

## NAG Toolbox

### nag\_linsys\_real\_posdef\_packed\_solve (f04be)

#### 1 Purpose

`nag_linsys_real_posdef_packed_solve` (f04be) computes the solution to a real system of linear equations  $AX = B$ , where  $A$  is an  $n$  by  $n$  symmetric positive definite matrix, stored in packed format, and  $X$  and  $B$  are  $n$  by  $r$  matrices. An estimate of the condition number of  $A$  and an error bound for the computed solution are also returned.

#### 2 Syntax

```
[ap, b, rcond, errbnd, ifail] = nag_linsys_real_posdef_packed_solve(uplo, ap, b,
'n', n, 'nrhs_p', nrhs_p)
[ap, b, rcond, errbnd, ifail] = f04be(uplo, ap, b, 'n', n, 'nrhs_p', nrhs_p)
```

#### 3 Description

The Cholesky factorization is used to factor  $A$  as  $A = U^T U$ , if **uplo** = 'U', or  $A = LL^T$ , if **uplo** = 'L', where  $U$  is an upper triangular matrix and  $L$  is a lower triangular matrix. The factored form of  $A$  is then used to solve the system of equations  $AX = B$ .

#### 4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia <http://www.netlib.org/lapack/lug>

Higham N J (2002) *Accuracy and Stability of Numerical Algorithms* (2nd Edition) SIAM, Philadelphia

#### 5 Parameters

##### 5.1 Compulsory Input Parameters

1: **uplo** – CHARACTER(1)

If **uplo** = 'U', the upper triangle of the matrix  $A$  is stored.

If **uplo** = 'L', the lower triangle of the matrix  $A$  is stored.

*Constraint:* **uplo** = 'U' or 'L'.

2: **ap**(:) – REAL (KIND=nag\_wp) array

The dimension of the array **ap** must be at least  $\max(1, n \times (n + 1)/2)$

The  $n$  by  $n$  symmetric matrix  $A$ . The upper or lower triangular part of the symmetric matrix is packed column-wise in a linear array. The  $j$ th column of  $A$  is stored in the array **ap** as follows:

More precisely,

if **uplo** = 'U', the upper triangle of  $A$  must be stored with element  $A_{ij}$  in **ap**( $i + j(j - 1)/2$ ) for  $i \leq j$ ;

if **uplo** = 'L', the lower triangle of  $A$  must be stored with element  $A_{ij}$  in **ap**( $i + (2n - j)(j - 1)/2$ ) for  $i \geq j$ .

- 3: **b**(*ldb*,:) – REAL (KIND=nag\_wp) array  
 The first dimension of the array **b** must be at least  $\max(1, \mathbf{n})$ .  
 The second dimension of the array **b** must be at least  $\max(1, \mathbf{nrhs\_p})$ .  
 The  $n$  by  $r$  matrix of right-hand sides  $B$ .

## 5.2 Optional Input Parameters

- 1: **n** – INTEGER  
*Default:* the first dimension of the array **b**.  
 The number of linear equations  $n$ , i.e., the order of the matrix  $A$ .  
*Constraint:*  $\mathbf{n} \geq 0$ .
- 2: **nrhs\_p** – INTEGER  
*Default:* the second dimension of the array **b**.  
 The number of right-hand sides  $r$ , i.e., the number of columns of the matrix  $B$ .  
*Constraint:*  $\mathbf{nrhs\_p} \geq 0$ .

## 5.3 Output Parameters

- 1: **ap**(:) – REAL (KIND=nag\_wp) array  
 The dimension of the array **ap** will be  $\max(1, \mathbf{n} \times (\mathbf{n} + 1)/2)$   
 If **ifail** = 0 or  $\mathbf{n} + 1$ , the factor  $U$  or  $L$  from the Cholesky factorization  $A = U^T U$  or  $A = LL^T$ , in the same storage format as  $A$ .
- 2: **b**(*ldb*,:) – REAL (KIND=nag\_wp) array  
 The first dimension of the array **b** will be  $\max(1, \mathbf{n})$ .  
 The second dimension of the array **b** will be  $\max(1, \mathbf{nrhs\_p})$ .  
 If **ifail** = 0 or  $\mathbf{n} + 1$ , the  $n$  by  $r$  solution matrix  $X$ .
- 3: **rcond** – REAL (KIND=nag\_wp)  
 If **ifail** = 0 or  $\mathbf{n} + 1$ , an estimate of the reciprocal of the condition number of the matrix  $A$ , computed as  $\mathbf{rcond} = 1 / (\|A\|_1 \|A^{-1}\|_1)$ .
- 4: **errbnd** – REAL (KIND=nag\_wp)  
 If **ifail** = 0 or  $\mathbf{n} + 1$ , an estimate of the forward error bound for a computed solution  $\hat{x}$ , such that  $\|\hat{x} - x\|_1 / \|x\|_1 \leq \mathbf{errbnd}$ , where  $\hat{x}$  is a column of the computed solution returned in the array **b** and  $x$  is the corresponding column of the exact solution  $X$ . If **rcond** is less than *machine precision*, then **errbnd** is returned as unity.
- 5: **ifail** – INTEGER  
**ifail** = 0 unless the function detects an error (see Section 5).

