NAG Library Routine Document

G13EAF

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

G13EAF performs a combined measurement and time update of one iteration of the time-varying Kalman filter using a square root covariance filter.

2 Specification

```
SUBROUTINE G13EAF (N, M, L, A, LDS, B, STQ, Q, LDQ, C, LDM, R, S, K, H,    &
                   TOL, IWK, WK, IFAIL)

INTEGER          N, M, L, LDS, LDQ, LDM, IWK(M), IFAIL
REAL (KIND=nag_wp) A(LDS,N), B(LDS,L), Q(LDQ,*), C(LDM,N), R(LDM,M),       &
                   S(LDS,N), K(LDS,M), H(LDM,M), TOL,                      &
                   WK((N+M)*(N+M+L))
LOGICAL          STQ
```

3 Description

The Kalman filter arises from the state space model given by:

$$X_{i+1} = A_i X_i + B_i W_i, \quad \text{Var}(W_i) = Q_i$$

$$Y_i = C_i X_i + V_i, \qquad \text{Var}(V_i) = R_i$$

where X_i is the state vector of length n at time i, Y_i is the observation vector of length m at time i, and W_i of length l and V_i of length m are the independent state noise and measurement noise respectively.

The estimate of X_i given observations Y_1 to Y_{i-1} is denoted by $\hat{X}_{i|i-1}$ with state covariance matrix $\text{Var}(\hat{X}_{i|i-1}) = P_{i|i-1} = S_i S_i^T$, while the estimate of X_i given observations Y_1 to Y_i is denoted by $\hat{X}_{i|i}$ with covariance matrix $\text{Var}(\hat{X}_{i|i}) = P_{i|i}$. The update of the estimate, $\hat{X}_{i|i-1}$, from time i to time $(i+1)$, is computed in two stages. First, the measurement-update is given by

$$\hat{X}_{i|i} = \hat{X}_{i|i-1} + K_i [Y_i - C_i \hat{X}_{i|i-1}] \tag{1}$$

and

$$P_{i|i} = [I - K_i C_i] P_{i|i-1} \tag{2}$$

where $K_i = P_{i|i-1} C_i^T [C_i P_{i|i-1} C_i^T + R_i]^{-1}$ is the Kalman gain matrix. The second stage is the time-update for X which is given by

$$\hat{X}_{i+1|i} = A_i \hat{X}_{i|i} + D_i U_i \tag{3}$$

and

$$P_{i+1|i} = A_i P_{i|i} A_i^T + B_i Q_i B_i^T \tag{4}$$

where $D_i U_i$ represents any deterministic control used.

The square root covariance filter algorithm provides a stable method for computing the Kalman gain matrix and the state covariance matrix. The algorithm can be summarised as

$$\begin{pmatrix} R_i^{1/2} & C_i S_i & 0 \\ 0 & A_i S_i & B_i Q_i^{1/2} \end{pmatrix} U = \begin{pmatrix} H_i^{1/2} & 0 & 0 \\ G_i & S_{i+1} & 0 \end{pmatrix} \tag{5}$$

where U is an orthogonal transformation triangularizing the left-hand pre-array to produce the right-hand post-array. The relationship between the Kalman gain matrix, K_i, and G_i is given by

$$A_i K_i = G_i \left(H_i^{1/2} \right)^{-1}.$$

G13EAF requires the input of the lower triangular Cholesky factors of the noise covariance matrices $R_i^{1/2}$ and, optionally, $Q_i^{1/2}$ and the lower triangular Cholesky factor of the current state covariance matrix, S_i, and returns the product of the matrices A_i and K_i, $A_i K_i$, the Cholesky factor of the updated state covariance matrix S_{i+1} and the matrix $H_i^{1/2}$ used in the computation of the likelihood for the model.

4   References

Vanbegin M, van Dooren P and Verhaegen M H G (1989) Algorithm 675: FORTRAN subroutines for computing the square root covariance filter and square root information filter in dense or Hessenberg forms *ACM Trans. Math. Software* **15** 243–256

Verhaegen M H G and van Dooren P (1986) Numerical aspects of different Kalman filter implementations *IEEE Trans. Auto. Contr.* **AC-31** 907–917

5   Arguments

1:    N – INTEGER   *Input*

   On entry: n, the size of the state vector.

