NAG Library Function Document

nag_zpptri (f07gwc)

1 Purpose

nag_zpptri (f07gwc) computes the inverse of a complex Hermitian positive definite matrix A, where A has been factorized by nag_zpptrf (f07grc), using packed storage.

2 Specification

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

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

3 Description

nag_zpptri (f07gwc) is used to compute the inverse of a complex Hermitian positive definite matrix A, the function must be preceded by a call to nag_zpptrf (f07grc), which computes the Cholesky factorization of A, using packed storage.

If **uplo** = Nag_Upper, $A = U^{\mathrm{H}}U$ and A^{-1} is computed by first inverting U and then forming $(U^{-1})U^{-\mathrm{H}}$.

If **uplo** = Nag_Lower, $A = LL^{\mathrm{H}}$ and A^{-1} is computed by first inverting L and then forming $L^{-\mathrm{H}}(L^{-1})$.

4 References

Du Croz J J and Higham N J (1992) Stability of methods for matrix inversion *IMA J. Numer. Anal.* **12** 1–19

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 how A has been factorized.

uplo = Nag_Upper
$A = U^{\mathrm{H}}U$, where U is upper triangular.

uplo = Nag_Lower
$A = LL^{\mathrm{H}}$, 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: **ap**[dim] – Complex *Input/Output*

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

On entry: the Cholesky factor of A stored in packed form, as returned by nag_zpptrf (f07grc).

On exit: the factorization is overwritten by the n by n matrix A^{-1}.

The storage of elements A_{ij} depends on the **order** and **uplo** arguments as follows:

if **order** = Nag_ColMajor and **uplo** = Nag_Upper,
A_{ij} is stored in **ap**$[(j-1) \times j/2 + i - 1]$, for $i \leq j$;
if **order** = Nag_ColMajor and **uplo** = Nag_Lower,
A_{ij} is stored in **ap**$[(2n-j) \times (j-1)/2 + i - 1]$, for $i \geq j$;
if **order** = Nag_RowMajor and **uplo** = Nag_Upper,
A_{ij} is stored in **ap**$[(2n-i) \times (i-1)/2 + j - 1]$, for $i \leq j$;
if **order** = Nag_RowMajor and **uplo** = Nag_Lower,
A_{ij} is stored in **ap**$[(i-1) \times i/2 + j - 1]$, for $i \geq j$.

5: **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 ⟨*value*⟩ had an illegal value.

NE_INT

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

Diagonal element ⟨*value*⟩ of the Cholesky factor is zero; the Cholesky factor is singular and the inverse of A cannot be computed.

7 Accuracy

The computed inverse X satisfies

$$\|XA - I\|_2 \leq c(n)\epsilon\kappa_2(A) \quad \text{and} \quad \|AX - I\|_2 \leq c(n)\epsilon\kappa_2(A),$$

where $c(n)$ is a modest function of n, ϵ is the ***machine precision*** and $\kappa_2(A)$ is the condition number of A defined by

$$\kappa_2(A) = \|A\|_2 \|A^{-1}\|_2.$$

8 Parallelism and Performance

nag_zpptri (f07gwc) is not threaded by NAG in any implementation.

nag_zpptri (f07gwc) 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 real floating-point operations is approximately $\frac{8}{3}n^3$.

The real analogue of this function is nag_dpptri (f07gjc).

10 Example

This example computes the inverse of the matrix A, where

$$A = \begin{pmatrix} 3.23+0.00i & 1.51-1.92i & 1.90+0.84i & 0.42+2.50i \\ 1.51+1.92i & 3.58+0.00i & -0.23+1.11i & -1.18+1.37i \\ 1.90-0.84i & -0.23-1.11i & 4.09+0.00i & 2.33-0.14i \\ 0.42-2.50i & -1.18-1.37i & 2.33+0.14i & 4.29+0.00i \end{pmatrix}.$$

Here A is Hermitian positive definite, stored in packed form, and must first be factorized by nag_zpptrf (f07grc).

10.1 Program Text

```
/* nag_zpptri (f07gwc) 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       ap_len, i, j, n;
  Integer       exit_status = 0;
  NagError      fail;
  Nag_UploType  uplo;
  Nag_OrderType order;
  /* Arrays */
  char          nag_enum_arg[40];
  Complex       *ap = 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]
  order = Nag_ColMajor;
#else
#define A_LOWER(I, J) ap[I*(I-1)/2 + J - 1]
#define A_UPPER(I, J) ap[(2*n-I)*(I-1)/2 + J - 1]
  order = Nag_RowMajor;
#endif

  INIT_FAIL(fail);

  printf("nag_zpptri (f07gwc) 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
  ap_len = n * (n + 1)/2;

  /* Allocate memory */
  if (!(ap = NAG_ALLOC(ap_len, Complex)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }
  /* Read A 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
        }
#ifdef _WIN32
      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 , %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
        }
#ifdef _WIN32
      scanf_s("%*[^\n] ");
#else
      scanf("%*[^\n] ");
#endif
    }

  /* Factorize A */
  /* nag_zpptrf (f07grc).
   * Cholesky factorization of complex Hermitian
   * positive-definite matrix, packed storage
   */
  nag_zpptrf(order, uplo, n, ap, &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_zpptrf (f07grc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Compute inverse of A */
  /* nag_zpptri (f07gwc).
   * Inverse of complex Hermitian positive-definite matrix,
   * matrix already factorized by nag_zpptrf (f07grc), packed
   * storage
   */
  nag_zpptri(order, uplo, n, ap, &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_zpptri (f07gwc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Print inverse */
  /* nag_pack_complx_mat_print_comp (x04ddc).
   * Print complex packed triangular matrix (comprehensive)
   */
  fflush(stdout);
  nag_pack_complx_mat_print_comp(order, uplo, Nag_NonUnitDiag, n, ap,
                                 Nag_BracketForm, "%7.4f", "Inverse",
                                 Nag_IntegerLabels, 0, Nag_IntegerLabels, 0,
                                 80, 0, 0, &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_pack_complx_mat_print_comp (x04ddc).\n%s\n",
             fail.message);
      exit_status = 1;
      goto END;
    }
 END:
  NAG_FREE(ap);

  return exit_status;
}
```

10.2 Program Data

```
nag_zpptri (f07gwc) Example Program Data
  4                                                    :Value of n
  Nag_Lower                                            :Value of uplo
 (3.23, 0.00)
 (1.51, 1.92) ( 3.58, 0.00)
 (1.90,-0.84) (-0.23,-1.11) ( 4.09, 0.00)
 (0.42,-2.50) (-1.18,-1.37) ( 2.33, 0.14) ( 4.29, 0.00)  :End of matrix A
```

10.3 Program Results

```
nag_zpptri (f07gwc) Example Program Results

 Inverse
                    1                   2                   3                   4
 1  ( 5.4691, 0.0000)
 2  (-1.2624,-1.5491)  ( 1.1024, 0.0000)
 3  (-2.9746,-0.9616)  ( 0.8989,-0.5672)  ( 2.1589, 0.0000)
 4  ( 1.1962, 2.9772)  (-0.9826,-0.2566)  (-1.3756,-1.4550)  ( 2.2934,-0.0000)
```