NAG Library Function Document

nag_zhbgvd (f08uqc)

1 Purpose

nag_zhbgvd (f08uqc) computes all the eigenvalues and, optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem, of the form

$$Az = \lambda Bz,$$

where A and B are Hermitian and banded, and B is also positive definite. If eigenvectors are desired, it uses a divide-and-conquer algorithm.

2 Specification

```
#include <nag.h>
#include <nagf08.h>
void nag_zhbgvd (Nag_OrderType order, Nag_JobType job, Nag_UploType uplo,
     Integer n, Integer ka, Integer kb, Complex ab[], Integer pdab,
     Complex bb[], Integer pdbb, double w[], Complex z[], Integer pdz,
     NagError *fail)
```

3 Description

The generalized Hermitian-definite band problem

$$Az = \lambda Bz$$

is first reduced to a standard band Hermitian problem

$$Cx = \lambda x,$$

where C is a Hermitian band matrix, using Wilkinson's modification to Crawford's algorithm (see Crawford (1973) and Wilkinson (1977)). The Hermitian eigenvalue problem is then solved for the eigenvalues and the eigenvectors, if required, which are then backtransformed to the eigenvectors of the original problem.

The eigenvectors are normalized so that the matrix of eigenvectors, Z, satisfies

$$Z^{\mathrm{H}}AZ = \Lambda \quad \text{and} \quad Z^{\mathrm{H}}BZ = I,$$

where Λ is the diagonal matrix whose diagonal elements are the eigenvalues.

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

Crawford C R (1973) Reduction of a band-symmetric generalized eigenvalue problem *Comm. ACM* **16** 41–44

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

Wilkinson J H (1977) Some recent advances in numerical linear algebra *The State of the Art in Numerical Analysis* (ed D A H Jacobs) Academic Press

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: **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.

3: **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.

4: **n** – Integer *Input*

On entry: n, the order of the matrices A and B.

Constraint: **n** ≥ 0.

5: **ka** – Integer *Input*

On entry: if **uplo** = Nag_Upper, the number of superdiagonals, k_a, of the matrix A.

If **uplo** = Nag_Lower, the number of subdiagonals, k_a, of the matrix A.

Constraint: **ka** ≥ 0.

6: **kb** – Integer *Input*

On entry: if **uplo** = Nag_Upper, the number of superdiagonals, k_b, of the matrix B.

If **uplo** = Nag_Lower, the number of subdiagonals, k_b, of the matrix B.

Constraint: **ka** $\geq$ **kb** ≥ 0.

7: **ab**[dim] – Complex *Input/Output*

Note: the dimension, *dim*, of the array **ab** must be at least $\max(1, \textbf{pdab} \times \textbf{n})$.

On entry: the upper or lower triangle of the n by n Hermitian band matrix A.

This is stored as a notional two-dimensional array with row elements or column elements stored contiguously. The storage of elements of A_{ij}, depends on the **order** and **uplo** arguments as follows:

if **order** = Nag_ColMajor and **uplo** = Nag_Upper,
A_{ij} is stored in **ab**$[k_a + i - j + (j-1) \times \textbf{pdab}]$, for $j = 1, \ldots, n$ and $i = \max(1, j - k_a), \ldots, j$;
if **order** = Nag_ColMajor and **uplo** = Nag_Lower,
A_{ij} is stored in **ab**$[i - j + (j-1) \times \textbf{pdab}]$, for $j = 1, \ldots, n$ and $i = j, \ldots, \min(n, j + k_a)$;

if **order** = Nag_RowMajor and **uplo** = Nag_Upper,
A_{ij} is stored in **ab**$[j-i+(i-1)\times$ **pdab**$]$, for $i=1,\ldots,n$ and $j=i,\ldots,\min(n,i+k_a)$;
if **order** = Nag_RowMajor and **uplo** = Nag_Lower,
A_{ij} is stored in **ab**$[k_a+j-i+(i-1)\times$ **pdab**$]$, for $i=1,\ldots,n$ and $j=\max(1,i-k_a),\ldots,i$.

On exit: the contents of **ab** are overwritten.