## 6 Error Indicators and Warnings

Errors or warnings detected by the function:

**ifail** > 0 and **ifail** ≤ **n**

The principal minor of order  $\langle value \rangle$  of the matrix  $A$  is not positive definite. The factorization has not been completed and the solution could not be computed.

**ifail** = **n** + 1 (*warning*)

A solution has been computed, but **rcond** is less than *machine precision* so that the matrix  $A$  is numerically singular.

**ifail** = -1

On entry, **uplo** not one of 'U' or 'u' or 'L' or 'l'.

**ifail** = -2

Constraint: **n** ≥ 0.

**ifail** = -3

Constraint: **nrhs\_p** ≥ 0.

**ifail** = -6

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

**ifail** = -99

An unexpected error has been triggered by this routine. Please contact NAG.

**ifail** = -399

Your licence key may have expired or may not have been installed correctly.

**ifail** = -999

Dynamic memory allocation failed.

*The integer allocatable memory required is **n**, and the double allocatable memory required is  $3 \times \mathbf{n}$ . Allocation failed before the solution could be computed.*

## 7 Accuracy

The computed solution for a single right-hand side,  $\hat{x}$ , satisfies an equation of the form

$$(A + E)\hat{x} = b,$$

where

$$\|E\|_1 = O(\epsilon)\|A\|_1$$

and  $\epsilon$  is the *machine precision*. An approximate error bound for the computed solution is given by

$$\frac{\|\hat{x} - x\|_1}{\|x\|_1} \leq \kappa(A) \frac{\|E\|_1}{\|A\|_1},$$

where  $\kappa(A) = \|A^{-1}\|_1 \|A\|_1$ , the condition number of  $A$  with respect to the solution of the linear equations. `nag_linsys_real_posdef_packed_solve` (f04be) uses the approximation  $\|E\|_1 = \epsilon \|A\|_1$  to estimate **errbnd**. See Section 4.4 of Anderson *et al.* (1999) for further details.

## 8 Further Comments

The packed storage scheme is illustrated by the following example when  $n = 4$  and **uplo** = 'U'. Two-dimensional storage of the symmetric matrix  $A$ :

$$\begin{array}{cccc} a_{11} & a_{12} & a_{13} & a_{14} \\ & a_{22} & a_{23} & a_{24} \\ & & a_{33} & a_{34} \\ & & & a_{44} \end{array} \quad (a_{ij} = a_{ji})$$

Packed storage of the upper triangle of  $A$ :

$$\mathbf{ap} = [a_{11}, a_{12}, a_{22}, a_{13}, a_{23}, a_{33}, a_{14}, a_{24}, a_{34}, a_{44}]$$

The total number of floating-point operations required to solve the equations  $AX = B$  is proportional to  $(\frac{1}{3}n^3 + n^2r)$ . The condition number estimation typically requires between four and five solves and never more than eleven solves, following the factorization.

In practice the condition number estimator is very reliable, but it can underestimate the true condition number; see Section 15.3 of Higham (2002) for further details.

The complex analogue of nag\_linsys\_real\_posdef\_packed\_solve (f04be) is nag\_linsys\_complex\_posdef\_packed\_solve (f04ce).

## 9 Example

This example solves the equations

$$AX = B,$$

where  $A$  is the symmetric positive definite matrix

$$A = \begin{pmatrix} 4.16 & -3.12 & 0.56 & -0.10 \\ -3.12 & 5.03 & -0.83 & 1.18 \\ 0.56 & -0.83 & 0.76 & 0.34 \\ -0.10 & 1.18 & 0.34 & 1.18 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 8.70 & 8.30 \\ -13.35 & 2.13 \\ 1.89 & 1.61 \\ -4.14 & 5.00 \end{pmatrix}.$$

An estimate of the condition number of  $A$  and an approximate error bound for the computed solutions are also printed.

### 9.1 Program Text

```
function f04be_example
    fprintf('f04be example results\n\n');

    % Solve Ax = b for positive definite A with error bound and condition number
    % A is stored in symmetric packed format.
    uplo = 'U';
    ap = [ 4.16           ...
          -3.12  5.03     ...
           0.56 -0.83  0.76 ...
          -0.10  1.18  0.34 1.18];
    b = [ 8.7, 8.30;
          -13.35, 2.13;
           1.89, 1.61;
          -4.14, 5.00];

    [ap, x, rcond, errbnd, ifail] = f04be(uplo, ap, b);

    disp('Solution');
    disp(x);
    disp('Estimate of condition number');
    fprintf('%10.1f\n\n', 1/rcond);
    disp('Estimate of error bound for computed solutions');
    fprintf('%10.1e\n\n', errbnd);
```

## 9.2 Program Results

f04be example results

Solution

1.0000	4.0000
-1.0000	3.0000
2.0000	2.0000
-3.0000	1.0000

Estimate of condition number

97.3

Estimate of error bound for computed solutions

1.1e-14

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