NAG C Library Function Document

nag_dpotrf (f07fdc)

1 Purpose

nag_dpotrf (f07fdc) computes the Cholesky factorization of a real symmetric positive-definite matrix.

2 Specification

```
void nag_dpotrf (Nag_OrderType order, Nag_UploType uplo, Integer n, double a[],
     Integer pda, NagError *fail)
```

3 Description

nag_dpotrf (f07fdc) forms the Cholesky factorization of a real symmetric positive-definite matrix A either as $A = U^TU$ if **uplo** = **Nag_Upper**, or $A = LL^T$ if **uplo** = **Nag_Lower**, where U is an upper triangular matrix and L is lower triangular.

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 **uplo** = **Nag_Upper**, the upper triangular part of A is stored and A is factorized as U^TU, where U is upper triangular;

if **uplo** = **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: **n** – Integer *Input*

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

Constraint: **n** ≥ 0.

4: **a**$[dim]$ – double *Input/Output*

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

If **order** = **Nag_ColMajor**, the (i, j)th element of the matrix A is stored in **a**$[(j-1) \times$ **pda** $+ i - 1]$ and if **order** = **Nag_RowMajor**, the (i, j)th element of the matrix A is stored in **a**$[(i-1) \times$ **pda** $+ j - 1]$.

On entry: the n by n symmetric positive-definite matrix A. If **uplo** = **Nag_Upper**, the upper triangle of A must be stored and the elements of the array below the diagonal are not referenced; if **uplo** = **Nag_Lower**, the lower triangle of A must be stored and the elements of the array above the diagonal are not referenced.

On exit: the upper or lower triangle of A is overwritten by the Cholesky factor U or L as specified by **uplo**.

5: **pda** – Integer *Input*

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

Constraint: **pda** $\geq \max(1,$ **n**$)$.

6: **fail** – NagError * *Output*

The NAG error parameter (see the Essential Introduction).

6 Error Indicators and Warnings

NE_INT

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

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

NE_INT_2

On entry, **pda** = ⟨*value*⟩, **n** = ⟨*value*⟩.
Constraint: **pda** $\geq \max(1,$ **n**$)$.

NE_POS_DEF

The leading minor of order ⟨*value*⟩ is not positive-definite and the factorization could not be completed. Hence A itself is not positive-definite. This may indicate an error in forming the matrix A. To factorize a symmetric matrix which is not positive-definite, call nag_dsytrf (f07mdc) instead.

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

$$|E| \leq c(n)\epsilon|U^T|\,|U|,$$

$c(n)$ is a modest linear function of n, and ϵ is the ***machine precision***. If **uplo** = **Nag_Lower**, a similar statement holds for the computed factor L. It follows that $|e_{ij}| \leq c(n)\epsilon\sqrt{a_{ii}a_{jj}}$.

8 Further Comments

The total number of floating-point operations is approximately $\frac{1}{3}n^3$.

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

nag_dpotrs (f07fec) to solve $AX = B$;

nag_dpocon (f07fgc) to estimate the condition number of A;

nag_dpotri (f07fjc) to compute the inverse of A.

The complex analogue of this function is nag_zpotrf (f07frc).

9 Example

To compute the Cholesky factorization of the matrix A, where

$$A = \begin{pmatrix} 4.16 & -3.12 & 0.56 & -0.10 \\ -3.12 & 5.03 & -0.83 & 1.18 \\ 0.56 & -0.83 & 0.76 & 0.34 \\ -0.10 & 1.18 & 0.34 & 1.18 \end{pmatrix}.$$

9.1 Program Text

```
/* nag_dpotrf (f07fdc) 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, n, pda;
  Integer exit_status=0;
  Nag_UploType uplo_enum;
  Nag_MatrixType matrix;

  NagError fail;
  Nag_OrderType order;
  /* Arrays */
  char   uplo[2];
  double *a=0;

#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;
#endif

  INIT_FAIL(fail);
  Vprintf("f07fdc Example Program Results\n\n");

  /* Skip heading in data file */
  Vscanf("%*[^\n] ");
  Vscanf("%ld%*[^\n] ", &n);
#ifdef NAG_COLUMN_MAJOR
  pda = n;
#else
```

```
  pda = n;
#endif
  /* Allocate memory */
  if ( !(a = NAG_ALLOC(n * 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;
     matrix = Nag_LowerMatrix;
   }
 else if (*(unsigned char *)uplo == 'U')
   {
     uplo_enum = Nag_Upper;
     matrix = Nag_UpperMatrix;
   }
 else
   {
     Vprintf("Unrecognised character for Nag_UploType type\n");
     exit_status = -1;
     goto END;
   }
  if (uplo_enum == Nag_Upper)
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = i; j <= n; ++j)
            Vscanf("%lf", &A(i,j));
        }
      Vscanf("%*[^\n] ");
    }
  else
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            Vscanf("%lf", &A(i,j));
        }
      Vscanf("%*[^\n] ");
    }

  /* Factorize A */
  f07fdc(order, uplo_enum, n, a, pda, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from f07fdc.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }

  /* Print factor */
  x04cac(order, matrix, Nag_NonUnitDiag, n, n, a, pda,
         "Factor", 0, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from x04cac.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
 END:
  if (a) NAG_FREE(a);
  return exit_status;
}
```

9.2 Program Data

```
f07fdc Example Program Data
  4                           :Value of N
  'L'                         :Value of UPLO
  4.16
 -3.12   5.03
  0.56  -0.83   0.76
 -0.10   1.18   0.34   1.18   :End of matrix A
```

9.3 Program Results

```
f07fdc Example Program Results

 Factor
             1           2           3           4
 1      2.0396
 2     -1.5297      1.6401
 3      0.2746     -0.2500      0.7887
 4     -0.0490      0.6737      0.6617      0.5347
```