

# NAG Fortran Library Routine Document

## G13CBF

**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

G13CBF calculates the smoothed sample spectrum of a univariate time series using spectral smoothing by the trapezium frequency (Daniell) window.

### 2 Specification

```
SUBROUTINE G13CBF(NX, MTX, PX, MW, PW, L, KC, LG, XG, NG, STATS, IFAIL)
INTEGER      NX, MTX, MW, L, KC, LG, NG, IFAIL
real       PX, PW, XG(KC), STATS(4)
```

### 3 Description

The supplied time series may be mean or trend corrected (by least-squares), and tapered, the tapering factors being those of the split cosine bell:

$$\begin{aligned} & \frac{1}{2} \left( 1 - \cos \left( \pi \left( t - \frac{1}{2} \right) / T \right) \right), & 1 \leq t \leq T \\ & \frac{1}{2} \left( 1 - \cos \left( \pi \left( n - t + \frac{1}{2} \right) / T \right) \right), & n + 1 - T \leq t \leq n \\ & 1, & \text{otherwise,} \end{aligned}$$

where  $T = \left\lceil \frac{np}{2} \right\rceil$  and  $p$  is the tapering proportion.

The unsmoothed sample spectrum

$$f^*(\omega) = \frac{1}{2\pi} \left| \sum_{t=1}^n x_t \exp(i\omega t) \right|^2$$

is then calculated for frequency values

$$\omega_k = \frac{2\pi k}{K}, \quad k = 0, 1, \dots, [K/2],$$

where  $[ ]$  denotes the integer part.

The smoothed spectrum is returned as a subset of these frequencies for which  $k$  is a multiple of a chosen value  $r$ , i.e.,

$$\omega_{rl} = \nu_l = \frac{2\pi l}{L}, \quad l = 0, 1, \dots, [L/2],$$

where  $K = r \times L$ . The user will normally fix  $L$  first, then choose  $r$  so that  $K$  is sufficiently large to provide an adequate representation for the unsmoothed spectrum, i.e.,  $K \geq 2 \times n$ . It is possible to take  $L = K$ , i.e.,  $r = 1$ .

The smoothing is defined by a trapezium window whose shape is supplied by the function

$$\begin{aligned} W(\alpha) &= 1, & |\alpha| \leq p \\ W(\alpha) &= \frac{1-|\alpha|}{1-p}, & p < |\alpha| \leq 1 \end{aligned}$$

the proportion  $p$  being supplied by the user.

The width of the window is fixed as  $2\pi/M$  by the user supplying  $M$ . A set of averaging weights are constructed:

$$W_k = g \times W\left(\frac{\omega_k M}{\pi}\right), \quad 0 \leq \omega_k \leq \frac{\pi}{M},$$

where  $g$  is a normalising constant, and the smoothed spectrum obtained is

$$\hat{f}(\nu_l) = \sum_{|\omega_k| < \frac{\pi}{M}} W_k f^*(\nu_l + \omega_k).$$

If no smoothing is required  $M$  should be set to  $n$ , in which case the values returned are  $\hat{f}(\nu_l) = f^*(\nu_l)$ . Otherwise, in order that the smoothing approximates well to an integration, it is essential that  $K \gg M$ , and preferable, but not essential, that  $K$  be a multiple of  $M$ . A choice of  $L > M$  would normally be required to supply an adequate description of the smoothed spectrum. Typical choices of  $L \simeq n$  and  $K \simeq 4n$  should be adequate for usual smoothing situations when  $M < n/5$ .

The sampling distribution of  $\hat{f}(\omega)$  is approximately that of a scaled  $\chi_d^2$  variate, whose degrees of freedom  $d$  is provided by the routine, together with multiplying limits  $mu$ ,  $ml$  from which approximate 95% confidence intervals for the true spectrum  $f(\omega)$  may be constructed as  $[ml \times \hat{f}(\omega), mu \times \hat{f}(\omega)]$ . Alternatively,  $\log \hat{f}(\omega)$  may be returned, with additive limits.

The bandwidth  $b$  of the corresponding smoothing window in the frequency domain is also provided. Spectrum estimates separated by (angular) frequencies much greater than  $b$  may be assumed to be independent.

