

NAG Fortran Library Routine Document

C02AKF

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

C02AKF determines the roots of a cubic equation with real coefficients.

2 Specification

```
SUBROUTINE C02AKF(U, R, S, T, ZEROR, ZEROI, ERREST, IFAIL)
INTEGER          IFAIL
real            U, R, S, T, ZEROR(3), ZEROI(3), ERREST(3)
```

3 Description

This routine attempts to find the roots of the cubic equation

$$uz^3 + rz^2 + sz + t = 0,$$

where u , r , s and t are real coefficients with $u \neq 0$. The roots are located by finding the eigenvalues of the associated 3 by 3 (upper Hessenberg) companion matrix H given by

$$H = \begin{pmatrix} 0 & 0 & -t/u \\ 1 & 0 & -s/u \\ 0 & 1 & -r/u \end{pmatrix}.$$

The eigenvalues are obtained by a call to F08PEF (SHSEQR/DHSEQR). Further details can be found in Section 8.

To obtain the roots of a quadratic equation, C02AJF can be used.

4 References

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

5 Parameters

- | | | |
|----|--|--------------|
| 1: | U – <i>real</i>
<i>On entry:</i> u , the coefficient of z^3 .
<i>Constraint:</i> $U \neq 0.0$. | <i>Input</i> |
| 2: | R – <i>real</i>
<i>On entry:</i> r , the coefficient of z^2 . | <i>Input</i> |
| 3: | S – <i>real</i>
<i>On entry:</i> s , the coefficient of z . | <i>Input</i> |
| 4: | T – <i>real</i>
<i>On entry:</i> t , the constant coefficient. | <i>Input</i> |

- 5: ZEROR(3) – *real* array Output
 6: ZEROI(3) – *real* array Output
On exit: ZEROR(*i*) and ZEROI(*i*) contain the real and imaginary parts, respectively, of the *i*th root.
- 7: ERREST(3) – *real* array Output
On exit: ERREST(*i*) contains an approximate error estimate for the *i*th root.
- 8: IFAIL – INTEGER Input/Output
On entry: IFAIL must be set to 0, –1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.
On exit: IFAIL = 0 unless the routine detects an error (see Section 6).
 For environments where it might be inappropriate to halt program execution when an error is detected, the value –1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, for users not familiar with this parameter the recommended value is 0. **When the value –1 or 1 is used it is essential to test the value of IFAIL on exit.**

6 Error Indicators and Warnings

If on entry IFAIL = 0 or –1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

On entry, U = 0.0.

IFAIL = 2

The companion matrix *H* cannot be formed without overflow.

IFAIL = 3

The iterative procedure used to determine the eigenvalues has failed to converge.

7 Accuracy

If IFAIL = 0 on exit, then the *i*th computed root should have approximately $|\log_{10}(\text{ERREST}(i))|$ correct significant digits.

8 Further Comments

The method used by the routine consists of the following steps, which are performed by routines from LAPACK in Chapter F08.

- (a) Form *H*.
- (b) Apply a diagonal similarity transformation to *H* (to give *H'*).
- (c) Calculate the eigenvalues and Schur factorization of *H'*.
- (d) Calculate the left and right eigenvectors of *H'*.
- (e) Estimate reciprocal condition numbers for all the eigenvalues of *H'*.
- (f) Calculate approximate error estimates for all the eigenvalues of *H'* (using the 1-norm).

9 Example

To find the roots of the cubic equation

$$z^3 + 3z^2 + 9z - 13 = 0.$$

9.1 Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*      C02AKF Example Program Text.
*      Mark 20 Release. NAG Copyright 2001.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*      .. Local Scalars ..
      real              R, S, T, U
      INTEGER          I, IFAIL
*      .. Local Arrays ..
      real              ERREST(3), ZEROI(3), ZEROR(3)
*      .. External Subroutines ..
      EXTERNAL         C02AKF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'C02AKF Example Program Results'
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) U, R, S, T
      IFAIL = 0

*
      CALL C02AKF(U,R,S,T,ZEROR,ZEROI,ERREST,IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,*) ' Roots of cubic equation          ',
+ '      Error estimates'
      WRITE (NOUT,*) '
+ '      (machine-dependent)'
      WRITE (NOUT,*)
      DO 20 I = 1, 3
          WRITE (NOUT,99999) ' z = ', ZEROR(I), ZEROI(I), '*i', ERREST(I)
20  CONTINUE
*
      STOP
*
99999  FORMAT (1X,A,1P,E12.4,SP,E12.4,A,8X,SS,E9.1)
      END
```

9.2 Program Data

C02AKF Example Program Data
1.0 3.0 9.0 -13.0 : Values of U, R, S and T

9.3 Program Results

C02AKF Example Program Results

Roots of cubic equation	Error estimates (machine-dependent)
z = 1.0000E+00 +0.0000E+00*i	1.8E-15
z = -2.0000E+00 +3.0000E+00*i	2.2E-15
z = -2.0000E+00 -3.0000E+00*i	2.2E-15
