NAG Library Function Document
nag_dsytrf (f07mdc)

1 Purpose
nag_dsytrf (f07mdc) computes the Bunch–Kaufman factorization of a real symmetric indefinite matrix.

2 Specification
#include <nag.h>
#include <nagf07.h>
void nag_dsytrf (Nag_OrderType order, Nag_UploType uplo, Integer n,
                  double a[], Integer pda, Integer ipiv[], NagError *fail)

3 Description
nag_dsytrf (f07mdc) factorizes a real symmetric matrix \( A \), using the Bunch–Kaufman diagonal pivoting method. \( A \) is factorized as either

\[
A = PUDU^T P^T \quad \text{if } \text{uplo} = \text{Nag_Upper}
\]

or

\[
A = PLDL^T P^T \quad \text{if } \text{uplo} = \text{Nag_Lower},
\]

where \( P \) is a permutation matrix, \( U \) (or \( L \)) is a unit upper (or lower) triangular matrix and \( D \) is a symmetric block diagonal matrix with 1 by 1 and 2 by 2 diagonal blocks; \( U \) (or \( L \)) has 2 by 2 unit diagonal blocks corresponding to the 2 by 2 blocks of \( D \). Row and column interchanges are performed to ensure numerical stability while preserving symmetry.

This method is suitable for symmetric matrices which are not known to be positive definite. If \( A \) is in fact positive definite, no interchanges are performed and no 2 by 2 blocks occur in \( D \).

4 References

5 Arguments
1: order – Nag_OrderType
   
   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 3.2.1.3 in the Essential Introduction for a more detailed explanation of the use of this argument.

   Constraint: order = Nag_RowMajor or Nag_ColMajor.

2: uplo – Nag_UploType
   
   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 \( PUDU^T P^T \), where \( U \) is upper triangular.

   uplo = Nag_Lower
   The lower triangular part of \( A \) is stored and \( A \) is factorized as \( PLDL^T P^T \), where \( L \) is lower triangular.

   Constraint: uplo = Nag_Upper or Nag_Lower.
3: \[ n \text{ – Integer} \]

\text{Input}

\text{On entry:} n, the order of the matrix \( A \).

\text{Constraint:} n \geq 0.

4: \[ a[\text{dim}] \text{ – double} \]

\text{Input/Output}

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

\text{On entry:} the \( n \) by \( n \) symmetric indefinite matrix \( A \).

If \( \text{order} = \text{Nag\_ColMajor} \), \( A_{ij} \) is stored in \( a[(j-1) \times pda + i - 1] \).

If \( \text{order} = \text{Nag\_RowMajor} \), \( A_{ij} \) is stored in \( a[(i-1) \times pda + j - 1] \).

If \( \text{uplo} = \text{Nag\_Upper} \), the upper triangular part of \( A \) must be stored and the elements of the array below the diagonal are not referenced.

If \( \text{uplo} = \text{Nag\_Lower} \), the lower triangular part of \( A \) must be stored and the elements of the array above the diagonal are not referenced.

\text{On exit:} the upper or lower triangle of \( A \) is overwritten by details of the block diagonal matrix \( D \) and the multipliers used to obtain the factor \( U \) or \( L \) as specified by \( \text{uplo} \).

5: \[ pda \text{ – Integer} \]

\text{Input}

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

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

6: \[ \text{ipiv}[\text{dim}] \text{ – Integer} \]

\text{Output}

\text{Note:} the dimension, \( \text{dim} \), of the array \( \text{ipiv} \) must be at least \( \max(1, n) \).

\text{On exit:} details of the interchanges and the block structure of \( D \). More precisely,

\begin{itemize}
  \item if \( \text{ipiv}[i-1] = k > 0 \), \( d_{ii} \) is a 1 by 1 pivot block and the \( i \)th row and column of \( A \) were interchanged with the \( k \)th row and column;
  \item if \( \text{uplo} = \text{Nag\_Upper} \) and \( \text{ipiv}[i-2] = \text{ipiv}[i-1] = -l < 0 \), \( \begin{pmatrix} d_{i-1,i-1} & \tilde{d}_{i,j-1} \\
\tilde{d}_{i,j-1} & d_{ij} \end{pmatrix} \) is a 2 by 2 pivot block and the \((i-1)\)th row and column of \( A \) were interchanged with the \( l \)th row and column;
  \item if \( \text{uplo} = \text{Nag\_Lower} \) and \( \text{ipiv}[i-1] = \text{ipiv}[i] = -m < 0 \), \( \begin{pmatrix} d_{ii} & d_{i+1,i} \\
\tilde{d}_{i+1,i} & d_{i+1,i+1} \end{pmatrix} \) is a 2 by 2 pivot block and the \((i+1)\)th row and column of \( A \) were interchanged with the \( m \)th row and column.
\end{itemize}

