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

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

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:

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

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

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

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

The smoothing window is defined by

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

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:

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

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

The sampling distribution of $\hat{f}(\omega)$ is approximately that of a scaled χ_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 $\left[ml \times \hat{f}(\omega), mu \times \hat{f}(\omega)\right]$. 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 Arguments

1: NX – INTEGER *Input*

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

Constraint: $NX \ge 1$.

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 $IC = 0$, $0 \le MTX \le 2$

If covariances are supplied ($IC \ne 0$), 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: $1 \leq$ IW ≤ 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: $1 \leq$ MW $\leq$ 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: MW $\leq$ NC $\leq$ 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 (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.

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

Constraint: KC $\geq$ NX $+$ NC.

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.

Constraint: $L \geq 2 \times MW - 1$.

11: LG – INTEGER *Input*

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

$LG = 0$
    Unlogged.

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

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 $LG = 1$). The elements $XG(i)$, for $i = NG + 1, \ldots, NXG$ 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 $LG = 1$), 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 argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation 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 argument, 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: 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, IC $= 0$ and MTX < 0: MTX $= \langle value \rangle$.

On entry, IC $= 0$ and MTX > 2: MTX $= \langle value \rangle$.

On entry, IW $= \langle value \rangle$.
Constraint: IW $= 1$, 2, 3 or 4.

On entry, MW $= \langle value \rangle$.
Constraint: MW ≥ 1.

On entry, MW $= \langle value \rangle$ and NX $= \langle value \rangle$.
Constraint: MW $\leq$ NX.

On entry, NC $= \langle value \rangle$ and MW $= \langle value \rangle$.
Constraint: NC $\geq$ MW.

On entry, NC $= \langle value \rangle$ and NX $= \langle value \rangle$.
Constraint: NC $\leq$ NX.

On entry, NX $= \langle value \rangle$.
Constraint: NX ≥ 1.

On entry, NXG $= \langle value \rangle$, KC $= \langle value \rangle$ and L $= \langle value \rangle$.
Constraint: if IC $= 0$, NXG $\geq \max(\text{KC}, \text{L})$.

On entry, NXG $= \langle value \rangle$ and L $= \langle value \rangle$.
Constraint: if IC $\neq 0$, NXG $\geq$ L.

On entry, PX $= \langle value \rangle$.
Constraint: PX ≥ 0.0.

On entry, PX $= \langle value \rangle$.
Constraint: PX ≤ 1.0.

IFAIL $= 2$

On entry, KC $= \langle value \rangle$, NX $= \langle value \rangle$ and NC $= \langle value \rangle$.
Constraint: if IC $= 0$, KC $\geq$ (NX $+$ NC).

IFAIL $= 3$

On entry, L $= \langle value \rangle$ and MW $= \langle value \rangle$.
Constraint: L $\geq 2 \times$ MW $- 1$.

IFAIL $= 4$

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

IFAIL $= 5$

The calculation of confidence limit factors has failed.
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 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL $= -399$

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

    See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL $= -999$

    Dynamic memory allocation failed.

    See Section 3.7 in How to Use the NAG Library and its Documentation 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

G13CAF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

G13CAF makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

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 26 Release. NAG Copyright 2016.

!     .. 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
```

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
```