The eigenvectors are normalized as follows:

if **itype** = 1 or 2,  $Z^T B Z = I$ ;

if **itype** = 3,  $Z^T B^{-1} Z = I$ ;

if an eigenvector fails to converge (**fail.code** = NE\_CONVERGENCE), then that column of  $Z$  contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in **jfail**.

If **job** = Nag\_EigVals, **z** is not referenced.

17: **pdz** – Integer Input

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

Constraints:

if **job** = Nag\_DoBoth, **pdz**  $\geq \max(1, \mathbf{n})$ ;  
otherwise **pdz**  $\geq 1$ .

18: **jfail**[*dim*] – Integer

Output

**Note:** the dimension, *dim*, of the array **jfail** must be at least  $\max(1, \mathbf{n})$ .

On exit: if **job** = Nag\_DoBoth, then

if **fail.code** = NE\_NOERROR, the first **m** elements of **jfail** are zero;

if **fail.code** = NE\_CONVERGENCE, **jfail** contains the indices of the eigenvectors that failed to converge.

If **job** = Nag\_EigVals, **jfail** is not referenced.

19: **fail** – NagError \*

Input/Output

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

### NE\_BAD\_PARAM

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

### NE\_CONVERGENCE

The algorithm failed to converge;  $\langle value \rangle$  eigenvectors failed to converge.

### NE\_ENUM\_INT\_2

On entry, **job** =  $\langle value \rangle$ , **pdz** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .

Constraint: if **job** = Nag\_DoBoth, **pdz**  $\geq \max(1, \mathbf{n})$ ;  
otherwise **pdz**  $\geq 1$ .

### NE\_ENUM\_INT\_3

On entry, **range** =  $\langle value \rangle$ , **il** =  $\langle value \rangle$ , **iu** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .

Constraint: if **range** = Nag\_Indices and **n** = 0, **il** = 1 and **iu** = 0;  
if **range** = Nag\_Indices and **n** > 0,  $1 \leq \mathbf{il} \leq \mathbf{iu} \leq \mathbf{n}$ .

### NE\_ENUM\_REAL\_2

On entry, **range** =  $\langle value \rangle$ , **vl** =  $\langle value \rangle$  and **vu** =  $\langle value \rangle$ .

Constraint: if **range** = Nag\_Interval, **vl** < **vu**.

### NE\_INT

On entry, **itype** =  $\langle value \rangle$ .

Constraint: **itype** = 1, 2 or 3.

On entry, **n** =  $\langle value \rangle$ .

Constraint: **n**  $\geq 0$ .

On entry, **pdz** =  $\langle value \rangle$ .

Constraint: **pdz** > 0.

**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.

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

See Section 2.7.6 in How to Use the NAG Library and its Documentation for further information.

**NE\_MAT\_NOT\_POS\_DEF**

If **fail.errnum** = **n** +  $\langle value \rangle$ , for  $1 \leq \langle value \rangle \leq \mathbf{n}$ , then the leading minor of order  $\langle value \rangle$  of  $B$  is not positive definite. The factorization of  $B$  could not be completed and no eigenvalues or eigenvectors were computed.

**NE\_NO\_LICENCE**

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

See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

**7 Accuracy**

If  $B$  is ill-conditioned with respect to inversion, then the error bounds for the computed eigenvalues and vectors may be large, although when the diagonal elements of  $B$  differ widely in magnitude the eigenvalues and eigenvectors may be less sensitive than the condition of  $B$  would suggest. See Section 4.10 of Anderson *et al.* (1999) for details of the error bounds.

**8 Parallelism and Performance**

nag\_dspgvx (f08tbc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag\_dspgvx (f08tbc) 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 x06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this function. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

**9 Further Comments**

The total number of floating-point operations is proportional to  $n^3$ .

The complex analogue of this function is nag\_zhpgvx (f08tpc).

