

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

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

where $[]$ denotes the integer part.

The autocovariances C_k may be supplied by you, or constructed from a time series x_1, x_2, \dots, 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:

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

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

The 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:

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

Parzen:

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

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

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 $[ml \times \hat{f}(\omega), mu \times \hat{f}(\omega)]$.

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

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: $NX \geq 1$.
- 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 $IC = 0$, $0 \leq MTX \leq 2$
 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: $0.0 \leq PX \leq 1.0$.

- 4: IW – INTEGER *Input*
On entry: the choice of lag window.
 IW = 1
 Rectangular.
 IW = 2
 Bartlett.
 IW = 3
 Tukey.
 IW = 4
 Parzen.
Constraint: $1 \leq IW \leq 4$.
- 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: $1 \leq MW \leq NX$.
- 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 $i = 0, 1, \dots, [L/2]$ in XG(1) to XG(NG) respectively (logged if LG = 1). The elements XG(i), for $i = NG + 1, \dots, NXG$ 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 \geq 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 \geq 1.

On entry, NXG = $\langle value \rangle$, KC = $\langle value \rangle$ and L = $\langle value \rangle$.

Constraint: if IC = 0, NXG \geq max(KC, 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 \geq 0.0.

On entry, PX = $\langle value \rangle$.

Constraint: PX \leq 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, unlogged 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, lxx, &
                          mtz, 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,*) mtz, 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
lxx = max(nxg,nx)
Allocate (xg(lxx),c(nc))

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

! Calculate smoothed spectrum
ifail = -1
Call g13caf(nx,mtz,px,iw,mw,ic,nc,c,kc,l,lg,nxx,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' &
  ' 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 g13caf

```

10.2 Program Data

G13CAF Example Program Data

```

256 100
1 0 0.1 4 100 200 0
360
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
:: NX,NC
:: MTX,IC,PX,IW,MW,L,LG
:: KC
:: 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 estimate	Spectrum estimate	Spectrum estimate	Spectrum 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						
