

NAG Toolbox

nag_linsys_complex_posdef_packed_solve (f04ce)

1 Purpose

nag_linsys_complex_posdef_packed_solve (f04ce) computes the solution to a complex system of linear equations $AX = B$, where A is an n by n Hermitian 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_complex_posdef_packed_solve(uplo, ap,
b, 'n', n, 'nrhs_p', nrhs_p)
[ap, b, rcond, errbnd, ifail] = f04ce(uplo, ap, b, 'n', n, 'nrhs_p', nrhs_p)
```

3 Description

The Cholesky factorization is used to factor A as $A = U^H U$, if **uplo** = 'U', or $A = LL^H$, 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**(:) – COMPLEX (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 Hermitian matrix A . The upper or lower triangular part of the Hermitian 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*,:) – COMPLEX (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**(:) – COMPLEX (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 $A = U^H U$ or $A = LL^H$, in the same storage format as A .
- 2: **b**(*ldb*,:) – COMPLEX (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** \neq -999

If **ifail** = $-i$, the i th argument had an illegal value.

ifail > 0 and **ifail** ≤ **n**

If **ifail** = i , the leading minor of order i of A is not positive definite. The factorization could not be completed, and the solution has not been computed.

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

rcond is less than *machine precision*, so that the matrix A is numerically singular. A solution to the equations $AX = B$ has nevertheless been computed.

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.

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 ϵ 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_complex_posdef_packed_solve` (f04ce) 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 Hermitian matrix A :

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

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 real analogue of `nag_linsys_complex_posdef_packed_solve` (f04ce) is `nag_linsys_real_posdef_packed_solve` (f04be).

9 Example

This example solves the equations

$$AX = B,$$

where A is the Hermitian positive definite matrix

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

and

$$B = \begin{pmatrix} 3.93 - 6.14i & 1.48 + 6.58i \\ 6.17 + 9.42i & 4.65 - 4.75i \\ -7.17 - 21.83i & -4.91 + 2.29i \\ 1.99 - 14.38i & 7.64 - 10.79i \end{pmatrix}.$$

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 f04ce_example

fprintf('f04ce example results\n\n');

% Solve complex Ax = b for Hermitian packed A with error and condition number
uplo = 'U';
ap = [3.23                                     ...
      1.51 - 1.92i   3.58 + 0i                 ...
      1.90 + 0.84i  -0.23 + 1.11i   4.09 + 0i   ...
      0.42 + 2.50i  -1.18 + 1.37i   2.33 - 0.14i  4.29 + 0i];
b = [ 3.93 - 6.14i,  1.48 + 6.58i;
      6.17 + 9.42i,  4.65 - 4.75i;
      -7.17 - 21.83i, -4.91 + 2.29i;
      1.99 - 14.38i,  7.64 - 10.79i];

[ap, x, rcond, errbnd, ifail] = ...
    f04ce(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

```
f04ce example results

Solution
 1.0000 - 1.0000i  -1.0000 + 2.0000i
-0.0000 + 3.0000i   3.0000 - 4.0000i
-4.0000 - 5.0000i  -2.0000 + 3.0000i
 2.0000 + 1.0000i   4.0000 - 5.0000i

Estimate of condition number
 151.4

Estimate of error bound for computed solutions
 1.7e-14
```
