# NAG Library Routine Document G13DDF

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

G13DDF fits a vector autoregressive moving average (VARMA) model to an observed vector of time series using the method of Maximum Likelihood (ML). Standard errors of parameter estimates are computed along with their appropriate correlation matrix. The routine also calculates estimates of the residual series.

# 2 Specification

# 3 Description

Let  $W_t = (w_{1t}, w_{2t}, \dots, w_{kt})^T$ , for  $t = 1, 2, \dots, n$ , denote a vector of k time series which is assumed to follow a multivariate ARMA model of the form

$$W_{t} - \mu = \phi_{1}(W_{t-1} - \mu) + \phi_{2}(W_{t-2} - \mu) + \dots + \phi_{p}(W_{t-p} - \mu) + \epsilon_{t} - \theta_{1}\epsilon_{t-1} - \theta_{2}\epsilon_{t-2} - \dots - \theta_{q}\epsilon_{t-q}$$

$$(1)$$

where  $\epsilon_t = (\epsilon_{1t}, \epsilon_{2t}, \dots, \epsilon_{kt})^{\mathrm{T}}$ , for  $t = 1, 2, \dots, n$ , is a vector of k residual series assumed to be Normally distributed with zero mean and positive definite covariance matrix  $\Sigma$ . The components of  $\epsilon_t$  are assumed to be uncorrelated at non-simultaneous lags. The  $\phi_i$  and  $\theta_j$  are k by k matrices of parameters.  $\{\phi_i\}$ , for  $i = 1, 2, \dots, p$ , are called the autoregressive (AR) parameter matrices, and  $\{\theta_i\}$ , for  $i = 1, 2, \dots, q$ , the moving average (MA) parameter matrices. The parameters in the model are thus the p (k by k)  $\phi$ -matrices, the p (k by k) p-matrices, the mean vector, p, and the residual error covariance matrix p. Let

where I denotes the k by k identity matrix.

The ARMA model (1) is said to be stationary if the eigenvalues of  $A(\phi)$  lie inside the unit circle. Similarly, the ARMA model (1) is said to be invertible if the eigenvalues of  $B(\theta)$  lie inside the unit circle.

The method of computing the exact likelihood function (using a Kalman filter algorithm) is discussed in Shea (1987). A quasi-Newton algorithm (see Gill and Murray (1972)) is then used to search for the maximum of the log-likelihood function. Stationarity and invertibility are enforced on the model using the reparameterisation discussed in Ansley and Kohn (1986). Conditional on the maximum likelihood estimates being equal to their true values the estimates of the residual series are uncorrelated with zero mean and constant variance  $\Sigma$ .

You have the option of setting a parameter (EXACT to .FALSE.) so that G13DDF calculates conditional maximum likelihood estimates (conditional on  $W_0 = W_{-1} = \cdots = W_{1-p} = \epsilon_0 = \epsilon_{-1} = \cdots = \epsilon_{1-q} = 0$ ). This may be useful if the exact maximum likelihood estimates are close to the boundary of the invertibility region.

You also have the option (see Section 5) of requesting G13DDF to constrain elements of the  $\phi$  and  $\theta$  matrices and  $\mu$  vector to have pre-specified values.

## 4 References

Ansley C F and Kohn R (1986) A note on reparameterising a vector autoregressive moving average model to enforce stationarity *J. Statist. Comput. Simulation* **24** 99–106

Gill P E and Murray W (1972) Quasi-Newton methods for unconstrained optimization *J. Inst. Math. Appl.* **9** 91–108

Shea B L (1987) Estimation of multivariate time series J. Time Ser. Anal. 8 95-110

# 5 Parameters

1: K – INTEGER Input

On entry: k, the number of observed time series.

Constraint: K > 1.

2: N – INTEGER Input

On entry: n, the number of observations in each time series.

3: IP – INTEGER Input

On entry: p, the number of AR parameter matrices.

Constraint:  $IP \geq 0$ .

4: IQ – INTEGER Input

On entry: q, the number of MA parameter matrices.

Constraint:  $IQ \ge 0$ .

IP = IQ = 0 is **not permitted**.