8: **pdab** – Integer *Input*

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

Constraint: **pdab** $\geq$ **ka** $+ 1$.

9: **bb**$[dim]$ – Complex *Input/Output*

Note: the dimension, *dim*, of the array **bb** must be at least $\max(1,$ **pdbb** $\times$ **n**$)$.

On entry: the upper or lower triangle of the n by n Hermitian band matrix B.

This is stored as a notional two-dimensional array with row elements or column elements stored contiguously. The storage of elements of B_{ij}, depends on the **order** and **uplo** arguments as follows:

if **order** = Nag_ColMajor and **uplo** = Nag_Upper,
B_{ij} is stored in **bb**$[k_b+i-j+(j-1)\times$ **pdbb**$]$, for $j=1,\ldots,n$ and $i=\max(1,j-k_b),\ldots,j$;
if **order** = Nag_ColMajor and **uplo** = Nag_Lower,
B_{ij} is stored in **bb**$[i-j+(j-1)\times$ **pdbb**$]$, for $j=1,\ldots,n$ and $i=j,\ldots,\min(n,j+k_b)$;
if **order** = Nag_RowMajor and **uplo** = Nag_Upper,
B_{ij} is stored in **bb**$[j-i+(i-1)\times$ **pdbb**$]$, for $i=1,\ldots,n$ and $j=i,\ldots,\min(n,i+k_b)$;
if **order** = Nag_RowMajor and **uplo** = Nag_Lower,
B_{ij} is stored in **bb**$[k_b+j-i+(i-1)\times$ **pdbb**$]$, for $i=1,\ldots,n$ and $j=\max(1,i-k_b),\ldots,i$.

On exit: the factor S from the split Cholesky factorization $B=S^{\mathrm{H}}S$, as returned by nag_zpbstf (f08utc).

10: **pdbb** – Integer *Input*

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

Constraint: **pdbb** $\geq$ **kb** $+ 1$.

11: **w**[**n**] – double *Output*

On exit: the eigenvalues in ascending order.

12: **z**$[dim]$ – Complex *Output*

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

$\max(1,$ **pdz** $\times$ **n**$)$ when **job** = Nag_DoBoth;
1 otherwise.

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

z$[(j-1)\times$ **pdz** $+i-1]$ when **order** = Nag_ColMajor;
z$[(i-1)\times$ **pdz** $+j-1]$ when **order** = Nag_RowMajor.

On exit: if **job** = Nag_DoBoth, **z** contains the matrix Z of eigenvectors, with the ith column of Z holding the eigenvector associated with $\mathbf{w}[i-1]$. The eigenvectors are normalized so that $Z^{\mathrm{H}}BZ = I$.

If **job** = Nag_EigVals, **z** is not referenced.

13: **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** ≥ 1.

14: **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 ⟨*value*⟩ had an illegal value.

NE_CONVERGENCE

The algorithm failed to converge; ⟨*value*⟩ off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

NE_ENUM_INT_2

On entry, **job** = ⟨*value*⟩, **pdz** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: if **job** = Nag_DoBoth, **pdz** $\geq \max(1, \mathbf{n})$;
otherwise **pdz** ≥ 1.

NE_INT

On entry, **ka** = ⟨*value*⟩.
Constraint: **ka** ≥ 0.

On entry, **n** = ⟨*value*⟩.
Constraint: **n** ≥ 0.

On entry, **pdab** = ⟨*value*⟩.
Constraint: **pdab** > 0.

On entry, **pdbb** = ⟨*value*⟩.
Constraint: **pdbb** > 0.

On entry, **pdz** = ⟨*value*⟩.
Constraint: **pdz** > 0.

NE_INT_2

On entry, **ka** = ⟨*value*⟩ and **kb** = ⟨*value*⟩.
Constraint: **ka** $\geq$ **kb** ≥ 0.

On entry, **pdab** $= \langle value \rangle$ and **ka** $= \langle value \rangle$.
Constraint: **pdab** $\geq$ **ka** $+ 1$.

