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

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

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

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

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:

$$\begin{array}{ll} \frac{1}{2}\big(1 - \cos\big(\pi\big(t - \frac{1}{2}\big)/T\big)\big), & 1 \le t \le T \\ \frac{1}{2}\big(1 - \cos\big(\pi\big(n - t + \frac{1}{2}\big)/T\big)\big), & n + 1 - T \le t \le n \\ 1, & \text{otherwise,} \end{array}$$

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

The smoothing window is defined by

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

which for the various windows is defined over $0 \le \alpha < 1$ 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: $0.0 \leq$ PX ≤ 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: $1 \leq \mathrm{IW} \leq 4$.

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: $1 \leq \mathrm{MW} \leq \mathrm{NX}$.

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: $\mathrm{MW} \leq \mathrm{NC} \leq \mathrm{NX}$.

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 $(\mathrm{NC}-1)$, 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 $2^m \geq \mathrm{NX} + \mathrm{NC}$, provided $m \leq 20$.

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

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

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

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 9 in C06PAF for further details).

10 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.

10.1 Program Text

```
    Program g13cafe

!     G13CAF Example Program Text

!     Mark 25 Release. NAG Copyright 2014.

!     .. 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 = 1
      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
```

10.2 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
```

10.3 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
```