5: MEAN – LOGICAL Input

On entry: MEAN = .TRUE., if components of  $\mu$  have been estimated and MEAN = .FALSE., if all elements of  $\mu$  are to be taken as zero.

Constraint: MEAN = .TRUE. or .FALSE..

6: PAR(NPAR) – REAL (KIND=nag\_wp) array Input/Output

On entry: initial parameter estimates read in row by row in the order  $\phi_1, \phi_2, \dots, \phi_p, \theta_1, \theta_2, \dots, \theta_q, \mu$ . Thus,

if IP > 0, PAR( $(l-1) \times k \times k + (i-1) \times k + j$ ) must be set equal to an initial estimate of the (i, j)th element of  $\phi_l$ , for l = 1, 2, ..., p, i = 1, 2, ..., k and j = 1, 2, ..., k;

if IQ > 0, PAR $(p \times k \times k + (l-1) \times k \times k + (i-1) \times k + j)$  must be set equal to an initial estimate of the (i, j)th element of  $\theta_l$ ,  $l = 1, 2, \ldots, q$  and  $i, j = 1, 2, \ldots, k$ ;

if MEAN = .TRUE., PAR( $(p+q) \times k \times k+i$ ) should be set equal to an initial estimate of the ith component of  $\mu$  ( $\mu(i)$ ). (If you set PAR( $(p+q) \times k \times k+i$ ) to 0.0 then G13DDF will calculate the mean of the ith series and use this as an initial estimate of  $\mu(i)$ .)

G13DDF.2 Mark 24

The first  $p \times k \times k$  elements of PAR must satisfy the stationarity condition and the next  $q \times k \times k$  elements of PAR must satisfy the invertibility condition.

If in doubt set all elements of PAR to 0.0.

On exit: if IFAIL = 0 or IFAIL  $\geq$  4 then all the elements of PAR will be overwritten by the latest estimates of the corresponding ARMA parameters.

# 7: NPAR – INTEGER Input

On entry: the dimension of the arrays PAR, PARHLD and G and the second dimension of the array CM as declared in the (sub)program from which G13DDF is called.NPAR is the number of initial parameter estimates.

Constraints:

```
if MEAN = .FALSE., NPAR must be set equal to (p+q) \times k \times k; if MEAN = .TRUE., NPAR must be set equal to (p+q) \times k \times k + k.
```

The total number of observations  $(n \times k)$  must exceed the total number of parameters in the model (NPAR + k(k+1)/2).

## 8: QQ(KMAX,K) – REAL (KIND=nag wp) array

Input/Output

On entry: QQ(i,j) must be set equal to an initial estimate of the (i,j)th element of  $\Sigma$ . The lower triangle only is needed. QQ must be positive definite. It is strongly recommended that on entry the elements of QQ are of the same order of magnitude as at the solution point. If you set QQ(i,j)=0.0, for  $i=1,2,\ldots,k$  and  $j=1,2,\ldots,i$ , then G13DDF will calculate the covariance matrix between the k time series and use this as an initial estimate of  $\Sigma$ .

On exit: if IFAIL = 0 or IFAIL  $\geq$  4 then QQ(i, j) will contain the latest estimate of the (i, j)th element of  $\Sigma$ . The lower triangle only is returned.

#### 9: KMAX – INTEGER

Input

On entry: the first dimension of the arrays QQ, W and V as declared in the (sub)program from which G13DDF is called.

Constraint:  $KMAX \ge K$ .

#### 10: W(KMAX,N) - REAL (KIND=nag wp) array

Input

On entry: W(i,t) must be set equal to the *i*th component of  $W_t$ , for  $i=1,2,\ldots,k$  and  $t=1,2,\ldots,n$ .

# 11: PARHLD(NPAR) – LOGICAL array

Input

On entry: PARHLD(i) must be set to .TRUE. if PAR(i) is to be held constant at its input value and .FALSE. if PAR(i) is a free parameter, for i = 1, 2, ..., NPAR.

If in doubt try setting all elements of PARHLD to .FALSE..