On entry, **pdbb** $= \langle value \rangle$ and **kb** $= \langle value \rangle$.
Constraint: **pdbb** $\geq$ **kb** $+ 1$.

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 $1 \leq \langle value \rangle \leq$ **n**, then nag_zpbstf (f08utc) returned **fail.errnum** $= \langle value \rangle$: 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_zhbgvd (f08uqc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_zhbgvd (f08uqc) 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 if **job** $=$ Nag_DoBoth and, assuming that $n \gg k_a$, is approximately proportional to $n^2 k_a$ otherwise.

The real analogue of this function is nag_dsbgvd (f08ucc).

10 Example

This example finds all the eigenvalues of the generalized band Hermitian eigenproblem $Az = \lambda Bz$, where

$$A = \begin{pmatrix} -1.13 & 1.94 - 2.10i & -1.40 + 0.25i & 0 \\ 1.94 + 2.10i & -1.91 & -0.82 - 0.89i & -0.67 + 0.34i \\ -1.40 - 0.25i & -0.82 + 0.89i & -1.87 & -1.10 - 0.16i \\ 0 & -0.67 - 0.34i & -1.10 + 0.16i & 0.50 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 9.89 & 1.08 - 1.73i & 0 & 0 \\ 1.08 + 1.73i & 1.69 & -0.04 + 0.29i & 0 \\ 0 & -0.04 - 0.29i & 2.65 & -0.33 + 2.24i \\ 0 & 0 & -0.33 - 2.24i & 2.17 \end{pmatrix}.$$

