NAG Library Routine Document F07CPF (ZGTSVX)

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of **bold italicised** terms and other implementation-dependent details.

1 Purpose

F07CPF (ZGTSVX) uses the LU factorization to compute the solution to a complex system of linear equations

$$AX = B$$
, $A^{\mathsf{T}}X = B$ or $A^{\mathsf{H}}X = B$,

where A is a tridiagonal matrix of order n and X and B are n by r matrices. Error bounds on the solution and a condition estimate are also provided.

2 Specification

```
SUBROUTINE FO7CPF (FACT, TRANS, N, NRHS, DL, D, DU, DLF, DF, DUF, DU2, IPIV, B, LDB, X, LDX, RCOND, FERR, BERR, WORK, RWORK, INFO)

INTEGER

N, NRHS, IPIV(*), LDB, LDX, INFO

REAL (KIND=nag_wp)

RCOND, FERR(NRHS), BERR(NRHS), RWORK(N)

COMPLEX (KIND=nag_wp)

DL(*), D(*), DU(*), DLF(*), DF(*), DUF(*), DU2(*), B(LDB,*), X(LDX,*), WORK(2*N)

CHARACTER(1)

FACT, TRANS
```

The routine may be called by its LAPACK name zgtsvx.

3 Description

F07CPF (ZGTSVX) performs the following steps:

- 1. If FACT = 'N', the LU decomposition is used to factor the matrix A as A = LU, where L is a product of permutation and unit lower bidiagonal matrices and U is upper triangular with nonzeros in only the main diagonal and first two superdiagonals.
- 2. If some $u_{ii} = 0$, so that U is exactly singular, then the routine returns with INFO = i. Otherwise, the factored form of A is used to estimate the condition number of the matrix A. If the reciprocal of the condition number is less than **machine precision**, INFO = N + 1 is returned as a warning, but the routine still goes on to solve for X and compute error bounds as described below.
- 3. The system of equations is solved for X using the factored form of A.
- 4. Iterative refinement is applied to improve the computed solution matrix and to calculate error bounds and backward error estimates for it.

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

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

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

Mark 26 F07CPF.1

5 Arguments

1: FACT - CHARACTER(1)

Input

On entry: specifies whether or not the factorized form of the matrix A has been supplied.

FACT = 'F'

DLF, DF, DUF, DU2 and IPIV contain the factorized form of the matrix A. DLF, DF, DUF, DU2 and IPIV will not be modified.

FACT = 'N

The matrix A will be copied to DLF, DF and DUF and factorized.

Constraint: FACT = 'F' or 'N'.

2: TRANS - CHARACTER(1)

Input

On entry: specifies the form of the system of equations.

TRANS = 'N'

AX = B (No transpose).

TRANS = 'T'

 $A^{\mathsf{T}}X = B$ (Transpose).

TRANS = 'C'

 $A^{H}X = B$ (Conjugate transpose).

Constraint: TRANS = 'N', 'T' or 'C'.

3: N – INTEGER

Input

On entry: n, the order of the matrix A.

Constraint: $N \ge 0$.

4: NRHS – INTEGER

Input

On entry: r, the number of right-hand sides, i.e., the number of columns of the matrix B.

Constraint: NRHS ≥ 0 .

5: DL(*) – COMPLEX (KIND=nag_wp) array

Input

Note: the dimension of the array DL must be at least max(1, N - 1).

On entry: the (n-1) subdiagonal elements of A.

6: D(*) - COMPLEX (KIND=nag_wp) array

Input

Note: the dimension of the array D must be at least max(1, N).

On entry: the n diagonal elements of A.

7: DU(*) - COMPLEX (KIND=nag wp) array

Input

Note: the dimension of the array DU must be at least max(1, N - 1).

On entry: the (n-1) superdiagonal elements of A.

8: DLF(*) - COMPLEX (KIND=nag wp) array

Input/Output

Note: the dimension of the array DLF must be at least max(1, N - 1).

On entry: if FACT = 'F', DLF contains the (n-1) multipliers that define the matrix L from the LU factorization of A.

On exit: if FACT = 'N', DLF contains the (n-1) multipliers that define the matrix L from the LU factorization of A.

F07CPF.2 Mark 26

9: DF(*) - COMPLEX (KIND=nag wp) array

Input/Output

Note: the dimension of the array DF must be at least max(1, N).

On entry: if FACT = 'F', DF contains the n diagonal elements of the upper triangular matrix U from the LU factorization of A.

On exit: if FACT = 'N', DF contains the n diagonal elements of the upper triangular matrix U from the LU factorization of A.

10: DUF(*) - COMPLEX (KIND=nag_wp) array

Input/Output

Note: the dimension of the array DUF must be at least max(1, N - 1).

On entry: if FACT = 'F', DUF contains the (n-1) elements of the first superdiagonal of U.

On exit: if FACT = 'N', DUF contains the (n-1) elements of the first superdiagonal of U.

11: DU2(*) - COMPLEX (KIND=nag wp) array

Input/Output

Note: the dimension of the array DU2 must be at least max(1, N-2).

