

NAG Library Function Document

nag_dpotrf (f07fdc)

1 Purpose

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

2 Specification

```
#include <nag.h>
#include <nagf07.h>

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 $A = U^T U$ if **uplo** = Nag_Upper or $A = L L^T$ 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 <http://www.netlib.org/lapack/lawnspdf/lawn14.pdf>

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: **uplo** – Nag_UploType *Input*
On entry: specifies whether the upper or lower triangular part of A is stored and how A is to be factorized.
uplo = Nag_Upper
The upper triangular part of A is stored and A is factorized as $U^T U$, where U is upper triangular.
uplo = Nag_Lower
The lower triangular part of A is stored and A is factorized as $L L^T$, 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: $n \geq 0$.
- 4: **a**[*dim*] – double *Input/Output*
 Note: the dimension, *dim*, of the array **a** must be at least $\max(1, \mathbf{pda} \times \mathbf{n})$.
 On entry: the n by n symmetric positive definite matrix A .
 If **order** = Nag_ColMajor, A_{ij} is stored in $\mathbf{a}[(j-1) \times \mathbf{pda} + i - 1]$.
 If **order** = Nag_RowMajor, A_{ij} is stored in $\mathbf{a}[(i-1) \times \mathbf{pda} + j - 1]$.
 If **uplo** = Nag_Upper, the upper triangular part of A must be stored and the elements of the array below the diagonal are not referenced.
 If **uplo** = Nag_Lower, the lower triangular part 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: $\mathbf{pda} \geq \max(1, \mathbf{n})$.
- 6: **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 $\langle \text{value} \rangle$ had an illegal value.

NE_INT

On entry, $\mathbf{n} = \langle \text{value} \rangle$.

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

On entry, $\mathbf{pda} = \langle \text{value} \rangle$.

Constraint: $\mathbf{pda} > 0$.

NE_INT_2

On entry, $\mathbf{pda} = \langle \text{value} \rangle$ and $\mathbf{n} = \langle \text{value} \rangle$.

Constraint: $\mathbf{pda} \geq \max(1, \mathbf{n})$.

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.

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_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.

NE_POS_DEF

The leading minor of order $\langle value \rangle$ 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.

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 Parallelism and Performance

nag_dpotr (f07fdc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_dpotr (f07fdc) 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 approximately $\frac{1}{3}n^3$.

A call to nag_dpotr (f07fdc) 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_zpotr (f07frc).

10 Example

This example computes the Cholesky factorization of the matrix A , where

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

10.1 Program Text

```

/* nag_dpotrf (f07fdc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#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;
    Nag_MatrixType matrix;
    NagError fail;
    Nag_OrderType order;
    /* Arrays */
    char nag_enum_arg[40];
    double *a = 0;
#ifdef NAG_LOAD_FP
    /* The following line is needed to force the Microsoft linker
       to load floating point support */
    float force_loading_of_ms_float_support = 0;
#endif /* NAG_LOAD_FP */

#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);

    printf("nag_dpotrf (f07fdc) 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
#ifdef NAG_COLUMN_MAJOR
    pda = n;
#else
    pda = n;
#endif
    /* Allocate memory */
    if (!(a = NAG_ALLOC(n * n, double)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
}

```

```

/* Read A from data file */
#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);

if (uplo == Nag_Upper) {
    matrix = Nag_UpperMatrix;
    for (i = 1; i <= n; ++i) {
        for (j = i; j <= n; ++j)
#ifdef _WIN32
            scanf_s("%lf", &A(i, j));
#else
            scanf("%lf", &A(i, j));
#endif
    }
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif
} else {
    matrix = Nag_LowerMatrix;
    for (i = 1; i <= n; ++i) {
        for (j = 1; j <= i; ++j)
#ifdef _WIN32
            scanf_s("%lf", &A(i, j));
#else
            scanf("%lf", &A(i, j));
#endif
    }
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif
}

/* Factorize A */
/* nag_dpotrf (f07fdc).
 * Cholesky factorization of real symmetric
 * positive-definite matrix
 */
nag_dpotrf(order, uplo, n, a, pda, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dpotrf (f07fdc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Print factor */
/* nag_gen_real_mat_print (x04cac).
 * Print real general matrix (easy-to-use)
 */
fflush(stdout);
nag_gen_real_mat_print(order, matrix, Nag_NonUnitDiag, n, n, a, pda,
    "Factor", 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(a);

    return exit_status;
}

```

10.2 Program Data

```

nag_dpotrf (f07fdc) Example Program Data
4                               :Value of n
Nag_Lower                      :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

```

10.3 Program Results

nag_dpotrf (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
