NAG Library Function Document

nag_zsptrf (f07qrc)

1 Purpose

nag_zsptrf (f07qrc) computes the Bunch–Kaufman factorization of a complex symmetric matrix, using packed storage.

2 Specification

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

void nag_zsptrf (Nag_OrderType order, Nag_UploType uplo, Integer n,
                 Complex ap[], Integer ipiv[], NagError *fail)
```

3 Description

nag_zsptrf (f07qrc) factorizes a complex symmetric matrix $A$, using the Bunch–Kaufman diagonal pivoting method and packed storage. $A$ is factorized as either $A = PUDU^T P^T$ if $\text{uplo} = \text{Nag_Upper}$ or $A = PLDL^T P^T$ 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.

4 References


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 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

   *Input*

   On entry: specifies whether the upper or lower triangular part of $A$ is stored and how $A$ is to be factorized.

   $\text{uplo} = \text{Nag_Upper}$

   The upper triangular part of $A$ is stored and $A$ is factorized as $PUDU^T P^T$, where $U$ is upper triangular.

   $\text{uplo} = \text{Nag_Lower}$

   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: \( n \) – Integer

*Input*

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

Constraint: \( n \geq 0 \).

4: \( \text{ap}[\text{dim}] \) – Complex

*Input/Output*

Note: the dimension, \( \text{dim} \), of the array \( \text{ap} \) must be at least \( \max(1, n \times (n + 1)/2) \).

On entry: the \( n \) by \( n \) symmetric matrix \( A \), packed by rows or columns.

The storage of elements \( A_{ij} \) depends on the \( \text{order} \) and \( \text{uplo} \) arguments as follows:

- If \( \text{order} = \text{Nag\_ColMajor} \) and \( \text{uplo} = \text{Nag\_Upper} \), \( A_{ij} \) is stored in \( \text{ap}[(j - 1) \times j/2 + i - 1] \), for \( i \leq j \);
- If \( \text{order} = \text{Nag\_ColMajor} \) and \( \text{uplo} = \text{Nag\_Lower} \), \( A_{ij} \) is stored in \( \text{ap}[(2n - j) \times (j - 1)/2 + i - 1] \), for \( i \geq j \);
- If \( \text{order} = \text{Nag\_RowMajor} \) and \( \text{uplo} = \text{Nag\_Upper} \), \( A_{ij} \) is stored in \( \text{ap}[(2n - i) \times (i - 1)/2 + j - 1] \), for \( i \leq j \);
- If \( \text{order} = \text{Nag\_RowMajor} \) and \( \text{uplo} = \text{Nag\_Lower} \), \( A_{ij} \) is stored in \( \text{ap}[(i - 1) \times i/2 + j - 1] \), for \( i \geq j \).

On exit: \( A \) 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: \( \text{ipiv}[\text{n}] \) – Integer

*Output*

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

- 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;

- If \( \text{uplo} = \text{Nag\_Upper} \) and \( \text{ipiv}[i - 2] = \text{ipiv}[i - 1] = -l < 0 \), \( \begin{pmatrix} d_{i-1,i-1} & \tilde{d}_{i,i-1} \\ \tilde{d}_{i,i-1} & d_{ii} \end{pmatrix} \) 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;

- If \( \text{uplo} = \text{Nag\_Lower} \) and \( \text{ipiv}[i - 1] = \text{ipiv}[i] = -m < 0 \), \( \begin{pmatrix} d_{ii} & d_{i+1,i} \\ d_{i+1,i} & d_{i+1,i+1} \end{pmatrix} \) 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.

6: \( \text{fail} \) – NagError*

*Input/Output*

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

6 Error Indicators and Warnings

**NE\_ALLOC\_FAIL**

Dynamic memory allocation failed.

See Section 3.2.1.2 in the Essential Introduction for further information.

**NE\_BAD\_PARAM**

On entry, argument \( \langle \text{value} \rangle \) had an illegal value.

**NE\_INT**

On entry, \( n = \langle \text{value} \rangle \).

Constraint: \( n \geq 0 \).
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 \((value)\) 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 \(\text{uplo} = \text{Nag\_Upper}\), the computed factors \(U\) and \(D\) are the exact factors of a perturbed matrix \(A + E\), where

\[
|E| \leq c(n)\epsilon \|U\|\|D\|\|U^T|P^T,
\]

\(c(n)\) is a modest linear function of \(n\), and \(\epsilon\) is the machine precision.

If \(\text{uplo} = \text{Nag\_Lower}\), a similar statement holds for the computed factors \(L\) and \(D\).

8 Parallelism and Performance
\n
\(\text{nag\_zsptrf (f07qrc)}\) is not threaded by NAG in any implementation.

\(\text{nag\_zsptrf (f07qrc)}\) 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 \(L\) overwrite elements in the corresponding columns of \(A\), but additional row interchanges must be applied to recover \(U\) or \(L\) explicitly (this is seldom necessary). If \(\text{ipiv}[i-1] = i\), for \(i = 1,2,\ldots,n\), then \(U\) or \(L\) are stored explicitly in packed form (except for their unit diagonal elements which are equal to 1).

The total number of real floating-point operations is approximately \(\frac{4}{3}n^3\).

A call to \(\text{nag\_zsptrf (f07qrc)}\) may be followed by calls to the functions:

\(\text{nag\_zsptrs (f07qsc)}\) to solve \(AX = B\);

\(\text{nag\_zspcon (f07quc)}\) to estimate the condition number of \(A\);

\(\text{nag\_zsptri (f07qwc)}\) to compute the inverse of \(A\).

The real analogue of this function is \(\text{nag\_dsptrf (f07pdc)}\).
10 Example

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

$$A = \begin{pmatrix} -0.39 - 0.71i & 5.14 - 0.64i & -7.86 - 2.96i & 3.80 + 0.92i \\ 5.14 - 0.64i & 8.86 + 1.81i & -3.52 + 0.58i & 5.32 - 1.59i \\ -7.86 - 2.96i & -3.52 + 0.58i & -2.83 - 0.03i & -1.54 - 2.86i \\ 3.80 + 0.92i & 5.32 - 1.59i & -1.54 - 2.86i & -0.56 + 0.12i \end{pmatrix},$$

using packed storage.

10.1 Program Text

/* nag_zsptrf (f07qrc) Example Program. * 
* Copyright 2014 Numerical Algorithms Group. * 
* Mark 7, 2001. * 
* Mark 7b revised, 2004. */

#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, pdb;
    Integer exit_status = 0;
    NagError fail;
    Nag_UploType uplo;
    Nag_OrderType order;
    /* Arrays */
    Integer *ipiv = 0;
    char nag_enum_arg[40];
    Complex *ap = 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_UPPER(I, J) ap[J*(J-1)/2 + I - 1]
    # define A_LOWER(I, J) ap[(2*n-J)*(J-1)/2 + I - 1]
    # define B(I, J) b[(J-1)*pdb + I - 1]
    # define A_UPPER(I, J) ap[I*(I-1)/2 + J - 1]
    # define A_LOWER(I, J) ap[(2*n-I)*(I-1)/2 + J - 1]
    # define B(I, J) b[(I-1)*pdb + J - 1]
    # elifdef NAG_COLUMN_MAJOR
    order = Nag_ColMajor;
    #else
    order = Nag_RowMajor;
    #endif

    INIT_FAIL(fail);

    printf("nag_zsptrf (f07qrc) Example Program Results\n\n");

    /* Skip heading in data file */
    #ifdef _WIN32
    scanf_s("%*[\n"]);
    #else
    scanf("%*[`\n"]);
    #endif
    #ifdef _WIN32

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```c
scanf_s("%"NAG_IFMT"%"NAG_IFMT"%[\n] ", &n, &nrhs);
#else
scanf("%"NAG_IFMT"%"NAG_IFMT"%[\n] ", &n, &nrhs);
#endif
#endif
#ifdef NAG_COLUMN_MAJOR
pdb = n;
#else
pdb = nrhs;
#endif

/* Allocate memory */
if (!(ipiv = NAG_ALLOC(n, Integer)) ||
!(ap = NAG_ALLOC(n * (n + 1)/2, Complex)) ||
!(b = NAG_ALLOC(n * nrhs, Complex)))
{
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
}
/* Read A and B from data file */
#ifdef _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 , %lf )", &A_UPPER(i, j).re,
                            &A_UPPER(i, j).im);
                #else
                    scanf(" ( %lf , %lf )", &A_UPPER(i, j).re,
                            &A_UPPER(i, j).im);
                #endif
            }
        }
    }
    else
    {
        for (i = 1; i <= n; ++i)
        {
            for (j = 1; j <= i; ++j)
            {
                #ifdef _WIN32
                    scanf_s(" ( %lf , %lf )", &A_LOWER(i, j).re,
                            &A_LOWER(i, j).im);
                #else
                    scanf(" ( %lf , %lf )", &A_LOWER(i, j).re,
                            &A_LOWER(i, j).im);
                #endif
            }
        }
    }
```
for (j = 1; j <= nrhs; ++j)
#else
    scanf_s(" ( %lf , %lf )", &B(i, j).re, &B(i, j).im);
#endif
scanf(" ( %lf , %lf )", &B(i, j).re, &B(i, j).im);
#endif