On entry: if FACT = 'F', DU2 contains the (n-2) elements of the second superdiagonal of U. On exit: if FACT = 'N', DU2 contains the (n-2) elements of the second superdiagonal of U.

12: IPIV(*) – INTEGER array

Input/Output

Note: the dimension of the array IPIV must be at least max(1, N).

On entry: if FACT = 'F', IPIV contains the pivot indices from the LU factorization of A.

On exit: if FACT = 'N', IPIV contains the pivot indices from the LU factorization of A; row i of the matrix was interchanged with row IPIV(i). IPIV(i) will always be either i or i+1; IPIV(i)=i indicates a row interchange was not required.

13: B(LDB,*) - COMPLEX (KIND=nag_wp) array

Input

Note: the second dimension of the array B must be at least max(1, NRHS).

On entry: the n by r right-hand side matrix B.

14: LDB - INTEGER

Input

On entry: the first dimension of the array B as declared in the (sub)program from which F07CPF (ZGTSVX) is called.

Constraint: LDB $\geq \max(1, N)$.

15: X(LDX,*) - COMPLEX (KIND=nag wp) array

Output

Note: the second dimension of the array X must be at least max(1, NRHS).

On exit: if INFO = 0 or N + 1, the n by r solution matrix X.

16: LDX – INTEGER

Input

On entry: the first dimension of the array X as declared in the (sub)program from which F07CPF (ZGTSVX) is called.

Constraint: LDX $\geq \max(1, N)$.

17: RCOND – REAL (KIND=nag wp)

Output

On exit: the estimate of the reciprocal condition number of the matrix A. If RCOND = 0.0, the matrix may be exactly singular. This condition is indicated by INFO > 0 and INFO \leq N. Otherwise, if RCOND is less than the **machine precision**, the matrix is singular to working precision. This condition is indicated by INFO = N + 1.

Mark 26 F07CPF.3

F07CPF NAG Library Manual

18: FERR(NRHS) – REAL (KIND=nag wp) array

Output

On exit: if INFO = 0 or N + 1, an estimate of the forward error bound for each computed solution vector, such that $\|\hat{x}_j - x_j\|_{\infty} / \|x_j\|_{\infty} \le \text{FERR}(j)$ where \hat{x}_j is the *j*th column of the computed solution returned in the array X and x_j is the corresponding column of the exact solution X. The estimate is as reliable as the estimate for RCOND, and is almost always a slight overestimate of the true error.

19: BERR(NRHS) - REAL (KIND=nag_wp) array

Output

On exit: if INFO = 0 or N + 1, an estimate of the component-wise relative backward error of each computed solution vector \hat{x}_j (i.e., the smallest relative change in any element of A or B that makes \hat{x}_j an exact solution).

20: $WORK(2 \times N) - COMPLEX (KIND=nag_wp) array$

Workspace

21: RWORK(N) - REAL (KIND=nag wp) array

Workspace

22: INFO - INTEGER

Output

On exit: INFO = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

INFO < 0

If INFO = -i, argument i had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0 and INFO < N

Element $\langle value \rangle$ of the diagonal is exactly zero. The factorization has not been completed, but the factor U is exactly singular, so the solution and error bounds could not be computed. RCOND = 0.0 is returned.

INFO > 0 and INFO = N

Element $\langle value \rangle$ of the diagonal is exactly zero. The factorization has been completed, but the factor U is exactly singular, so the solution and error bounds could not be computed. RCOND = 0.0 is returned.

INFO = N + 1

U is nonsingular, but RCOND is less than *machine precision*, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of RCOND would suggest.

7 Accuracy

For each right-hand side vector b, the computed solution \hat{x} is the exact solution of a perturbed system of equations $(A+E)\hat{x}=b$, where

$$|E| \le c(n)\epsilon |L||U|,$$

c(n) is a modest linear function of n, and ϵ is the **machine precision**. See Section 9.3 of Higham (2002) for further details.

If x is the true solution, then the computed solution \hat{x} satisfies a forward error bound of the form

$$\frac{\|x-\hat{x}\|_{\infty}}{\|\hat{x}\|_{\infty}} \leq w_{c}\operatorname{cond}(A,\hat{x},b)$$

F07CPF.4 Mark 26

where $\operatorname{cond}(A, \hat{x}, b) = \| |A^{-1}| (|A||\hat{x}| + |b|) \|_{\infty} / \|\hat{x}\|_{\infty} \le \operatorname{cond}(A) = \| |A^{-1}| |A| \|_{\infty} \le \kappa_{\infty}(A)$. If \hat{x} is the jth column of X, then w_c is returned in BERR(j) and a bound on $\|x - \hat{x}\|_{\infty} / \|\hat{x}\|_{\infty}$ is returned in FERR(j). See Section 4.4 of Anderson et al. (1999) for further details.

8 Parallelism and Performance

F07CPF (ZGTSVX) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F07CPF (ZGTSVX) 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 routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

The total number of floating-point operations required to solve the equations AX = B is proportional to nr.