10.1 Program Text

```
/* nag_zhbgvd (f08uqc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

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

int main(void)
{
  /* Scalars */
  Integer i, j, ka, kb, n, pdab, pdbb, pdz, zsize;
  Integer exit_status = 0;
  /* Arrays */
  Complex *ab = 0, *bb = 0, *z = 0;
  double *w = 0;
  char nag_enum_arg[40];

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

#ifdef NAG_COLUMN_MAJOR
#define AB_UPPER(I, J) ab[(J-1)*pdab + ka + I - J]
#define AB_LOWER(I, J) ab[(J-1)*pdab + I - J]
#define BB_UPPER(I, J) bb[(J-1)*pdbb + kb + I - J]
#define BB_LOWER(I, J) bb[(J-1)*pdbb + I - J]
  order = Nag_ColMajor;
#else
#define AB_UPPER(I, J) ab[(I-1)*pdab + J - I]
#define AB_LOWER(I, J) ab[(I-1)*pdab + ka + J - I]
#define BB_UPPER(I, J) bb[(I-1)*pdbb + J - I]
#define BB_LOWER(I, J) bb[(I-1)*pdbb + kb + J - I]
  order = Nag_RowMajor;
#endif

  INIT_FAIL(fail);

  printf("nag_zhbgvd (f08uqc) 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 "%" NAG_IFMT "%" NAG_IFMT "%*[^\n]", &n, &ka, &kb);
#else
  scanf("%" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[^\n]", &n, &ka, &kb);
#endif
```

```
  if (n < 0 || ka < kb || kb < 0) {
    printf("Invalid n, ka or kb\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);
#ifdef _WIN32
  scanf_s(" %39s%*[^\n]", nag_enum_arg, (unsigned)_countof(nag_enum_arg));
#else
  scanf(" %39s%*[^\n]", nag_enum_arg);
#endif
  job = (Nag_JobType) nag_enum_name_to_value(nag_enum_arg);
  if (job == Nag_EigVals) {
    zsize = 1;
    pdz = 1;
  }
  else {
    zsize = n * n;
    pdz = n;
  }

  pdab = ka + 1;
  pdbb = kb + 1;
  /* Allocate memory */
  if (!(ab = NAG_ALLOC((ka + 1) * n, Complex)) ||
      !(bb = NAG_ALLOC((kb + 1) * n, Complex)) ||
      !(z = NAG_ALLOC(zsize, Complex)) || !(w = NAG_ALLOC(n, double)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }

  /* Read the triangular parts of the matrices A and B from data file */
  if (uplo == Nag_Upper) {
    for (i = 1; i <= n; ++i)
      for (j = i; j <= MIN(i + ka, n); ++j)
#ifdef _WIN32
        scanf_s(" ( %lf , %lf )", &AB_UPPER(i, j).re, &AB_UPPER(i, j).im);
#else
        scanf(" ( %lf , %lf )", &AB_UPPER(i, j).re, &AB_UPPER(i, j).im);
#endif
#ifdef _WIN32
    scanf_s("%*[^\n]");
#else
    scanf("%*[^\n]");
#endif
    for (i = 1; i <= n; ++i)
      for (j = i; j <= MIN(i + kb, n); ++j)
#ifdef _WIN32
        scanf_s(" ( %lf , %lf )", &BB_UPPER(i, j).re, &BB_UPPER(i, j).im);
#else
        scanf(" ( %lf , %lf )", &BB_UPPER(i, j).re, &BB_UPPER(i, j).im);
#endif
  }
  else {
    for (i = 1; i <= n; ++i)
      for (j = MAX(1, i - ka); j <= i; ++j)
#ifdef _WIN32
        scanf_s(" ( %lf , %lf )", &AB_LOWER(i, j).re, &AB_LOWER(i, j).im);
#else
        scanf(" ( %lf , %lf )", &AB_LOWER(i, j).re, &AB_LOWER(i, j).im);
#endif
```

```
#ifdef _WIN32
    scanf_s("%*[^\n]");
#else
    scanf("%*[^\n]");
#endif
    for (i = 1; i <= n; ++i)
      for (j = MAX(1, i - kb); j <= i; ++j)
#ifdef _WIN32
        scanf_s(" ( %lf , %lf )", &BB_LOWER(i, j).re, &BB_LOWER(i, j).im);
#else
        scanf(" ( %lf , %lf )", &BB_LOWER(i, j).re, &BB_LOWER(i, j).im);
#endif
  }
#ifdef _WIN32
  scanf_s("%*[^\n]");
#else
  scanf("%*[^\n]");
#endif

  /* Solve the generalized Hermitian band eigenvalue problem A*x = lambda*B*x
   * using nag_zhbgvd (f08uqc).
   */
  nag_zhbgvd(order, job, uplo, n, ka, kb, ab, pdab, bb, pdbb, w, z, pdz,
             &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_zhbgvd (f08uqc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Print eigensolution */
  printf(" Eigenvalues\n   ");
  for (j = 0; j < n; ++j)
    printf(" %10.4f%s", w[j], j % 6 == 5 ? "\n" : " ");
  printf("\n");
  if (job == Nag_DoBoth) {
    /* nag_gen_complx_mat_print (x04dac): Print Matrix of eigenvectors Z. */
    printf("\n");
    fflush(stdout);
    nag_gen_complx_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, n,
                             z, pdz, "Eigenvectors", 0, &fail);
    if (fail.code != NE_NOERROR) {
      printf("Error from nag_gen_complx_mat_print (x04dac).\n%s\n",
             fail.message);
      exit_status = 1;
    }
  }

END:
  NAG_FREE(ab);
  NAG_FREE(bb);
  NAG_FREE(z);
  NAG_FREE(w);

  return exit_status;
}
```

10.2 Program Data

```
nag_zhbgvd (f08uqc) Example Program Data

   4            2            1                          : n, ka and kb

   Nag_Upper                                            : uplo
   Nag_EigVals                                          : job

 (-1.13, 0.00) ( 1.94,-2.10) (-1.40, 0.25)
               (-1.91, 0.00) (-0.82,-0.89) (-0.67, 0.34)
                             (-1.87, 0.00) (-1.10,-0.16)
                                           ( 0.50, 0.00) : matrix A
```

```
 ( 9.89, 0.00) ( 1.08,-1.73)
               ( 1.69, 0.00) (-0.04, 0.29)
                             ( 2.65, 0.00) (-0.33, 2.24)
                                           ( 2.17, 0.00) : matrix B
```

10.3 Program Results

```
nag_zhbgvd (f08uqc) Example Program Results

 Eigenvalues
       -6.6089     -2.0416      0.1603      1.7712
```