NAG C Library Function Document nag dpbtrf (f07hdc)

1 Purpose

nag dpbtrf (f07hdc) computes the Cholesky factorization of a real symmetric positive-definite band matrix.

2 Specification

3 Description

nag_dpbtrf (f07hdc) forms the Cholesky factorization of a real symmetric positive-definite band matrix A either as $A = U^T U$ if $\mathbf{uplo} = \mathbf{Nag_Upper}$, or $A = LL^T$ if $\mathbf{uplo} = \mathbf{Nag_Lower}$, where U (or L) is an upper (or lower) triangular band matrix with the same number of super-diagonals (or sub-diagonals) as A.

4 References

Demmel J W (1989) On floating-point errors in Cholesky *LAPACK Working Note No. 14* University of Tennessee, Knoxville

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

5 Parameters

1: **order** – Nag OrderType

Input

On entry: the **order** parameter 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 2.2.1.4 of the Essential Introduction for a more detailed explanation of the use of this parameter.

Constraint: order = Nag_RowMajor or Nag_ColMajor.

2: **uplo** – Nag_UploType

Input

On entry: indicates whether the upper or lower triangular part of A is stored and how A is factorized, as follows:

if $\mathbf{uplo} = \mathbf{Nag_Upper}$, the upper triangular part of A is stored and A is factorized as U^TU , where U is upper triangular;

if $\mathbf{uplo} = \mathbf{Nag_Lower}$, the lower triangular part of A is stored and A is factorized as LL^T , where L is lower triangular.

Constraint: uplo = Nag_Upper or Nag_Lower.

3: \mathbf{n} - Integer Input

On entry: n, the order of the matrix A.

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

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4: **kd** – Integer *Input*

On entry: k, the number of super-diagonals or sub-diagonals of the matrix A.

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

5: $\mathbf{ab}[dim] - \text{double}$

Input/Output

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

On entry: the n by n symmetric band matrix A. This is stored as a notional two-dimensional array with row elements or column elements stored contiguously. The storage of elements a_{ij} depends on the **order** and **uplo** parameters as follows:

```
if order = Nag_ColMajor and uplo = Nag_Upper, a_{ij} is stored in \mathbf{ab}[k+i-j+(j-1)\times\mathbf{pdab}], for i=1,\ldots,n and j=i,\ldots,\min(n,i+k); if order = Nag_ColMajor and uplo = Nag_Lower, a_{ij} is stored in \mathbf{ab}[i-j+(j-1)\times\mathbf{pdab}], for i=1,\ldots,n and j=\max(1,i-k),\ldots,i; if order = Nag_RowMajor and uplo = Nag_Upper, a_{ij} is stored in \mathbf{ab}[j-i+(i-1)\times\mathbf{pdab}], for i=1,\ldots,n and j=i,\ldots,\min(n,i+k); if order = Nag_RowMajor and uplo = Nag_Lower, a_{ij} is stored in \mathbf{ab}[k+j-i+(i-1)\times\mathbf{pdab}], for i=1,\ldots,n and j=\max(1,i-k),\ldots,i.
```

On exit: the upper or lower triangle of A is overwritten by the Cholesky factor U or L as specified by **uplo**, using the same storage format as described above.

6: **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: $pdab \ge kd + 1$.

7: **fail** – NagError *

Output

The NAG error parameter (see the Essential Introduction).

6 Error Indicators and Warnings

NE INT

```
On entry, \mathbf{n} = \langle value \rangle.
Constraint: \mathbf{n} \geq 0.
On entry, \mathbf{kd} = \langle value \rangle.
Constraint: \mathbf{kd} \geq 0.
On entry, \mathbf{pdab} = \langle value \rangle.
Constraint: \mathbf{pdab} > 0.
```

NE_INT_2

```
On entry, \mathbf{pdab} = \langle value \rangle, \mathbf{kd} = \langle value \rangle.
Constraint: \mathbf{pdab} \geq \mathbf{kd} + 1.
```

NE POS DEF

The matrix A is not positive definite.

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NE ALLOC FAIL

Memory allocation failed.

NE BAD PARAM

On entry, parameter (value) had an illegal value.

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 consult NAG for assistance.

7 Accuracy

If **uplo** = Nag_Upper, the computed factor U is the exact factor of a perturbed matrix A + E, where

$$|E| \le c(k+1)\epsilon |U^T| |U|,$$

c(k+1) is a modest linear function of k+1, and ϵ is the *machine precision*.

