NAG 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 (KIND=nag_wp) 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:

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

where $T=\left[\frac{np}{2}\right]$ 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

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

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.,

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

where $K=r\times L$. You 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

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

the proportion p being supplied by you.

The width of the window is fixed as $2\pi/M$ by you 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 normalizing 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 χ^2_d 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 $\left[ml \times \hat{f}(\omega) mu \times \hat{f}(\omega)\right]$. 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

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

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

5 Parameters

1: NX – INTEGER *Input*

On entry: n, the length of the time series.

Constraint: NX ≥ 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 ≤ 2.

3: PX – REAL (KIND=nag_wp) *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 ≤ 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: $1 \leq \text{MW} \leq \text{NX}$.

5: PW – REAL (KIND=nag_wp) *Input*

On entry: p, the shape parameter of the trapezium frequency window.

A value of 0.0 gives a triangular window, and a value of 1.0 a rectangular window.

If $\text{MW} = \text{NX}$ (i.e., no smoothing is carried out), PW is not used.

Constraint: $0.0 \leq \text{PW} \leq 1.0$.

6: L – INTEGER *Input*

On entry: L, the frequency division of smoothed spectral estimates as $2\pi/L$.

Constraints:

$\text{L} \geq 1$;
L must be a factor of KC.

7: KC – INTEGER *Input*

On entry: K, the order of the fast Fourier transform (FFT) 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:

$\text{KC} \geq 2 \times \text{NX}$;
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 the internal FFT algorithm used.

8: LG – INTEGER *Input*

On entry: indicates whether unlogged or logged spectral estimates and confidence limits are required.

$\text{LG} = 0$
For unlogged.

$\text{LG} \neq 0$
For logged.

9: XG(KC) – REAL (KIND=nag_wp) array *Input/Output*

On entry: the n data points.

On exit: contains the NG spectral estimates $\hat{f}(\omega_i)$, for $i = 0, 1, \ldots, [L/2]$, in XG(1) to XG(NG) (logged if $\text{LG} \neq 0$). The elements XG(i), for $i = \text{NG} + 1, \ldots, \text{KC}$, contain 0.0.

10: NG – INTEGER *Output*

On exit: the number of spectral estimates, $[L/2] + 1$, in XG.

11: STATS(4) – REAL (KIND=nag_wp) 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 $\text{LG} \neq 0$), and the bandwidth in STATS(4).

12: IFAIL – INTEGER *Input/Output*

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

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 $\text{IFAIL} \neq 0$ 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.**

On exit: $\text{IFAIL} = 0$ unless the routine detects an error or a warning has been flagged (see Section 6).

6 Error Indicators and Warnings

If on entry $\text{IFAIL} = 0$ or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Note: G13CBF may return useful information for one or more of the following detected errors or warnings.

Errors or warnings detected by the routine:

$\text{IFAIL} = 1$

On entry, $\text{NX} < 1$,
or $\text{MTX} < 0$,
or $\text{MTX} > 2$,
or $\text{PX} < 0.0$,
or $\text{PX} > 1.0$,
or $\text{MW} < 1$,
or $\text{MW} > \text{NX}$,
or $\text{PW} < 0.0$ and $\text{MW} \neq \text{NX}$,
or $\text{PW} > 1.0$ and $\text{MW} \neq \text{NX}$,
or $\text{L} < 1$.

$\text{IFAIL} = 2$

On entry, $\text{KC} < 2 \times \text{NX}$,
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.

$\text{IFAIL} = 3$

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

$\text{IFAIL} = 4$

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.

$\text{IFAIL} = 5$

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.

IFAIL = −99

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.8 in the Essential Introduction for further information.

IFAIL = −399

Your licence key may have expired or may not have been installed correctly.

See Section 3.7 in the Essential Introduction for further information.

IFAIL = −999

Dynamic memory allocation failed.

See Section 3.6 in the Essential Introduction for further information.

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 Parallelism and Performance

Not applicable.

9 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 $\mathrm{KC} \times \log(\mathrm{KC})$ (but see Section 9 in C06PAF for further details).

10 Example

This example reads a time series of length 131. It then calls G13CBF to calculate the univariate spectrum and prints the logged spectrum together with 95% confidence limits.

10.1 Program Text

```
    Program g13cbfe

!     G13CBF Example Program Text

!     Mark 25 Release. NAG Copyright 2014.

!     .. Use Statements ..
      Use nag_library, Only: g13cbf, nag_wp
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: pw, px
      Integer                          :: i, ifail, kc, l, lg, lxg, mtx, mw,   &
                                          ng, nx
!     .. Local Arrays ..
      Real (Kind=nag_wp)               :: stats(4)
      Real (Kind=nag_wp), Allocatable  :: xg(:)
!     .. Intrinsic Procedures ..
      Intrinsic                        :: max
!     .. Executable Statements ..
      Write (nout,*) 'G13CBF Example Program Results'
      Write (nout,*)
```

```
!     Skip heading in data file
      Read (nin,*)

!     Read in the problem size
      Read (nin,*) nx

!     Read in smoothing parameters
      Read (nin,*) mtx, px, mw, l, kc, lg
      If (mw/=nx) Then
        Read (nin,*) pw
      End If

      lxg = max(kc,nx)
      Allocate (xg(lxg))

!     Read in series
      Read (nin,*) xg(1:nx)

!     Calculate smooth spectrum
      ifail = -1
      Call g13cbf(nx,mtx,px,mw,pw,l,kc,lg,xg,ng,stats,ifail)
      If (ifail/=0) Then
        If (ifail<4) Then
          Go To 100
        End If
      End If

!     Display results
      If (mw==nx) Then
        Write (nout,*) 'No smoothing'
      Else
        Write (nout,99999) 'Frequency width of smoothing window = 1/', mw
      End If
      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'
      Write (nout,*) &
        '      estimate       estimate       estimate       estimate'
      Write (nout,99996)(i,xg(i),i=1,ng)
      Write (nout,*)

100   Continue

99999 Format (1X,A,I0)
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 Program g13cbfe
```

10.2 Program Data

```
G13CBF Example Program Data
 131                                                  :: NX
1 0.2 30 100 400 1                                    :: MTX,PX,MW,L,KC,LG
0.5                                                   :: PW
 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                                          :: End of XG
```

10.3 Program Results

```
 G13CBF Example Program Results

 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       Spectrum       Spectrum       Spectrum
       estimate       estimate       estimate       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
```