

NAG Library Routine Document

C06PAF

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

C06PAF calculates the discrete Fourier transform of a sequence of n real data values or of a Hermitian sequence of n complex data values.

2 Specification

```
SUBROUTINE C06PAF(DIRECT, X, N, WORK, IFAIL)
INTEGER          N, IFAIL
double precision X(N+2), WORK(*)
CHARACTER*1      DIRECT
```

3 Description

Given a sequence of n real data values x_j , for $j = 0, 1, \dots, n-1$, C06PAF calculates their discrete Fourier transform (in the **Forward** direction) defined by

$$\hat{z}_k = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} x_j \times \exp\left(-i \frac{2\pi jk}{n}\right), \quad k = 0, 1, \dots, n-1.$$

The transformed values $\hat{z}_k$ are complex, but they form a Hermitian sequence (i.e., $\hat{z}_{n-k}$ is the complex conjugate of $\hat{z}_k$), so they are completely determined by n real numbers (since $\hat{z}_0$ is real, as is $\hat{z}_{n/2}$ for n even).

Alternatively, given a Hermitian sequence of n complex data values z_j , this routine calculates their inverse (**backward**) discrete Fourier transform defined by

$$\hat{x}_k = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} z_j \times \exp\left(i \frac{2\pi jk}{n}\right), \quad k = 0, 1, \dots, n-1.$$

The transformed values $\hat{x}_k$ are real.

(Note the scale factor of $\frac{1}{\sqrt{n}}$ in the above definitions.)

A call of C06PAF with DIRECT = 'F' followed by a call with DIRECT = 'B' will restore the original data.

C06PAF uses a variant of the fast Fourier transform (FFT) algorithm (see Brigham (1974)) known as the Stockham self-sorting algorithm, which is described in Temperton (1983).

4 References

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

Temperton C (1983) Self-sorting mixed-radix fast Fourier transforms *J. Comput. Phys.* **52** 1–23

5 Parameters

- 1: DIRECT – CHARACTER*1 *Input*
- On entry:* if the forward transform as defined in Section 3 is to be computed, then DIRECT must be set equal to 'F'.

If the backward transform is to be computed then DIRECT must be set equal to 'B'.

Constraint: DIRECT = 'F' or 'B'.

- 2: $X(N+2)$ – *double precision* array *Input/Output*

On entry: if X is declared with bounds $(0 : N+1)$ in the subroutine from which C06PAF is called, then:

if DIRECT is set to 'F', $X(j)$ must contain x_j , for $j = 0, 1, \dots, n-1$;

if DIRECT is set to 'B', $X(2 \times k)$ and $X(2 \times k + 1)$ must contain the real and imaginary parts respectively of $\hat{z}_k$, for $k = 0, 1, \dots, n/2$. (Note that for the sequence $\hat{z}_k$ to be Hermitian, the imaginary part of $\hat{z}_0$, and of $\hat{z}_{n/2}$ for n even, must be zero.)

On exit:

if DIRECT is set to 'F' and X is declared with bounds $(0 : N+1)$ then $X(2 \times k)$ and $X(2 \times k + 1)$ will contain the real and imaginary parts respectively of $\hat{z}_k$, for $k = 0, 1, \dots, n/2$;

if DIRECT is set to 'B' and X is declared with bounds $(0 : N+1)$ then $X(j)$ will contain x_j , for $j = 0, 1, \dots, n-1$.

- 3: N – INTEGER *Input*

On entry: n , the number of data values. The total number of prime factors of N, counting repetitions, must not exceed 30.

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

Note: the dimension of the array WORK must be at least $3 \times N + 15$.

The workspace requirements as documented for C06PAF 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 value of 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, $N \leq 1$.

IFAIL = 2

On entry, DIRECT $\neq$ 'F' or 'B'.

IFAIL = 4

On entry, N has more than 30 prime factors.

IFAIL = 5

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 is approximately proportional to $n \times \log n$, but also depends on the factorization of n . C06PAF is faster if the only prime factors of n are 2, 3 or 5; and fastest of all if n is a power of 2.

9 Example

This example reads in a sequence of real data values and prints their discrete Fourier transform (as computed by C06PAF with DIRECT set to 'F'), after expanding it from complex Hermitian form into a full complex sequence. It then performs an inverse transform using C06PAF with DIRECT = 'B', and prints the sequence so obtained alongside the original data values.

9.1 Program Text

```
*      C06PAF Example Program Text
*      Mark 19 Release. NAG Copyright 1999.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX
      PARAMETER        (NMAX=20)
*      .. Local Scalars ..
      INTEGER          IFAIL, J, N, NJ
*      .. Local Arrays ..
      DOUBLE PRECISION WORK(3*NMAX+15), X(0:NMAX+1), XX(0:NMAX-1)
*      .. External Subroutines ..
      EXTERNAL         C06PAF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'C06PAF Example Program Results'
*      Skip heading in data file
      READ (NIN,*)
20  CONTINUE
      READ (NIN,*,END=120) N
      IF (N.GT.1 .AND. N.LE.NMAX) THEN
        DO 40 J = 0, N - 1
          READ (NIN,*) X(J)
          XX(J) = X(J)
40    CONTINUE
      IFAIL = 1

*      CALL C06PAF('F',X,N,WORK,IFAIL)

*      IF (IFAIL.EQ.0) THEN
        WRITE (NOUT,*)
        WRITE (NOUT,*) 'Components of discrete Fourier transform'
        WRITE (NOUT,*)
        WRITE (NOUT,*) '          Real          Imag'
        WRITE (NOUT,*)
        DO 60 J = 0, N/2
          WRITE (NOUT,99999) J, X(2*J), X(2*J+1)
60    CONTINUE
```

```

      DO 80 J = N/2 + 1, N - 1
        NJ = N - J
        WRITE (NOUT,99999) J, X(2*NJ), -X(2*NJ+1)
80    CONTINUE
*
      CALL C06PAF('B',X,N,WORK,IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,*)
      +      'Original sequence as restored by inverse transform'
      WRITE (NOUT,*)
      WRITE (NOUT,*) '          Original   Restored'
      WRITE (NOUT,*)
      DO 100 J = 0, N - 1
        WRITE (NOUT,99999) J, XX(J), X(J)
100    CONTINUE
      GO TO 20
    ELSE
      WRITE (NOUT,*)
      WRITE (NOUT,99998) ' ** C06PAF returned with IFAIL = ',
      +      IFAIL
      END IF
    ELSE
      WRITE (NOUT,*) 'Invalid value of N'
    END IF
120 CONTINUE
*
99999 FORMAT (1X,I5,2F10.5)
99998 FORMAT (1X,A,I5)
      END

```

9.2 Program Data

C06PAF Example Program Data

```

7
0.34907
0.54890
0.74776
0.94459
1.13850
1.32850
1.51370

```

9.3 Program Results

C06PAF Example Program Results

Components of discrete Fourier transform

	Real	Imag
0	2.48361	0.00000
1	-0.26599	0.53090
2	-0.25768	0.20298
3	-0.25636	0.05806
4	-0.25636	-0.05806
5	-0.25768	-0.20298
6	-0.26599	-0.53090

Original sequence as restored by inverse transform

	Original	Restored
0	0.34907	0.34907
1	0.54890	0.54890

2	0.74776	0.74776
3	0.94459	0.94459
4	1.13850	1.13850
5	1.32850	1.32850
6	1.51370	1.51370