ifdef _WIN32
scanf_s("%*
" );
#else
scanf("%*
" );
#endif

/* Factorize A */
/* nag_zsptrf (f07qrc). */
/* Bunch-Kaufman factorization of complex symmetric matrix, */
/* packed storage */
nag_zsptrf(order, uplo, n, ap, ipiv, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_zsptrf (f07qrc).\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Compute solution */
/* nag_zsptrs (f07qsc). */
/* Solution of complex symmetric system of linear equations, */
/* multiple right-hand sides, matrix already factorized by */
/* nag_zsptrf (f07qrc), packed storage */
nag_zsptrs(order, uplo, n, nrhs, ap, ipiv, b, pdb, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_zsptrs (f07qsc).\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Print solution */
/* nag_gen_complx_mat_print_comp (x04dbc). */
/* Print complex general matrix (comprehensive) */
fflush(stdout);
nag_gen_complx_mat_print_comp(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, nrhs, b, pdb, Nag_BracketForm, "%7.4f",
   "Solution(s)", Nag_IntegerLabels, 0, Nag_IntegerLabels, 0, 80, 0, 0, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_gen_complx_mat_print_comp (x04dbc).\n", fail.message);
    exit_status = 1;
    goto END;
}

END:
NAG_FREE(ipiv);
NAG_FREE(ap);
NAG_FREE(b);
return exit_status;

10.2 Program Data
nag_zsptrf (f07qrc) Example Program Data
  4 2
  Nag_Lower
(-0.39,-0.71)
( 5.14,-0.64) ( 8.86, 1.81)
(-7.86,-2.96) (-3.52, 0.58) (-2.83,-0.03)
nag_zsptrf (f07qrc) Example Program Results

Solution(s)

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