If **uplo** = **Nag_Lower**, a similar statement holds for the computed factor L. It follows that $|e_{ij}| \le c(k+1)\epsilon \sqrt{a_{ii}a_{jj}}$.

8 Further Comments

The total number of floating-point operations is approximately $n(k+1)^2$, assuming $n \gg k$.

A call to this function may be followed by calls to the functions:

```
nag dpbtrs (f07hec) to solve AX = B;
```

nag_dpbcon (f07hgc) to estimate the condition number of A.

The complex analogue of this function is nag zpbtrf (f07hrc).

9 Example

To compute the Cholesky factorization of the matrix A, where

$$A = \begin{pmatrix} 5.49 & 2.68 & 0.00 & 0.00 \\ 2.68 & 5.63 & -2.39 & 0.00 \\ 0.00 & -2.39 & 2.60 & -2.22 \\ 0.00 & 0.00 & -2.22 & 5.17 \end{pmatrix}$$

9.1 Program Text

```
/* nag_dpbtrf (f07hdc) Example Program.

*
 * Copyright 2001 Numerical Algorithms Group.

*
 * Mark 7, 2001.
 */

#include <stdio.h>
#include <nag.h>
#include <nag.stdlib.h>
#include <nagf07.h>
#include <nagx04.h>

int main(void)
{
    /* Scalars */
    Integer i, j, k, kd, n, pdab;
    Integer exit_status=0;
    Nag_UploType uplo_enum;
```

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```
NagError fail;
  Nag_OrderType order;
  /* Arrays */
  char uplo[2];
  double *ab=0;
#ifdef NAG_COLUMN_MAJOR
#define AB_UPPER(I,J) ab[(J-1)*pdab + k + I - J - 1]
#define AB_LOWER(I,J) ab[(J-1)*pdab + 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 + k + J - I - 1]
 order = Nag_RowMajor;
#endif
  INIT_FAIL(fail);
  Vprintf("f07hdc Example Program Results\n\n");
  /* Skip heading in data file */
  Vscanf("%*[^\n] ");
  Vscanf("%ld%ld%*[^\n] ", &n, &kd);
  pdab = kd + 1;
  /* Allocate memory */
  if ( !(ab = NAG\_ALLOC((kd+1) * n, double)) )
      Vprintf("Allocation failure\n");
      exit_status = -1;
      goto END;
 /* Read A from data file */
Vscanf(" ' %1s '%*[^\n] ", uplo);
if (*(unsigned char *)uplo == 'L')
    uplo_enum = Nag_Lower;
  else if (*(unsigned char *)uplo == 'U')
    uplo_enum = Nag_Upper;
  else
      Vprintf("Unrecognised character for Nag_UploType type\n");
      exit_status = -1;
      goto END;
  k = kd + 1;
  if (uplo_enum == Nag_Upper)
    {
      for (i = 1; i \le n; ++i)
          for (j = i; j \le MIN(i+kd,n); ++j)
            Vscanf("%lf", &AB_UPPER(i,j));
      Vscanf("%*[^\n] ");
    }
  else
      for (i = 1; i \le n; ++i)
          for (j = MAX(1,i-kd); j \le i; ++j)
            Vscanf("%lf", &AB_LOWER(i,j));
      Vscanf("%*[^\n] ");
    }
  /* Factorize A */
  f07hdc(order, uplo_enum, n, kd, ab, pdab, &fail);
  if (fail.code != NE_NOERROR)
      Vprintf("Error from f07hdc.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
```

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```
/* Print details of factorization */
if (uplo_enum == Nag_Upper)
   x04cec(order, n, n, 0, kd, ab, pdab, "Factor", 0, &fail);
else
   x04cec(order, n, n, kd, 0, ab, pdab, "Factor", 0, &fail);
if (fail.code != NE_NOERROR)

{
    Vprintf("Error from x04cec.\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}
END:
if (ab) NAG_FREE(ab);
return exit_status;
}
```

9.2 Program Data

```
f07hdc Example Program Data
4 1 :Values of N and KD
'L' :Value of UPLO
5.49
2.68 5.63
-2.39 2.60
-2.22 5.17 :End of matrix A
```

9.3 Program Results

f07hdc Example Program Results

```
Factor

1 2 3 4 4

1 2.3431
2 1.1438 2.0789
3 -1.1497 1.1306
4 -1.9635 1.1465
```

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