7: \[ \text{fail} \text{ – NagError} * \]

\text{Input/Output}

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 \hspace{1cm} \textbf{Error Indicators and Warnings}

\textbf{NE\_ALLOC\_FAIL}

Dynamic memory allocation failed.

See Section 3.2.1.2 in the Essential Introduction for further information.

\textbf{NE\_BAD\_PARAM}

On entry, argument \( \langle \text{value} \rangle \) had an illegal value.
NE_INT
On entry, \( n = \langle \text{value} \rangle \).
Constraint: \( n \geq 0 \).
On entry, \( pda = \langle \text{value} \rangle \).
Constraint: \( pda > 0 \).

NE_INT_2
On entry, \( pda = \langle \text{value} \rangle \) and \( n = \langle \text{value} \rangle \).
Constraint: \( pda \geq \max(1,n) \).

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 3.6.6 in the Essential Introduction for further information.

NE_NO_LICENCE
Your licence key may have expired or may not have been installed correctly.
See Section 3.6.5 in the Essential Introduction for further information.

NE_SINGULAR
Element \( \langle \text{value} \rangle \) of the diagonal is exactly zero. The factorization has been completed, but the block diagonal matrix \( D \) is exactly singular, and division by zero will occur if it is used to solve a system of equations.

7 Accuracy
If \( \text{uplo} = \text{Nag}_\text{Upper} \), the computed factors \( U \) and \( D \) are the exact factors of a perturbed matrix \( A + E \), where
\[
|E| \leq c(n)\epsilon P||U||D||U^T|F^T,
\]
\( c(n) \) is a modest linear function of \( n \), and \( \epsilon \) is the machine precision.
If \( \text{uplo} = \text{Nag}_\text{Lower} \), a similar statement holds for the computed factors \( L \) and \( D \).

8 Parallelism and Performance
nag_dsytrf (f07mdc) is not threaded by NAG in any implementation.
nag_dsytrf (f07mdc) 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 elements of \( D \) overwrite the corresponding elements of \( A \); if \( D \) has 2 by 2 blocks, only the upper or lower triangle is stored, as specified by \( \text{uplo} \).
The unit diagonal elements of \( U \) or \( L \) and the 2 by 2 unit diagonal blocks are not stored. The remaining elements of \( U \) or \( L \) are stored in the corresponding columns of the array \( a \), but additional row interchanges must be applied to recover \( U \) or \( L \) explicitly (this is seldom necessary). If \( \text{ipiv}[i-1] = i \),
for $i = 1, 2, \ldots, n$ (as is the case when $A$ is positive definite), then $U$ or $L$ is stored explicitly (except for its unit diagonal elements which are equal to 1).

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

A call to nag_dsytrf (f07mdc) may be followed by calls to the functions:

- nag_dsytrs (f07mec) to solve $AX = B$;
- nag_dsycon (f07mgc) to estimate the condition number of $A$;
- nag_dsytri (f07mjc) to compute the inverse of $A$.

The complex analogues of this function are nag_zhetrf (f07mrc) for Hermitian matrices and nag_zsytrf (f07nrc) for symmetric matrices.

10 Example

This example computes the Bunch–Kaufman factorization of the matrix $A$, where

$$
A = \begin{pmatrix}
2.07 & 3.87 & 4.20 & -1.15 \\
3.87 & -0.21 & 1.87 & 0.63 \\
4.20 & 1.87 & 1.15 & 2.06 \\
-1.15 & 0.63 & 2.06 & -1.81
\end{pmatrix}
$$

10.1 Program Text

/* nag_dsytrf (f07mdc) Example Program. */
/* Copyright 2014 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, nrhs, pda, pdb;
    Integer exit_status = 0;
    NagError fail;
    Nag_UploType uplo;
    Nag_OrderType order;
    /* Arrays */
    char nag_enum_arg[40];
    Integer *ipiv = 0;
    double *a = 0, *b = 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]
    #define B(I, J) b[(J-1)*pdb + I - 1]
    order = Nag_ColMajor;
    #else
    #define A(I, J) a[(J-1)*pda + I - 1]
    #define B(I, J) b[(J-1)*pdb + I - 1]
    order = Nag_RowMajor;
    #endif

