NAG Library Routine Document

G13CAF

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

G13CAF calculates the smoothed sample spectrum of a univariate time series using one of four lag windows – rectangular, Bartlett, Tukey or Parzen window.

2 Specification

```
SUBROUTINE G13CAF (NX, MTX, PX, IW, MW, IC, NC, C, KC, L, LG, NXG, XG, NG,      &
                   STATS, IFAIL)

INTEGER            NX, MTX, IW, MW, IC, NC, KC, L, LG, NXG, NG, IFAIL
REAL (KIND=nag_wp) PX, C(NC), XG(NXG), STATS(4)
```

3 Description

The smoothed sample spectrum is defined as

$$\hat{f}(\omega) = \frac{1}{2\pi}\left(C_0 + 2\sum_{k=1}^{M-1} w_k C_k \cos(\omega k)\right),$$

where M is the window width, and is calculated for frequency values

$$\omega_i = \frac{2\pi i}{L}, \qquad i = 0, 1, \ldots, [L/2],$$

where [] denotes the integer part.

The autocovariances C_k may be supplied by you, or constructed from a time series $x_1, x_2, \ldots, x_n$, as

$$C_k = \frac{1}{n}\sum_{t=1}^{n-k} x_t x_{t+k},$$

the fast Fourier transform (FFT) being used to carry out the convolution in this formula.

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

$$\frac{1}{2}\left(1 - \cos\left(\pi\left(t - \frac{1}{2}\right)/T\right)\right), \qquad 1 \leq t \leq T$$

$$\frac{1}{2}\left(1 - \cos\left(\pi\left(n - t + \frac{1}{2}\right)/T\right)\right), \qquad n + 1 - T \leq t \leq n$$

$$1, \qquad \text{otherwise,}$$

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

The smoothing window is defined by

$$w_k = W\left(\frac{k}{M}\right), \qquad k \leq M - 1,$$

which for the various windows is defined over $0 \leq \alpha < 1$ by rectangular:

$$W(\alpha) = 1$$

Bartlett:

$$W(\alpha) = 1 - \alpha$$

Tukey:

$$W(\alpha) = \tfrac{1}{2}(1 + \cos(\pi\alpha))$$

Parzen:

$$W(\alpha) = 1 - 6\alpha^2 + 6\alpha^3, \quad 0 \leq \alpha \leq \tfrac{1}{2}$$

$$W(\alpha) = 2(1 - \alpha)^3, \qquad \tfrac{1}{2} < \alpha < 1.$$

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: if covariances are to be calculated by the routine (IC $= 0$), MTX must specify 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: if IC $= 0$, $0 \leq$ MTX ≤ 2

If covariances are supplied (IC $\neq 0$), MTX is not used.

3: PX – REAL (KIND=nag_wp) *Input*

On entry: if covariances are to be calculated by the routine (IC $= 0$), PX must specify the proportion of the data (totalled over both ends) to be initially tapered by the split cosine bell taper.

If covariances are supplied (IC $\neq 0$), PX must specify the proportion of data tapered before the supplied covariances were calculated and after any mean or trend correction. PX is required for the calculation of output statistics. A value of 0.0 implies no tapering.

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

4: IW – INTEGER *Input*

On entry: the choice of lag window.

IW = 1
Rectangular.

IW = 2
Bartlett.

IW = 3
Tukey.

IW = 4
Parzen.

Constraint: $1 \leq \text{IW} \leq 4$.

5: MW – INTEGER *Input*

On entry: M, the 'cut-off' point of the lag window. Windowed covariances at lag M or greater are zero.

Constraint: $1 \leq \text{MW} \leq \text{NX}$.

6: IC – INTEGER *Input*

On entry: indicates whether covariances are to be calculated in the routine or supplied in the call to the routine.

IC = 0
Covariances are to be calculated.

IC $\neq$ 0
Covariances are to be supplied.

7: NC – INTEGER *Input*

On entry: the number of covariances to be calculated in the routine or supplied in the call to the routine.