### 12: EXACT – LOGICAL

Input

On entry: must be set equal to .TRUE. if you wish G13DDF to compute exact maximum likelihood estimates. EXACT must be set equal to .FALSE. if only conditional likelihood estimates are required.

#### 13: IPRINT – INTEGER

Input

On entry: the frequency with which the automatic monitoring routine is to be called.

IPRINT > 0

The ML search procedure is monitored once every IPRINT iterations and just before exit from the search routine.

IPRINT = 0

The search routine is monitored once at the final point.

IPRINT < 0

The search routine is not monitored at all.

## 14: CGETOL – REAL (KIND=nag wp)

Input

On entry: the accuracy to which the solution in PAR and QQ is required.

If CGETOL is set to  $10^{-l}$  and on exit IFAIL = 0 or IFAIL  $\geq$  6, then all the elements in PAR and QQ should be accurate to approximately l decimal places. For most practical purposes the value  $10^{-4}$  should suffice. You should be wary of setting CGETOL too small since the convergence criteria may then have become too strict for the machine to handle.

If CGETOL has been set to a value which is less than the *machine precision*,  $\epsilon$ , then G13DDF will use the value  $10.0 \times \sqrt{\epsilon}$  instead.

## 15: MAXCAL – INTEGER

Input

On entry: the maximum number of likelihood evaluations to be permitted by the search procedure.

Suggested value:  $MAXCAL = 40 \times NPAR \times (NPAR + 5)$ .

Constraint:  $MAXCAL \ge 1$ .

#### 16: ISHOW – INTEGER

Input

On entry: specifies which of the following two quantities are to be printed.

- (i) table of maximum likelihood estimates and their standard errors (as returned in the output arrays PAR, QQ and CM);
- (ii) table of residual series (as returned in the output array V).

ISHOW = 0

None of the above are printed.

ISHOW = 1

(i) only is printed.

ISHOW = 2

(i) and (ii) are printed.

Constraint:  $0 \le ISHOW \le 2$ .

## 17: NITER - INTEGER

Output

On exit: if IFAIL = 0 or IFAIL  $\geq$  4 then NITER contains the number of iterations performed by the search routine.

## 18: RLOGL - REAL (KIND=nag wp)

Output

On exit: if IFAIL = 0 or IFAIL  $\geq$  4 then RLOGL contains the value of the log-likelihood function corresponding to the final point held in PAR and QQ.

19:  $V(KMAX,N) - REAL (KIND=nag_wp)$  array

Output

On exit: if IFAIL = 0 or IFAIL  $\geq$  4 then V(i,t) will contain an estimate of the ith component of  $\epsilon_t$ , for  $i=1,2,\ldots,k$  and  $t=1,2,\ldots,n$ , corresponding to the final point held in PAR and QQ.

## 20: G(NPAR) - REAL (KIND=nag wp) array

Output

On exit: if IFAIL = 0 or IFAIL  $\geq$  4 then G(i) will contain the estimated first derivative of the log-likelihood function with respect to the ith element in the array PAR. If the gradient cannot be computed then all the elements of G are returned as zero.

G13DDF.4 Mark 24

# 21: CM(LDCM,NPAR) - REAL (KIND=nag\_wp) array

Output

On exit: if IFAIL = 0 or IFAIL  $\geq$  4 then CM(i,j) will contain an estimate of the correlation coefficient between the ith and jth elements in the PAR array for  $1 \leq i \leq \text{NPAR}$ ,  $1 \leq j \leq \text{NPAR}$ . If i = j, then CM(i,j) will contain the estimated standard error of PAR(i). If the lth component of PAR has been held constant, i.e., PARHLD(l) was set to .TRUE., then the lth row and column of CM will be set to zero. If the second derivative matrix cannot be computed then all the elements of CM are returned as zero.

#### 22: LDCM - INTEGER

Input

On entry: the first dimension of the array CM as declared in the (sub)program from which G13DDF is called.

*Constraint*: LDCM  $\geq$  NPAR.

#### 23: 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 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: 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).