    "07mdc.4 Mark 25"
INIT_FAIL(fail);

printf("nag_dsytrf (f07mdc) Example Program Results\n\n");
/* Skip heading in data file */
#endif _WIN32
scanf_s("%*[\n ] ");
#else
scanf("%*[\n ] ");
#endif _WIN32
scanf_s("%"NAG_IFMT"%"NAG_IFMT"%*[\n ] ", &n, &nrhs);
#else
scanf("%"NAG_IFMT"%"NAG_IFMT"%*[\n ] ", &n, &nrhs);
#endif _WIN32
#endif NAG_COLUMN_MAJOR
pda = n;
pdb = n;
#else
pda = n;
pdb = nrhs;
#endif
/* Allocate memory */
if (!(ipiv = NAG_ALLOC(n, Integer)) ||
!(a = NAG_ALLOC(n * n, double)) ||
!(b = NAG_ALLOC(n * nrhs, double)))
{
printf("Allocation failure\n");
exit_status = -1;
goto END;
}
/* Read A and B from data file */
#endif _WIN32
scanf_s(" %39s%*[\n ] ", nag_enum_arg, _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)
{
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
}
#else
 scanf_s("%*[\n ] ");
#else
scanf("%*[\n ] ");
#endif
} else
{
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
} 
#endif _WIN32
for (i = 1; i <= n; ++i)
{
    for (j = 1; j <= nrhs; ++j)
        #ifdef _WIN32
            scanf_s("%lf", &B(i, j));
        #else
            scanf("%lf", &B(i, j));
        #endif
    #ifdef _WIN32
        scanf_s("%*[\n"]
    #else
        scanf("%*[\n"]
    #endif
}

/* Factorize A */
/* nag_dsytrf (f07mdc). *
 * Bunch-Kaufman factorization of real symmetric indefinite
 * matrix *
*/
#ifdef _WIN32
    scanf_s("%*[\n"]
#else
    scanf("%*[\n"]
#endif
nag_dsytrf(order, uplo, n, a, pda, ipiv, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_dsytrf (f07mdc).
%s
", fail.message);
    exit_status = 1;
    goto END;
}

/* Compute solution */
/* nag_dsytrs (f07mec). *
 * Solution of real symmetric indefinite system of linear
 * equations, multiple right-hand sides, matrix already
 * factorized by nag_dsytrf (f07mdc)
*/
#ifdef _WIN32
    scanf_s("%*[\n"]
#else
    scanf("%*[\n"]
#endif
nag_dsytrs(order, uplo, n, nrhs, a, pda, ipiv, b, pdb,
&fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_dsytrs (f07mec).
%s
", fail.message);
    exit_status = 1;
    goto END;
}

/* Print solution */
/* nag_gen_real_mat_print (x04cac). *
 * Print real general matrix (easy-to-use) *
 */
fflush(stdout);
nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, nrhs, b,
    pdb, "Solution(s)", 0, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_gen_real_mat_print (x04cac).
%s
", fail.message);
    exit_status = 1;
    goto END;
}
END:
NAG_FREE(ipiv);
NAG_FREE(a);
NAG_FREE(b);
return exit_status;
10.2 Program Data

nag_dsytrf (f07mdc) Example Program Data

4 2 :Values of n and nrhs
Nag_Lower :Value of uplo
2.07
3.87 -0.21
4.20 1.87 1.15
-1.15 0.63 2.06 -1.81 :End of matrix A
-9.50 27.85
-8.38 9.90
-6.07 19.25
-0.96 3.93 :End of matrix B

10.3 Program Results

nag_dsytrf (f07mdc) Example Program Results

Solution(s)

<table>
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<tr>
<th></th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
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<td>1.0000</td>
</tr>
<tr>
<td>2</td>
<td>-1.0000</td>
<td>4.0000</td>
</tr>
<tr>
<td>3</td>
<td>2.0000</td>
<td>3.0000</td>
</tr>
<tr>
<td>4</td>
<td>5.0000</td>
<td>2.0000</td>
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