Constraint: $\text{MW} \leq \text{NC} \leq \text{NX}$.

8: C(NC) – REAL (KIND=nag_wp) array *Input/Output*

On entry: if IC $\neq 0$, C must contain the NC covariances for lags from 0 to $(\text{NC} - 1)$, otherwise C need not be set.

On exit: if IC $= 0$, C will contain the NC calculated covariances.

If IC $\neq 0$, the contents of C will be unchanged.

9: KC – INTEGER *Input*

On entry: if IC $= 0$, KC must specify the order of the fast Fourier transform (FFT) used to calculate the covariances. KC should be a product of small primes such as 2^m where m is the smallest integer such that $2^m \geq \text{NX} + \text{NC}$, provided $m \leq 20$.

If IC $\neq 0$, that is covariances are supplied, KC is not used.

Constraint: $\text{KC} \geq \text{NX} + \text{NC}$. 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.

10: L – INTEGER *Input*

On entry: L, the frequency division of the spectral estimates as $\frac{2\pi}{L}$. Therefore it is also the order of the FFT used to construct the sample spectrum from the covariances. L should be a product of small primes such as 2^m where m is the smallest integer such that $2^m \geq 2M - 1$, provided $m \leq 20$.

Constraint: $\mathrm{L} \geq 2 \times \mathrm{MW} - 1$. The largest prime factor of L must not exceed 19, and the total number of prime factors of L, counting repetitions, must not exceed 20. These two restrictions are imposed by the internal FFT algorithm used.

11: LG – INTEGER *Input*

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

$\mathrm{LG} = 0$
Unlogged.

$\mathrm{LG} \neq 0$
Logged.

12: NXG – INTEGER *Input*

On entry: the dimension of the array XG as declared in the (sub)program from which G13CAF is called.

Constraints:

if $\mathrm{IC} = 0$, $\mathrm{NXG} \geq \max(\mathrm{KC}, \mathrm{L})$;
if $\mathrm{IC} \neq 0$, $\mathrm{NXG} \geq \mathrm{L}$.

13: XG(NXG) – REAL (KIND=nag_wp) array *Input/Output*

On entry: if the covariances are to be calculated, then XG must contain the NX data points. If covariances are supplied, XG may contain any values.

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

14: NG – INTEGER *Output*

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

15: 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 $\mathrm{LG} = 1$), and the bandwidth in STATS(4).

16: 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, 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.**

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

6 Error Indicators and Warnings

If on entry 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 and IC $= 0$,
or MTX > 2 and IC $= 0$,
or PX < 0.0,
or PX > 1.0,
or IW < 1,
or IW > 4,
or MW < 1,
or MW $>$ NX,
or NC $<$ MW,
or NC $>$ NX,
or NXG $< \max(\mathrm{KC}, \mathrm{L})$ and IC $= 0$,
or NXG $<$ L and IC $\neq 0$.

IFAIL $= 2$

On entry, KC $<$ NX $+$ NC,
or KC has a prime factor exceeding 19,
or KC has more than 20 prime factors, counting repetitions.

This error only occurs when IC $= 0$.

IFAIL $= 3$

On entry, L $< 2 \times$ MW $- 1$,
or L has a prime factor exceeding 19,
or L has more than 20 prime factors, counting repetitions.

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

G13CAF carries out two FFTs of length KC to calculate the covariances and one FFT of length L to calculate the sample spectrum. The time taken by the routine for an FFT of length n is approximately proportional to $n \log(n)$ (but see Section 8 in C06PAF for further details).

9 Example

This example reads a time series of length 256. It selects the mean correction option, a tapering proportion of 0.1, the Parzen smoothing window and a cut-off point for the window at lag 100. It chooses to have 100 auto-covariances calculated and unlogged spectral estimates at a frequency division of $2\pi/200$. It then calls G13CAF to calculate the univariate spectrum and statistics and prints the autocovariances and the spectrum together with its 95% confidence multiplying limits.