## 4 References

Jenkins G M and Watts D G (1968) *Spectral Analysis and its Applications* Holden-Day

Bloomfield P (1976) *Fourier Analysis of Time Series: An Introduction* Wiley

## 5 Parameters

- 1: NX – INTEGER *Input*  
*On entry:* the length of the time series,  $n$ .  
*Constraint:*  $NX \geq 1$ .
  
- 2: MTX – INTEGER *Input*  
*On entry:* whether the data are to be initially mean or trend corrected.  
 MTX = 0  
     For no correction,  
 MTX = 1  
     For mean correction.  
 MTX = 2  
     For trend correction.  
*Constraint:*  $0 \leq MTX \leq 2$ .
  
- 3: PX – *real* *Input*  
*On entry:* the proportion of the data (totalled over both ends) to be initially tapered by the split cosine bell taper. (A value of 0.0 implies no tapering.)  
*Constraint:*  $0.0 \leq PX \leq 1.0$ .

- 4: MW – INTEGER *Input*  
*On entry:* the value of  $M$  which determines the frequency width of the smoothing window as  $2\pi/M$ . A value of  $n$  implies no smoothing is to be carried out.  
*Constraint:*  $1 \leq MW \leq NX$ .
- 5: PW – *real* *Input*  
*On entry:* the shape parameter,  $p$ , of the trapezium frequency window.  
 A value of 0.0 gives a triangular window, and a value of 1.0 a rectangular window.  
 If  $MW = NX$  (i.e., no smoothing is carried out), then PW is not used.  
*Constraint:*  $0.0 \leq PW \leq 1.0$ .
- 6: L – INTEGER *Input*  
*On entry:* the frequency division,  $L$ , of smoothed spectral estimates as  $2\pi/L$ .  
*Constraints:*  
 $L \geq 1$ ,  
 $L$  must be a factor of KC (see below).
- 7: KC – INTEGER *Input*  
*On entry:* the order of the fast Fourier transform (FFT),  $K$ , used to calculate the spectral estimates. KC should be a multiple of small primes such as  $2^m$  where  $m$  is the smallest integer such that  $2^m \geq 2n$ , provided  $m \leq 20$ .  
*Constraints:*  
 $KC \geq 2 \times NX$ ,  
 KC must be a multiple of L. The largest prime factor of KC must not exceed 19, and the total number of prime factors of KC, counting repetitions, must not exceed 20. These two restrictions are imposed by C06EAF which performs the FFT.
- 8: LG – INTEGER *Input*  
*On entry:* indicates whether unlogged or logged spectral estimates and confidence limits are required.  
 $LG = 0$   
 For unlogged.  
 $LG \neq 0$   
 For logged.
- 9: XG(KC) – *real* array *Input/Output*  
*On entry:* the  $n$  data points.  
*On exit:* contains the NG spectral estimates  $\hat{f}(\omega_i)$ , for  $i = 0, 1, \dots, [L/2]$ , in XG(1) to XG(NG) (logged if  $LG \neq 0$ ). The elements XG( $i$ ), for  $i = NG + 1, \dots, KC$  contain 0.0.
- 10: NG – INTEGER *Output*  
*On exit:* the number of spectral estimates,  $[L/2] + 1$ , in XG.
- 11: STATS(4) – *real* array *Output*  
*On exit:* four associated statistics. These are the degrees of freedom in STATS(1), the lower and upper 95% confidence limit factors in STATS(2) and STATS(3) respectively (logged if  $LG \neq 0$ ), and the bandwidth in STATS(4).

## 12: 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, because for this routine the values of the output parameters may be useful even if IFAIL  $\neq$  0 on exit, the recommended value is -1. **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, NX < 1,  
 or MTX < 0,  
 or MTX > 2,  
 or PX < 0.0,  
 or PX > 1.0,  
 or MW < 1,  
 or MW > NX,  
 or PW < 0.0 and MW  $\neq$  NX,  
 or PW > 1.0 and MW  $\neq$  NX,  
 or L < 1.

IFAIL = 2

On entry, KC < 2  $\times$  NX,  
 or KC is not a multiple of L,  
 or KC has a prime factor exceeding 19,  
 or KC has more than 20 prime factors, counting repetitions.

