NAG C Library Function Document

nag_dsptrf (f07pdc)

1 Purpose

nag_dsptrf (f07pdc) computes the Bunch–Kaufman factorization of a real symmetric indefinite matrix, using packed storage.

2 Specification

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

3 Description

nag_dsptrf (f07pdc) factorizes a real symmetric matrix A, using the Bunch–Kaufman diagonal pivoting method and packed storage. A is factorized as either $A = PUDU^TP^T$ if **uplo** $=$ **Nag_Upper**, or $A = PLDL^TP^T$ if **uplo** $=$ **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

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 to be factorized, as follows:

if **uplo** $=$ **Nag_Upper**, the upper triangular part of A is stored and A is factorized as $PUDU^TP^T$, where U is upper triangular;

if **uplo** $=$ **Nag_Lower**, the lower triangular part of A is stored and A is factorized as $PLDL^TP^T$, 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: **ap**[dim] – double *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 symmetric indefinite matrix A, packed by rows or columns. The storage of elements a_{ij} depends on the **order** and **uplo** parameters 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 $i \geq j$.

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 **uplo**.

5: **ipiv**[dim] – Integer *Output*

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

On exit: details of the interchanges and the block structure of D.

More precisely, if **ipiv**$[i-1] = k > 0$, d_{ii} is a 1 by 1 pivot block and the ith row and column of A were interchanged with the kth row and column.

If **uplo** = **Nag_Upper** and **ipiv**$[i-2]$ = **ipiv**$[i-1] = -l < 0$, $\begin{pmatrix} d_{i-1,i-1} & d_{i,i-1} \\ d_{i,i-1} & d_{ii} \end{pmatrix}$ is a 2 by 2 pivot block and the $(i-1)$th row and column of A were interchanged with the lth row and column.

If **uplo** = **Nag_Lower** and **ipiv**$[i-1]$ = **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 mth row and column.

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.

NE_SINGULAR

The block diagonal matrix D is exactly singular.

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 factors U and D are the exact factors of a perturbed matrix $A + E$, where

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

$c(n)$ is a modest linear function of n, and ϵ is the ***machine precision***.

If **uplo** $= $ **Nag_Lower**, a similar statement holds for the computed factors L and D.

8 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 **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 **ipiv**$[i-1] = i$, for $i = 1, 2, \ldots, n$ (as is the case when A is positive-definite), 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 floating-point operations is approximately $\frac{1}{3}n^3$.

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

nag_dsptrs (f07pec) to solve $AX = B$;

nag_dspcon (f07pgc) to estimate the condition number of A;

nag_dsptri (f07pjc) to compute the inverse of A.

The complex analogues of this function are nag_zhptrf (f07prc) for Hermitian matrices and nag_zsptrf (f07qrc) for symmetric matrices.

9 Example

To compute the Bunch–Kaufman factorization of the matrix A, where

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

using packed storage.

9.1 Program Text

```
/* nag_dsptrf (f07pdc) 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  ap_len, i, j, n;
  Integer  exit_status=0;
  Nag_UploType uplo_enum;
```

```
  NagError fail;
  Nag_OrderType order;

  /* Arrays */
  char   uplo[2];
  Integer *ipiv=0;
  double *ap=0;

#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);
  Vprintf("f07pdc Example Program Results\n\n");

  /* Skip heading in data file */
  Vscanf("%*[^\n] ");
  Vscanf("%ld%*[^\n] ", &n);
  ap_len = n*(n+1)/2;

  /* Allocate memory */
  if ( !(ipiv = NAG_ALLOC(n, Integer)) ||
       !(ap = NAG_ALLOC(ap_len, 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;
  else if (*(unsigned char *)uplo == 'U')
    uplo_enum = Nag_Upper;
  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_UPPER(i,j));
        }
      Vscanf("%*[^\n] ");
    }
  else
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = 1; j <= i; ++j)
            Vscanf("%lf", &A_LOWER(i,j));
        }
      Vscanf("%*[^\n] ");
    }
  /* Factorize A */
  f07pdc(order, uplo_enum, n, ap, ipiv, &fail);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from f07pdc.\n%s\n", fail.message);
      exit_status = 1;
```

```
      goto END;
    }
  /* Print factor */
  x04ccc(order, uplo_enum, Nag_NonUnitDiag, n, ap,
         "Factor", 0, NAGERR_DEFAULT);
  if (fail.code != NE_NOERROR)
    {
      Vprintf("Error from x04ccc.\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Print pivot indices */
  Vprintf("\nIPIV\n");
  for (i = 1; i <= n; ++i)
    Vprintf("%6ld%s", ipiv[i-1], i%7==0 ?"\n":" ");
  Vprintf("\n");
 END:
  if (ap) NAG_FREE(ap);
  if (ipiv) NAG_FREE(ipiv);
  return exit_status;
}
```

9.2 Program Data

```
f07pdc Example Program Data
  4                            :Value of N
  'U'                          :Value of UPLO
  2.07   3.87   4.20  -1.15
        -0.21   1.87   0.63
                1.15   2.06
                      -1.81   :End of matrix A
```

9.3 Program Results

```
f07pdc Example Program Results

 Factor
            1          2          3          4
 1      2.0700     4.2000     0.2230     0.6537
 2                 1.1500     0.8115    -0.5960
 3                           -2.5907     0.3031
 4                                       0.4074

IPIV
    -3     -3      3      4
```