9.1 Program Text

```
    Program g13cafe

!     G13CAF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: g13caf, nag_wp
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: px
      Integer                          :: i, ic, ifail, iw, kc, l, lg, lxg,    &
                                          mtx, mw, nc, ng, nx, nxg
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: c(:), xg(:)
      Real (Kind=nag_wp)               :: stats(4)
!     .. Intrinsic Procedures ..
      Intrinsic                        :: max
!     .. Executable Statements ..
      Write (nout,*) 'G13CAF Example Program Results'
      Write (nout,*)

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

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

!     Read in smoothing parameters
      Read (nin,*) mtx, ic, px, iw, mw, l, lg
      If (ic==0) Then
        Read (nin,*) kc
      End If

      If (ic==0) Then
        nxg = max(kc,l)
      Else
        nxg = l
      End If
      lxg = max(nxg,nx)
      Allocate (xg(lxg),c(nc))

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

!     Calculate smoothed spectrum
      ifail = -1
      Call g13caf(nx,mtx,px,iw,mw,ic,nc,c,kc,l,lg,nxg,xg,ng,stats,ifail)
      If (ifail/=0) Then
        If (ifail<4) Then
          Go To 100
        End If
      End If

!     Display results
      Write (nout,*) 'Covariances'
```

```
      Write (nout,99999) c(1:nc)
      Write (nout,*)
      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)

100   Continue

99999 Format (1X,6F11.4)
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 g13cafe
```

9.2 Program Data

```
G13CAF Example Program Data
 256 100                                                     :: NX,NC
1  0  0.1  4  100  200  0                                    :: MTX,IC,PX,IW,MW,L,LG
360                                                          :: KC
  5.0  11.0  16.0  23.0  36.0  58.0  29.0  20.0  10.0
  8.0   3.0   0.0   0.0   2.0  11.0  27.0  47.0  63.0
 60.0  39.0  28.0  26.0  22.0  11.0  21.0  40.0  78.0
122.0 103.0  73.0  47.0  35.0  11.0   5.0  16.0  34.0
 70.0  81.0 111.0 101.0  73.0  40.0  20.0  16.0   5.0
 11.0  22.0  40.0  60.0  80.9  83.4  47.7  47.8  30.7
 12.2   9.6  10.2  32.4  47.6  54.0  62.9  85.9  61.2
 45.1  36.4  20.9  11.4  37.8  69.8 106.1 100.8  81.6
 66.5  34.8  30.6   7.0  19.8  92.5 154.4 125.9  84.8
 68.1  38.5  22.8  10.2  24.1  82.9 132.0 130.9 118.1
 89.9  66.6  60.0  46.9  41.0  21.3  16.0   6.4   4.1
  6.8  14.5  34.0  45.0  43.1  47.5  42.2  28.1  10.1
  8.1   2.5   0.0   1.4   5.0  12.2  13.9  35.4  45.8
 41.1  30.1  23.9  15.6   6.6   4.0   1.8   8.5  16.6
 36.3  49.6  64.2  67.0  70.9  47.8  27.5   8.5  13.2
 56.9 121.5 138.3 103.2  85.7  64.6  36.7  24.2  10.7
 15.0  40.1  61.5  98.5 124.7  96.3  66.6  64.5  54.1
 39.0  20.6   6.7   4.3  22.7  54.8  93.8  95.8  77.2
 59.1  44.0  47.0  30.5  16.3   7.3  37.6  74.0 139.0
111.2 101.6  66.2  44.7  17.0  11.3  12.4   3.4   6.0
 32.3  54.3  59.7  63.7  63.5  52.2  25.4  13.1   6.8
  6.3   7.1  35.6  73.0  85.1  78.0  64.0  41.8  26.2
 26.7  12.1   9.5   2.7   5.0  24.4  42.0  63.5  53.8
 62.0  48.5  43.9  18.6   5.7   3.6   1.4   9.6  47.4
 57.1 103.9  80.6  63.6  37.6  26.1  14.2   5.8  16.7
 44.3  63.9  69.0  77.8  64.9  35.7  21.2  11.1   5.7
  8.7  36.1  79.7 114.4 109.6  88.8  67.8  47.5  30.6
 16.3   9.6  33.2  92.6 151.6 136.3 134.7  83.9  69.4
 31.5  13.9   4.4  38.0                                      :: End of XG
```