IFAIL = 3

This indicates that a serious error has occurred. Check all array subscripts and subroutine parameter lists in calls to G13CBF. Seek expert help.

IFAIL = 4

One or more spectral estimates are negative. Unlogged spectral estimates are returned in XG, and the degrees of freedom, unlogged confidence limit factors and bandwidth in STATS.

IFAIL = 5

The calculation of confidence limit factors has failed. This error will not normally occur. Spectral estimates (logged if requested) are returned in XG, and degrees of freedom and bandwidth in STATS.

## 7 Accuracy

The FFT is a numerically stable process, and any errors introduced during the computation will normally be insignificant compared with uncertainty in the data.

## 8 Further Comments

G13CBF carries out a FFT of length KC to calculate the sample spectrum. The time taken by the routine for this is approximately proportional to  $KC \times \log(KC)$  (but see Section 8 of the document for C06EAF for further details).

## 9 Example

The example program reads a time series of length 131. It selects the mean correction option, a tapering proportion of 0.2, the option of no smoothing and a frequency division for logged spectral estimates of  $2\pi/100$ . It then calls G13CBF to calculate the univariate spectrum and prints the logged spectrum together with 95% confidence limits. The program then selects a smoothing window with frequency width  $2\pi/30$  and shape parameter 0.5 and recalculates and prints the logged spectrum and 95% confidence limits.

### 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.

```
*      G13CBF Example Program Text
*      Mark 14 Revised.  NAG Copyright 1989.
*      .. Parameters ..
      INTEGER          KCMAX, NXMAX
      PARAMETER       (KCMAX=400,NXMAX=KCMAX/2)
      INTEGER          NIN, NOUT
      PARAMETER       (NIN=5,NOUT=6)
*      .. Local Scalars ..
      real            PW, PX
      INTEGER          I, IFAIL, KC, L, LG, MTX, MW, NG, NX
*      .. Local Arrays ..
      real            STATS(4), XG(KCMAX), XH(NXMAX)
*      .. External Subroutines ..
      EXTERNAL        G13CBF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'G13CBF Example Program Results'
*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) NX
      IF (NX.GT.0 .AND. NX.LE.NXMAX) THEN
          READ (NIN,*) (XH(I),I=1,NX)
          MTX = 1
          PX = 0.2e0
          MW = NX
          PW = 0.5e0
          KC = 400
          L = 100
          LG = 1
20      READ (NIN,*,END=60) MW
          IF (MW.GT.0 .AND. MW.LE.NX) THEN
              DO 40 I = 1, NX
                  XG(I) = XH(I)
40      CONTINUE
          IFAIL = 1
*
          CALL G13CBF(NX,MTX,PX,MW,PW,L,KC,LG,XG,NG,STATS,IFAIL)
*
          WRITE (NOUT,*)
          IF (MW.EQ.NX) THEN
              WRITE (NOUT,*) 'No smoothing'
          ELSE
              WRITE (NOUT,99999)
              +      'Frequency width of smoothing window = 1/', MW
          END IF
          WRITE (NOUT,*)
          IF (IFAIL.NE.0) THEN
              WRITE (NOUT,99999) 'G13CBF fails. IFAIL =', IFAIL
              WRITE (NOUT,*)
          END IF
      END IF
```

```

      END IF
      IF (IFAIL.EQ.0 .OR. IFAIL.GE.4) THEN
        WRITE (NOUT,99998) 'Degrees of freedom =', STATS(1),
+         ' Bandwidth =', STATS(4)
        WRITE (NOUT,*)
        WRITE (NOUT,99997)
+         '95 percent confidence limits - Lower =', STATS(2),
+         ' Upper =', STATS(3)
        WRITE (NOUT,*)
        WRITE (NOUT,*)
+         ' Spectrum      Spectrum      Spectrum      Spectrum'
+         ' estimate      estimate      estimate      estimate'
        WRITE (NOUT,99996) (I,XG(I),I=1,NG)
      END IF
      GO TO 20
    END IF
  END IF
60 STOP
*
99999 FORMAT (1X,A,I3)
99998 FORMAT (1X,A,F4.1,A,F7.4)
99997 FORMAT (1X,A,F7.4,A,F7.4)
99996 FORMAT (1X,I4,F10.4,I5,F10.4,I5,F10.4,I5,F10.4)
      END