**Note**: G13DDF may return useful information for one or more of the following detected errors or warnings.

Errors or warnings detected by the routine:

## IFAIL = 1

```
On entry, K < 1,
          IP < 0,
or
          IQ < 0,
or
          IP = IO = 0,
or
          NPAR \neq (IP + IQ) \times K \times K + \Delta \times K, where \Delta = 1 if MEAN = .TRUE. or \Delta = 0 if
or
          MEAN = .FALSE.,
          N \times K \leq NPAR + K \times (K+1)/2,
or
          KMAX < K,
or
          MAXCAL < 1,
or
          ISHOW < 0,
or
          ISHOW > 2,
or
          LDCM < NPAR,
or
```

#### IFAIL = 2

On entry, either the initial estimate of  $\Sigma$  is not positive definite, or the initial estimates of the AR parameters are such that the model is non-stationary, or the initial estimates of the MA parameters are such that the model is non-invertible. To proceed, you must try a different starting point.

#### IFAIL = 3

The routine cannot compute a sufficiently accurate estimate of the gradient vector at the user-supplied starting point. This usually occurs if either the initial parameter estimates are very close to the ML parameter estimates, or you have supplied a very poor estimate of  $\Sigma$  or the starting point is very close to the boundary of the stationarity or invertibility region. To proceed, you must try a different starting point.

#### IFAIL = 4

There have been MAXCAL log-likelihood evaluations made in the routine. If steady increases in the log-likelihood function were monitored up to the point where this exit occurred, then the exit probably simply occurred because MAXCAL was set too small, so the calculations should be restarted from the final point held in PAR and QQ. This type of exit may also indicate that there is no maximum to the likelihood surface. Output quantities (as described in Section 5) are computed at the final point held in PAR and QQ, except that if G or CM cannot be computed, in which case they are set to zero.

#### IFAIL = 5

The conditions for a solution have not all been met, but a point at which the log-likelihood took a larger value could not be found.

Provided that the estimated first derivatives are sufficiently small, and that the estimated condition number of the second derivative (Hessian) matrix, as printed when  $IPRINT \geq 0$ , is not too large, this error exit may simply mean that, although it has not been possible to satisfy the specified requirements, the algorithm has in fact found the solution as far as the accuracy of the machine permits.

Such a condition can arise, for instance, if CGETOL has been set so small that rounding error in evaluating the likelihood function makes attainment of the convergence conditions impossible.

If the estimated condition number at the final point is large, it could be that the final point is a solution but that the smallest eigenvalue of the Hessian matrix is so close to zero at the solution that it is not possible to recognize it as a solution. Output quantities (as described in Section 5) are computed at the final point held in PAR and QQ, except that if G or CM cannot be computed, in which case they are set to zero.

#### IFAIL = 6

The ML solution is so close to the boundary of either the stationarity region or the invertibility region that G13DDF cannot evaluate the Hessian matrix. The elements of CM will then be set to zero on exit. The elements of G will also be set to zero. All other output quantities will be correct.

#### IFAIL = 7

This is an unlikely exit, which could occur in E04XAA, which computes an estimate of the second derivative matrix and the gradient vector at the solution point. Either the Hessian matrix was found to be too ill-conditioned to be evaluated accurately or the gradient vector could not be computed to an acceptable degree of accuracy. In this case the elements of CM will be set to zero on exit as will the elements of G. All other output quantities will be correct.

#### IFAIL = 8

The second derivative matrix at the solution point is not positive definite. In this case the elements of CM will be set to zero on exit. All other output quantities will be correct.

## IFAIL = -999

Internal memory allocation failed.

G13DDF.6 Mark 24

# 7 Accuracy

On exit from G13DDF, if IFAIL = 0 or IFAIL  $\geq 6$  and CGETOL has been set to  $10^{-l}$ , then all the parameters should be accurate to approximately l decimal places. If CGETOL was set equal to a value less than the **machine precision**,  $\epsilon$ , then all the parameters should be accurate to approximately  $10.0 \times \sqrt{\epsilon}$ .

If IFAIL = 4 on exit (i.e., MAXCAL likelihood evaluations have been made but the convergence conditions of the search routine have not been satisfied), then the elements in PAR and QQ may still be good approximations to the ML estimates. Inspection of the elements of G may help you determine whether this is likely.

