

NAG Library Routine Document

C06RAF

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

C06RAF computes the discrete Fourier sine transforms of m sequences of real data values.

2 Specification

```
SUBROUTINE C06RAF(M, N, X, WORK, IFAIL)
INTEGER          M, N, IFAIL
double precision X(M*(N+2)), WORK(*)
```

3 Description

Given m sequences of $n - 1$ real data values x_j^p , for $j = 1, 2, \dots, n - 1$ and $p = 1, 2, \dots, m$, C06RAF simultaneously calculates the Fourier sine transforms of all the sequences defined by

$$\hat{x}_k^p = \sqrt{\frac{2}{n}} \sum_{j=1}^{n-1} x_j^p \times \sin\left(jk\frac{\pi}{n}\right), \quad k = 1, 2, \dots, n - 1 \text{ and } p = 1, 2, \dots, m.$$

(Note the scale factor $\sqrt{\frac{2}{n}}$ in this definition.)

Since the Fourier sine transform defined above is its own inverse, two consecutive calls of this routine will restore the original data.

The transform calculated by this routine can be used to solve Poisson's equation when the solution is specified at both left and right boundaries (see Swarztrauber (1977)).

The routine uses a variant of the fast Fourier transform (FFT) algorithm (see Brigham (1974)) known as the Stockham self-sorting algorithm, described in Temperton (1983), together with pre- and post-processing stages described in Swarztrauber (1982). Special coding is provided for the factors 2, 3, 4 and 5.

4 References

Brigham E O (1974) *The Fast Fourier Transform* Prentice-Hall

Swarztrauber P N (1977) The methods of cyclic reduction, Fourier analysis and the FACR algorithm for the discrete solution of Poisson's equation on a rectangle *SIAM Rev.* **19** (3) 490–501

Swarztrauber P N (1982) Vectorizing the FFT's *Parallel Computation* (ed G Rodrigue) 51–83 Academic Press

Temperton C (1983) Fast mixed-radix real Fourier transforms *J. Comput. Phys.* **52** 340–350

5 Parameters

- 1: M – INTEGER *Input*
On entry: m , the number of sequences to be transformed.
Constraint: $M \geq 1$.

2: N – INTEGER Input

On entry: one more than the number of real values in each sequence, i.e., the number of values in each sequence is $n - 1$.

Constraint: $N \geq 1$.

3: X($M \times (N + 2)$) – **double precision** array Input/Output

On entry: the data must be stored in X as if in a two-dimensional array of dimension $(1 : M, 1 : N + 2)$; each of the m sequences is stored in a **row** of the array. In other words, if the $n - 1$ data values of the p th sequence to be transformed are denoted by x_j^p , for $j = 1, 2, \dots, n - 1$ and $p = 1, 2, \dots, m$, then the first $m(n - 1)$ elements of the array X must contain the values

$$x_1^1, x_1^2, \dots, x_1^m, x_2^1, x_2^2, \dots, x_2^m, \dots, x_{n-1}^1, x_{n-1}^2, \dots, x_{n-1}^m.$$

The n th to $(n + 2)$ th elements of each row $x_n^p, \dots, x_{n+2}^p$, for $p = 1, 2, \dots, m$, are required as workspace. These $3m$ elements may contain arbitrary values as they are set to zero by the routine.

On exit: the m Fourier sine transforms stored as if in a two-dimensional array of dimension $(1 : M, 1 : N + 2)$. Each of the m transforms is stored in a **row** of the array, overwriting the corresponding original sequence. If the $(n - 1)$ components of the p th Fourier sine transform are denoted by $\hat{x}_k^p$, for $k = 1, 2, \dots, n - 1$ and $p = 1, 2, \dots, m$, then the $m(n + 2)$ elements of the array X contain the values

$$\hat{x}_1^1, \hat{x}_1^2, \dots, \hat{x}_1^m, \hat{x}_2^1, \hat{x}_2^2, \dots, \hat{x}_2^m, \dots, \hat{x}_{n-1}^1, \hat{x}_{n-1}^2, \dots, \hat{x}_{n-1}^m, 0, 0, \dots, 0 \text{ (3m times)}.$$

4: WORK(*) – **double precision** array Workspace

Note: the dimension of the array WORK must be at least $M \times N + 2 \times N + 15$.

The workspace requirements as documented for C06RAF may be an overestimate in some implementations. For full details of the workspace required by this routine please refer to the Users' Note for your implementation.