9.3 Program Results

```
 G13CAF Example Program Results

 Covariances
   1152.9733   937.3289   494.9243    14.8648  -342.8548  -514.6479
   -469.2733  -236.6896   109.0608   441.3498   637.4571   641.9954
    454.0505   154.5960  -136.8016  -343.3911  -421.8441  -374.4095
   -241.1943   -55.6140   129.4067   267.4248   311.8293   230.2807
     56.4402  -146.4689  -320.9948  -406.4077  -375.6384  -273.5936
   -132.6214    11.0791   126.4843   171.3391   122.6284   -11.5482
   -169.2623  -285.2358  -331.4567  -302.2945  -215.4832  -107.8732
```

```
   -3.4126    73.2521    98.0831    71.8949    17.0985   -27.5632
  -76.7900  -110.5354  -126.1383  -121.1043  -103.9362   -67.4619
  -10.8678    58.5009   116.4587   140.0961   129.5928    66.3211
  -35.5487  -135.3894  -203.7149  -216.2161  -152.7723   -30.4361
   99.3397   188.9594   204.9047   148.4056    34.4975  -103.7840
 -208.5982  -252.4128  -223.7600  -120.8640    23.3565   156.0956
  227.7642   228.5123   172.3820    87.4911   -21.2170  -117.5282
 -176.3634  -165.1218   -75.1308    67.1634   195.7290   279.3039
  290.8258   225.3811   104.0784   -44.4731  -162.7355  -207.7480
 -165.2444   -48.5473   118.8872   265.0045

Degrees of freedom = 9.0      Bandwidth = 0.1165

95 percent confidence limits -     Lower = 0.4731  Upper = 3.3329

      Spectrum       Spectrum      Spectrum       Spectrum
      estimate       estimate      estimate       estimate
   1  210.4696    2  428.2020    3  810.1419    4  922.5900
   5  706.1605    6  393.4052    7  207.6481    8  179.0657
   9  170.1320   10  133.0442   11  103.6752   12  103.0644
  13  141.5173   14  194.3041   15  266.5730   16  437.0181
  17  985.3130   18 2023.1574   19 2681.8980   20 2363.7439
  21 1669.9001   22 1012.1320   23  561.4822   24  467.2741
  25  441.9977   26  300.1985   27  172.0184   28  114.7823
  29   79.1533   30   49.4882   31   27.0902   32   16.8081
  33   27.5111   34   59.4429   35   97.0145   36  119.3664
  37  116.6737   38   87.3142   39   54.9570   40   42.9781
  41   46.6097   42   53.6206   43   50.6050   44   36.7780
  45   25.6285   46   24.8555   47   30.2626   48   31.5642
  49   27.3351   50   22.4443   51   18.5418   52   15.2425
  53   12.0207   54   12.6846   55   18.3975   56   19.3058
  57   12.6103   58    7.9511   59    7.1333   60    5.4996
  61    3.4182   62    3.2359   63    5.3836   64    8.5225
  65   10.0610   66    7.9483   67    4.2261   68    3.2631
  69    5.5751   70    7.8491   71    9.3694   72   11.0791
  73   10.1386   74    6.3158   75    3.6375   76    2.6561
  77    1.8026   78    1.0103   79    1.0693   80    2.3950
  81    4.0822   82    4.6221   83    4.0672   84    3.8460
  85    4.8489   86    6.3964   87    6.4762   88    4.9457
  89    4.4444   90    5.2131   91    5.0389   92    4.6141
  93    5.8722   94    7.9268   95    7.9486   96    5.7854
  97    4.5495   98    5.2696   99    6.3893  100    6.5216
 101    6.2129
```