The condition number estimation typically requires between four and five solves and never more than eleven solves, following the factorization. The solution is then refined, and the errors estimated, using iterative refinement.

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 this routine is F07CBF (DGTSVX).

10 Example

This example solves the equations

$$AX = B$$
,

where A is the tridiagonal matrix

$$A = \begin{pmatrix} -1.3 + 1.3i & 2.0 - 1.0i & 0 & 0 & 0\\ 1.0 - 2.0i & -1.3 + 1.3i & 2.0 + 1.0i & 0 & 0\\ 0 & 1.0 + 1.0i & -1.3 + 3.3i & -1.0 + 1.0i & 0\\ 0 & 0 & 2.0 - 3.0i & -0.3 + 4.3i & 1.0 - 1.0i\\ 0 & 0 & 0 & 1.0 + 1.0i & -3.3 + 1.3i \end{pmatrix}$$

and

$$B = \begin{pmatrix} 2.4 - 5.0i & 2.7 + 6.9i \\ 3.4 + 18.2i & -6.9 - 5.3i \\ -14.7 + 9.7i & -6.0 - 0.6i \\ 31.9 - 7.7i & -3.9 + 9.3i \\ -1.0 + 1.6i & -3.0 + 12.2i \end{pmatrix}.$$

Estimates for the backward errors, forward errors and condition number are also output.

10.1 Program Text

```
Program f07cpfe
```

- ! FO7CPF Example Program Text
- ! Mark 26 Release. NAG Copyright 2016.
- ! .. Use Statements ..

Mark 26 F07CPF.5

F07CPF NAG Library Manual

```
Use nag_library, Only: nag_wp, x04dbf, zgtsvx
      .. Implicit None Statement ..
     Implicit None
!
      .. Parameters ..
                                       :: nin = 5, nout = 6
     Integer, Parameter
      .. Local Scalars ..
     Real (Kind=nag_wp)
                                        :: rcond
                                        :: i, ifail, info, ldb, ldx, n, nrhs
     Integer
!
      .. Local Arrays ..
     Complex (Kind=nag_wp), Allocatable :: b(:,:), d(:), df(:), dl(:),
                                           dlf(:), du(:), du2(:), duf(:),
                                           work(:), x(:,:)
     Real (Kind=nag_wp), Allocatable :: berr(:), ferr(:), rwork(:)
     Integer, Allocatable
                                        :: ipiv(:)
     Character (1)
                                        :: clabs(1), rlabs(1)
      .. Executable Statements ..
1
     Write (nout,*) 'FO7CPF Example Program Results'
     Write (nout, *)
     Flush (nout)
!
     Skip heading in data file
     Read (nin,*)
     Read (nin,*) n, nrhs
     ldb = n
     ldx = n
     Allocate (b(ldb,nrhs),d(n),df(n),dl(n-1),dlf(n-1),du(n-1),du2(n-2),
        duf(n-1),work(2*n),x(ldx,nrhs),berr(nrhs),ferr(nrhs),rwork(n),ipiv(n))
     Read the tridiagonal matrix A from data file
     Read (nin,*) du(1:n-1)
     Read (nin,*) d(1:n)
     Read (nin,*) dl(1:n-1)
     Read the right hand matrix B
1
     Read (nin,*)(b(i,1:nrhs),i=1,n)
!
     Solve the equations AX = B
     The NAG name equivalent of zgtsvx is f07cpf
     Call zgtsvx('No factors','No transpose',n,nrhs,dl,d,du,dlf,df,duf,du2,
        ipiv,b,ldb,x,ldx,rcond,ferr,berr,work,rwork,info)
     If ((info==0) .Or. (info==n+1)) Then
       Print solution, error bounds and condition number
!
1
        ifail: behaviour on error exit
!
              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
        ifail = 0
        Call x04dbf('General',' ',n,nrhs,x,ldx,'Bracketed','F7.4'
          'Solution(s)','Integer',rlabs,'Integer',clabs,80,0,ifail)
        Write (nout,*)
        Write (nout,*) 'Backward errors (machine-dependent)'
        Write (nout, 99999) berr(1:nrhs)
        Write (nout,*)
        Write (nout,*) 'Estimated forward error bounds (machine-dependent)'
        Write (nout, 99999) ferr(1:nrhs)
        Write (nout,*)
        Write (nout,*) 'Estimate of reciprocal condition number'
        Write (nout, 99999) rcond
        If (info==n+1) Then
          Write (nout,*)
          Write (nout,*) 'The matrix A is singular to working precision'
        End If
     Else
       Write (nout,99998) 'The (', info, ',', info, ')',
   ' element of the factor U is zero'
```

F07CPF.6 Mark 26

```
End If

99999 Format ((3X,1P,7E11.1))

99998 Format (1X,A,I3,A,I3,A,A)

End Program f07cpfe
```

10.2 Program Data

10.3 Program Results

```
FO7CPF Example Program Results
```

Mark 26 F07CPF.7 (last)