**10 Example**

This example finds the eigenvalues in the half-open interval  $(-1.0, 1.0]$ , and corresponding eigenvectors, of the generalized symmetric eigenproblem  $Az = \lambda Bz$ , where

$$A = \begin{pmatrix} 0.24 & 0.39 & 0.42 & -0.16 \\ 0.39 & -0.11 & 0.79 & 0.63 \\ 0.42 & 0.79 & -0.25 & 0.48 \\ -0.16 & 0.63 & 0.48 & -0.03 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 4.16 & -3.12 & 0.56 & -0.10 \\ -3.12 & 5.03 & -0.83 & 1.09 \\ 0.56 & -0.83 & 0.76 & 0.34 \\ -0.10 & 1.09 & 0.34 & 1.18 \end{pmatrix}.$$

The example program for nag\_dspgvd (f08tcc) illustrates solving a generalized symmetric eigenproblem of the form  $ABz = \lambda z$ .

## 10.1 Program Text

```

/* nag_dspgvx (f08tbc) Example Program.
*
* NAGPRODCODE Version.
*
* Copyright 2016 Numerical Algorithms Group.
*
* Mark 26, 2016.
*/

#include <stdio.h>
#include <nag.h>
#include <nagx04.h>
#include <nag_stdlib.h>
#include <nagf08.h>

int main(void)
{
    /* Scalars */
    double abstol, vl, vu;
    Integer i, il = 0, iu = 0, j, m, n, pdz;
    Integer exit_status = 0;
    /* Arrays */
    double *ap = 0, *bp = 0, *w = 0, *z = 0;
    Integer *index = 0;
    char nag_enum_arg[40];

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

#ifdef NAG_COLUMN_MAJOR
#define A_UPPER(I, J) ap[J*(J-1)/2 + I - 1]
#define A_LOWER(I, J) ap[(2*n-J)*(J-1)/2 + I - 1]
#define B_UPPER(I, J) bp[J*(J-1)/2 + I - 1]
#define B_LOWER(I, J) bp[(2*n-J)*(J-1)/2 + I - 1]
#define Z(I, J) z[(J-1)*pdz + I - 1]
    order = Nag_ColMajor;
#else
#define A_UPPER(I, J) ap[(2*n-I)*(I-1)/2 + J - 1]
#define A_LOWER(I, J) ap[I*(I-1)/2 + J - 1]
#define B_UPPER(I, J) bp[(2*n-I)*(I-1)/2 + J - 1]
#define B_LOWER(I, J) bp[I*(I-1)/2 + J - 1]
#define Z(I, J) z[(I-1)*pdz + J - 1]
    order = Nag_RowMajor;
#endif

    INIT_FAIL(fail);

    printf("nag_dspgvx (f08tbc) Example Program Results\n\n");

    /* Skip heading in data file */
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "%*[\n]", &n);
#else
    scanf("%" NAG_IFMT "%*[\n]", &n);
#endif
    if (n < 0) {
        printf("Invalid n\n");
        exit_status = 1;
        goto END;;
    }
#ifdef _WIN32
    scanf_s("%39s%*[\n]", nag_enum_arg, (unsigned)_countof(nag_enum_arg));