#### **8 Further Comments**

# 8.1 Memory Usage

Let  $r = \max(\text{IP}, \text{IQ})$  and  $s = \text{NPAR} + \text{K} \times (\text{K} + 1)/2$ . Local workspace arrays of fixed lengths are allocated internally by G13DDF. The total size of these arrays amounts to  $s + \text{K} \times r + 52$  integer elements and  $2 \times s^2 + s \times (s-1)/2 + 15 \times s + \text{K}^2 \times \left(2 \times \text{IP} + \text{IQ} + (r+3)^2\right) + \text{K} \times \left(2 \times r^2 + 2 \times r + 3 \times \text{N} + 4\right) + 10$  real elements.

## 8.2 Timing

The number of iterations required depends upon the number of parameters in the model and the distance of the user-supplied starting point from the solution.

## 8.3 Constraining for Stationarity and Invertibility

If the solution lies on the boundary of the admissibility region (stationarity and invertibility region) then G13DDF may get into difficulty and exit with IFAIL = 5. If this exit occurs you are advised to either try a different starting point or a different setting for EXACT. If this still continues to occur then you are urged to try fitting a more parsimonious model.

#### 8.4 Over-parameterisation

You are advised to try and avoid fitting models with an excessive number of parameters since overparameterisation can cause the maximization problem to become ill-conditioned.

## 8.5 Standardizing the Residual Series

The standardized estimates of the residual series  $\epsilon_t$  (denoted by  $\hat{e}_t$ ) can easily be calculated by forming the Cholesky decomposition of  $\Sigma$ , e.g.,  $GG^{\mathsf{T}}$  and setting  $\hat{e}_t = G^{-1}\hat{\epsilon}_t$ . F07FDF (DPOTRF) may be used to calculate the array G. The components of  $\hat{e}_t$  which are now uncorrelated at **all** lags can sometimes be more easily interpreted.

# 8.6 Assessing the Fit of the Model

If your time series model provides a good fit to the data then the residual series should be approximately white noise, i.e., exhibit no serial cross-correlation. An examination of the residual cross-correlation matrices should confirm whether this is likely to be so. You are advised to call G13DSF to provide information for diagnostic checking. G13DSF returns the residual cross-correlation matrices along with their asymptotic standard errors. G13DSF also computes a portmanteau statistic and its asymptotic significance level for testing model adequacy. If IFAIL = 0 or  $5 \le IFAIL \le 8$  on exit from G13DDF then the quantities output K, N, V, KMAX, IP, IQ, PAR, PARHLD, and QQ will be suitable for input to G13DSF.

# 9 Example

This example shows how to fit a bivariate AR(1) model to two series each of length 48.  $\mu$  will be estimated and  $\phi_1(2,1)$  will be constrained to be zero.

## 9.1 Program Text

```
Program g13ddfe
      G13DDF Example Program Text
!
1
     Mark 24 Release. NAG Copyright 2012.
      .. Use Statements ..
!
     Use nag_library, Only: g13ddf, nag_wp, x04abf
!
      .. Implicit None Statement ..
     Implicit None
!
      .. Parameters ..
     Integer, Parameter
                                        :: iset = 1, nin = 5, nout = 6
      .. Local Scalars ..
!
     Real (Kind=nag_wp)
                                        :: cgetol, rlogl
                                         :: i, ifail, ip, iprint, iq, ishow, k, &
   kmax, ldcm, maxcal, n, nadv, niter, &
     Integer
                                            npar
     Logical
                                         :: exact, mean
!
      .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable :: cm(:,:), g(:), par(:), qq(:,:),
                                           v(:,:), w(:,:)
     Logical, Allocatable
                                         :: parhld(:)
     .. Executable Statements ..
!
      Write (nout,*) 'G13DDF Example Program Results'
     Write (nout,*)
     Flush (nout)
!
     Skip heading in data file
     Read (nin,*)
!
     Read in problem size
     Read (nin,*) k, ip, iq, n, mean
!
     Calculate NPAR
     npar = (ip+iq)*k*k
      If (mean) Then
       npar = npar + k
     End If
     ldcm = npar
     kmax = k
      Allocate (par(npar),qq(kmax,k),w(kmax,n),v(kmax,n),q(npar), &
        cm(ldcm,npar),parhld(npar))
1
     Read in series
     Read (nin,*)(w(i,1:n),i=1,k)
!
     Read in control parameters
     Read (nin,*) iprint, cgetol, maxcal, ishow
     Read in exact likelihood flag
     Read (nin,*) exact
     Read in initial parameter estimates and free parameter flags
      Read (nin,*) par(1:npar)
     Read (nin,*) parhld(1:npar)
!
     Read in initial values for covariance matrix QQ
     Read (nin,*)(qq(i,1:i),i=1,k)
      Set the advisory channel to NOUT for monitoring information
!
      If (iprint \ge 0 .Or. ishow = 0) Then
       nadv = nout
        Call x04abf(iset,nadv)
     End If
```