```

## 9.2 Program Data

G13CBF Example Program Data

```

131
11.500  9.890  8.728  8.400  8.230  8.365  8.383  8.243
 8.080  8.244  8.490  8.867  9.469  9.786 10.100 10.714
11.320 11.900 12.390 12.095 11.800 12.400 11.833 12.200
12.242 11.687 10.883 10.138  8.952  8.443  8.231  8.067
 7.871  7.962  8.217  8.689  8.989  9.450  9.883 10.150
10.787 11.000 11.133 11.100 11.800 12.250 11.350 11.575
11.800 11.100 10.300  9.725  9.025  8.048  7.294  7.070
 6.933  7.208  7.617  7.867  8.309  8.640  9.179  9.570
10.063 10.803 11.547 11.550 11.800 12.200 12.400 12.367
12.350 12.400 12.270 12.300 11.800 10.794  9.675  8.900
 8.208  8.087  7.763  7.917  8.030  8.212  8.669  9.175
 9.683 10.290 10.400 10.850 11.700 11.900 12.500 12.500
12.800 12.950 13.050 12.800 12.800 12.800 12.600 11.917
10.805  9.240  8.777  8.683  8.649  8.547  8.625  8.750
 9.110  9.392  9.787 10.340 10.500 11.233 12.033 12.200
12.300 12.600 12.800 12.650 12.733 12.700 12.259 11.817
10.767  9.825  9.150
131
30

```

## 9.3 Program Results

G13CBF Example Program Results

No smoothing

Degrees of freedom = 2.0      Bandwidth = 0.0480

95 percent confidence limits -      Lower = -1.3053      Upper = 3.6762

	Spectrum estimate		Spectrum estimate		Spectrum estimate		Spectrum estimate
1	-5.9354	2	-0.1662	3	-0.8250	4	-0.9452
5	3.2137	6	0.2738	7	-1.0690	8	-1.0401
9	-1.2388	10	-3.5434	11	-5.2568	12	-3.2450
13	-2.4294	14	-3.9987	15	-2.9853	16	-4.6631
17	-4.3317	18	-4.6982	19	-4.6335	20	-3.6732
21	-5.8411	22	-4.7727	23	-3.9747	24	-4.8351
25	-5.9979	26	-6.1169	27	-5.5245	28	-4.4774
29	-5.6331	30	-4.0707	31	-4.6921	32	-5.6515

33	-9.2919	34	-4.6302	35	-4.1700	36	-4.7829
37	-6.6058	38	-5.8145	39	-5.2714	40	-5.8736
41	-10.2188	42	-5.7887	43	-7.0751	44	-7.4055
45	-8.2774	46	-7.8966	47	-6.4435	48	-5.7844
49	-5.4690	50	-6.8709	51	-8.7123		

Frequency width of smoothing window = 1/ 30

Degrees of freedom = 7.0      Bandwidth = 0.1767

95 percent confidence limits -      Lower = -0.8275      Upper = 1.4213

	Spectrum estimate		Spectrum estimate		Spectrum estimate		Spectrum estimate
1	-0.1776	2	-0.4561	3	-0.1784	4	1.9042
5	2.1094	6	1.7061	7	-0.7659	8	-1.4734
9	-1.5939	10	-2.1157	11	-2.9151	12	-2.7055
13	-2.8200	14	-3.4077	15	-3.8813	16	-3.6607
17	-4.0601	18	-4.4756	19	-4.2700	20	-4.3092
21	-4.5711	22	-4.8111	23	-4.5658	24	-4.7285
25	-5.4386	26	-5.5081	27	-5.2325	28	-5.0262
29	-4.4539	30	-4.4764	31	-4.9152	32	-5.8492
33	-5.5872	34	-4.9804	35	-4.8904	36	-5.2666
37	-5.7643	38	-5.8620	39	-5.5011	40	-5.7129
41	-6.3894	42	-6.4027	43	-6.1352	44	-6.5766
45	-7.3676	46	-7.1405	47	-6.1674	48	-5.8600
49	-6.1036	50	-6.2673	51	-6.4321		

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