```

```

#else
    scanf(" %39s%*[\n]", nag_enum_arg);
#endif
/* nag_enum_name_to_value (x04nac).
 * Converts NAG enum member name to value
 */
uplo = (Nag_UploType) nag_enum_name_to_value(nag_enum_arg);

m = n;
pdz = n;
/* Allocate memory */
if (!(ap = NAG_ALLOC(n * (n + 1) / 2, double)) ||
    !(bp = NAG_ALLOC(n * (n + 1) / 2, double)) ||
    !(w = NAG_ALLOC(n, double)) ||
    !(z = NAG_ALLOC(n * m, double)) || !(index = NAG_ALLOC(n, Integer)))
{
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
}

/* Read the lower and upper bounds of the interval to be searched. */
#ifdef _WIN32
    scanf_s("%lf%lf%*[\n]", &vl, &vu);
#else
    scanf("%lf%lf%*[\n]", &vl, &vu);
#endif
/* Read the triangular parts of the matrices A and B from data file. */
if (uplo == Nag_Upper) {
    for (i = 1; i <= n; ++i)
#ifdef _WIN32
        for (j = i; j <= n; ++j)
            scanf_s("%lf", &A_UPPER(i, j));
#else
        for (j = i; j <= n; ++j)
            scanf("%lf", &A_UPPER(i, j));
#endif
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif
    for (i = 1; i <= n; ++i)
#ifdef _WIN32
        for (j = i; j <= n; ++j)
            scanf_s("%lf", &B_UPPER(i, j));
#else
        for (j = i; j <= n; ++j)
            scanf("%lf", &B_UPPER(i, j));
#endif
    }
    else if (uplo == Nag_Lower) {
        for (i = 1; i <= n; ++i)
#ifdef _WIN32
            for (j = 1; j <= i; ++j)
                scanf_s("%lf", &A_LOWER(i, j));
#else
            for (j = 1; j <= i; ++j)
                scanf("%lf", &A_LOWER(i, j));
#endif
#ifdef _WIN32
            scanf_s("%*[\n]");
#else
            scanf("%*[\n]");
#endif
        for (i = 1; i <= n; ++i)
#ifdef _WIN32
            for (j = 1; j <= i; ++j)
                scanf_s("%lf", &B_LOWER(i, j));
#else
            for (j = 1; j <= i; ++j)

```



```

        scanf("%lf", &B_LOWER(i, j));
#endif
    }
#ifdef _WIN32
    scanf_s("%*[^\\n]");
#else
    scanf("%*[^\\n]");
#endif

    /* use the default absolute error tolerance for eigenvalues. */
    abstol = 0.0;

    /* Solve the generalized symmetric eigenvalue problem A*x = lambda*B*x
     * using nag_dspgvx (f08tbc).
     */
    nag_dspgvx(order, 1, Nag_DoBoth, Nag_Interval, uplo, n, ap, bp, vl, vu, il,
               iu, abstol, &m, w, z, pdz, index, &fail);

    if (fail.code != NE_NOERROR) {
        printf("Error from nag_dspgvx (f08tbc).\\n%s\\n", fail.message);
        exit_status = 1;
        goto END;
    }

    /* Normalize the eigenvectors */
    for (j = 1; j <= m; j++)
        for (i = n; i >= 1; i--)
            z(i, j) = z(i, j) / z(1, j);

    /* Print eigensolution */
    printf("Number of eigenvalues found =%5" NAG_IFMT "\\n\\n", m);
    printf(" Eigenvalues\\n    ");
    for (j = 0; j < m; ++j)
        printf(" %8.4f%s", w[j], j % 8 == 7 ? "\\n" : "");
    printf("\\n");

    /* Print normalized vectors using nag_gen_real_mat_print (x04cac). */
    fflush(stdout);
    nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, m,
                           z, pdz, "Selected eigenvectors", 0, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_gen_real_mat_print (x04cac).\\n%s\\n", fail.message);
        exit_status = 1;
        goto END;
    }
}

END:
    NAG_FREE(ap);
    NAG_FREE(bp);
    NAG_FREE(w);
    NAG_FREE(z);
    NAG_FREE(index);

    return exit_status;
}

```

## 10.2 Program Data

nag\_dspgvx (f08tbc) Example Program Data

```

4                               : n

Nag_Upper                       : uplo

-1.0    1.0                     : VL and VU

0.24    0.39    0.42   -0.16
      -0.11    0.79    0.63
           -0.25    0.48
              -0.03   : matrix A

```

```
4.16  -3.12  0.56  -0.10
      5.03  -0.83  1.09
           0.76  0.34
           1.18 : matrix B
```

### 10.3 Program Results

nag\_dspgvx (f08tbc) Example Program Results

Number of eigenvalues found = 2

Eigenvalues

-0.4548 0.1001

Selected eigenvectors

	1	2
1	1.0000	1.0000
2	1.7303	0.0830
3	-1.1354	-0.1129
4	-2.0169	-1.0611

---