G13DDF.8 Mark 24

Fit a VARMA model

```
ifail = 0
Call g13ddf(k,n,ip,iq,mean,par,npar,qq,kmax,w,parhld,exact,iprint, &
    cgetol,maxcal,ishow,niter,rlogl,v,g,cm,ldcm,ifail)
```

End Program g13ddfe

# 9.2 Program Data

```
G13DDF Example Program Data
2 1 0 48 T
                                                :: K, IP, IQ, N, MEAN
               5.200 6.230 6.210 5.860
2.620 1.490 1.170 0.850
-1.490 -1.620
4.090 3.180
-0.350 0.240 2.440 2.580 2.040 0.400
 2.260 3.340 5.090 5.000 4.780 4.110
 3.450 1.650 1.290 4.090 6.320 7.500
 3.890
        1.580
               5.210
                      5.250 4.930
                                      7.380
 5.870 5.810 9.680 9.070 7.290 7.840
 7.550 7.320 7.970 7.760 7.000 8.350
 7.340 6.350 6.960 8.540 6.620 4.970
4.550 4.810 4.750 4.760 10.880 10.010 11.620 10.360 6.400 6.240 7.930 4.040
 3.730 5.600 5.350 6.810 8.270 7.680
 6.650 6.080 10.250 9.140 17.750 13.300
 9.630 6.800 4.080 5.060 4.940 6.650 7.940 10.760 11.890 5.850 9.010 7.500
10.020 10.380 8.150 8.370 10.730 12.140
                                                :: End of W
-1 0.0001 3000 2
                                                :: IPRINT, CGETOL, MAXCAL, ISHOW
Т
                                                :: EXACT
0.0 0.0 0.0 0.0 0.0
                                                 :: PAR
F F
        \mathbf{T}
            F F F
                                                 :: PARHLD
0.0
0.0 0.0
                                                :: End of QQ
```

## 9.3 Program Results

G13DDF Example Program Results

```
VALUE OF LOG LIKELIHOOD FUNCTION ON EXIT = -0.20280E+03
```

MAXIMUM LIKELIHOOD ESTIMATES OF AR PARAMETER MATRICES

```
PHI(1) ROW-WISE: 0.802 0.065
( 0.091)( 0.102)
0.000 0.575
( 0.000)( 0.121)
```

MAXIMUM LIKELIHOOD ESTIMATE OF PROCESS MEAN

4.271 7.825 (1.219) (0.776)

MAXIMUM LIKELIHOOD ESTIMATE OF SIGMA MATRIX

2.964

0.637 5.380

RESIDUAL SERIES NUMBER 1

	T V(T)		18 -2.09			23 -0.01	
	T V(T)		26 <b>-</b> 1.89			31 -3.32	
	T V(T)		34 0.47			39 3.99	
	T V(T)		42 1.07				
RESIDUAL SERIES NUMBER				2			
	Т V(Т)		2 -1.20				
	T V(T)		10 -1.30			15 -2.88	
	T V(T)		18 -3.85			23 1.03	
	T V(T)		26 -1.07				
	T V(T)		34 -0.61			39 2.38	
	T V(T)		42 -1.01			47 2.59	

G13DDF.10 (last) Mark 24