On exit: WORK(1) contains the minimum workspace required for the current values of M and N with this implementation.

5: IFAIL – INTEGER Input/Output

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction 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, if you are 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, $M < 1$.

IFAIL = 2

On entry, $N < 1$.

IFAIL = 3

An unexpected error has occurred in an internal call. Check all subroutine calls and array dimensions. Seek expert help.

7 Accuracy

Some indication of accuracy can be obtained by performing a subsequent inverse transform and comparing the results with the original sequence (in exact arithmetic they would be identical).

8 Further Comments

The time taken by C06RAF is approximately proportional to $nm \log n$, but also depends on the factors of n . C06RAF is fastest if the only prime factors of n are 2, 3 and 5, and is particularly slow if n is a large prime, or has large prime factors.

9 Example

This example reads in sequences of real data values and prints their Fourier sine transforms (as computed by C06RAF). It then calls C06RAF again and prints the results which may be compared with the original sequence.

9.1 Program Text

```
*      C06RAF Example Program Text
*      Mark 19 Release. NAG Copyright 1998.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=5,NMAX=20)
*      .. Local Scalars ..
      INTEGER          I, IFAIL, J, M, N
*      .. Local Arrays ..
      DOUBLE PRECISION WORK(MMAX*NMAX+2*NMAX+15), X((NMAX+2)*MMAX)
*      .. External Subroutines ..
      EXTERNAL         C06RAF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'C06RAF Example Program Results'
*      Skip heading in data file
      READ (NIN,*)
20  CONTINUE
      READ (NIN,*,END=120) M, N
      IF (M.LE.MMAX .AND. N.LE.NMAX) THEN
        DO 40 J = 1, M
          READ (NIN,*) (X((I-1)*M+J),I=1,N-1)
40     CONTINUE
          WRITE (NOUT,*)
          WRITE (NOUT,*) 'Original data values'
          WRITE (NOUT,*)
          DO 60 J = 1, M
            WRITE (NOUT,99999) (X((I-1)*M+J),I=1,N-1)
60     CONTINUE
          IFAIL = 1
*
*      -- Compute transform
          CALL C06RAF(M,N,X,WORK,IFAIL)
*
          IF (IFAIL.EQ.0) THEN
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Discrete Fourier sine transforms'
            WRITE (NOUT,*)
            DO 80 J = 1, M
              WRITE (NOUT,99999) (X((I-1)*M+J),I=1,N-1)
80         CONTINUE
          *

```

```

*          -- Compute inverse transform
          CALL C06RAF(M,N,X,WORK,IFAIL)
*
          WRITE (NOUT,*)
          WRITE (NOUT,*)
+         'Original data as restored by inverse transform'
          WRITE (NOUT,*)
          DO 100 J = 1, M
            WRITE (NOUT,99999) (X((I-1)*M+J),I=1,N-1)
100        CONTINUE
          GO TO 20
        ELSE
          WRITE (NOUT,*)
          WRITE (NOUT,99998) ' ** C06RAF returned with IFAIL = ',
+         IFAIL
          END IF
        ELSE
          WRITE (NOUT,*) 'Invalid value of M or N'
          END IF
120 CONTINUE
*
99999 FORMAT (6X,6F10.4)
99998 FORMAT (1X,A,I5)
        END

```

9.2 Program Data

C06RAF Example Program Data

```

3  6 : Number of sequences, M, (number of values in each sequence)+1, N
0.6772 0.1138 0.6751 0.6362 0.1424 : X, sequence 1
0.2983 0.1181 0.7255 0.8638 0.8723 : X, sequence 2
0.0644 0.6037 0.6430 0.0428 0.4815 : X, sequence 3

```

9.3 Program Results

C06RAF Example Program Results

Original data values

0.6772	0.1138	0.6751	0.6362	0.1424
0.2983	0.1181	0.7255	0.8638	0.8723
0.0644	0.6037	0.6430	0.0428	0.4815

Discrete Fourier sine transforms

1.0014	0.0062	0.0834	0.5286	0.2514
1.2477	-0.6599	0.2570	0.0859	0.2658
0.8521	0.0719	-0.0561	-0.4890	0.2056

Original data as restored by inverse transform

0.6772	0.1138	0.6751	0.6362	0.1424
0.2983	0.1181	0.7255	0.8638	0.8723
0.0644	0.6037	0.6430	0.0428	0.4815