   Constraint: $N \geq 1$.

2:    M – INTEGER   *Input*

   On entry: m, the size of the observation vector.

   Constraint: $M \geq 1$.

3:    L – INTEGER   *Input*

   On entry: l, the dimension of the state noise.

   Constraint: $L \geq 1$.

4:    A(LDS, N) – REAL (KIND=nag_wp) array   *Input*

   On entry: the state transition matrix, A_i.

5:    LDS – INTEGER   *Input*

   On entry: the first dimension of the arrays A, B, S and K as declared in the (sub)program from which G13EAF is called.

   Constraint: $LDS \geq N$.

6:    B(LDS, L) – REAL (KIND=nag_wp) array   *Input*

   On entry: the noise coefficient matrix B_i.

7: STQ – LOGICAL *Input*

On entry: if STQ = .TRUE., the state noise covariance matrix Q_i is assumed to be the identity matrix. Otherwise the lower triangular Cholesky factor, $Q_i^{1/2}$, must be provided in Q.

8: Q(LDQ, ∗) – REAL (KIND=nag_wp) array *Input*

Note: the second dimension of the array Q must be at least L if STQ = .FALSE. and at least 1 if STQ = .TRUE..

On entry: if STQ = .FALSE., Q must contain the lower triangular Cholesky factor of the state noise covariance matrix, $Q_i^{1/2}$. Otherwise Q is not referenced.

9: LDQ – INTEGER *Input*

On entry: the first dimension of the array Q as declared in the (sub)program from which G13EAF is called.

Constraints:

if STQ = .FALSE., LDQ ≥ L;
otherwise LDQ ≥ 1.

10: C(LDM, N) – REAL (KIND=nag_wp) array *Input*

On entry: the measurement coefficient matrix, C_i.

11: LDM – INTEGER *Input*

On entry: the first dimension of the arrays C, R and H as declared in the (sub)program from which G13EAF is called.

Constraint: LDM ≥ M.

12: R(LDM, M) – REAL (KIND=nag_wp) array *Input*

On entry: the lower triangular Cholesky factor of the measurement noise covariance matrix $R_i^{1/2}$.

13: S(LDS, N) – REAL (KIND=nag_wp) array *Input/Output*

On entry: the lower triangular Cholesky factor of the state covariance matrix, S_i.

On exit: the lower triangular Cholesky factor of the state covariance matrix, S_{i+1}.

14: K(LDS, M) – REAL (KIND=nag_wp) array *Output*

On exit: the Kalman gain matrix, K_i, premultiplied by the state transition matrix, A_i, A_iK_i.

15: H(LDM, M) – REAL (KIND=nag_wp) array *Output*

On exit: the lower triangular matrix $H_i^{1/2}$.

16: TOL – REAL (KIND=nag_wp) *Input*

On entry: the tolerance used to test for the singularity of $H_i^{1/2}$. If $0.0 \le \text{TOL} < m^2 \times$ ***machine precision***, then $m^2 \times$ ***machine precision*** is used instead. The inverse of the condition number of $H^{1/2}$ is estimated by a call to F07TGF (DTRCON). If this estimate is less than TOL then $H^{1/2}$ is assumed to be singular.

Suggested value: TOL = 0.0.

Constraint: TOL ≥ 0.0.

17:	IWK(M) – INTEGER array	*Workspace*
18:	WK$((N + M) \times (N + M + L))$ – REAL (KIND=nag_wp) array	*Workspace*

19: 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, N < 1,
or   M < 1,
or   L < 1,
or   LDS < N,
or   LDM < M,
or   STQ = .TRUE. and LDQ < 1,
or   STQ = .FALSE. and LDQ < L,
or   TOL < 0.0.

IFAIL = 2

The matrix $H_i^{1/2}$ is singular.

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 use of the square root algorithm improves the stability of the computations as compared with the direct coding of the Kalman filter. The accuracy will depend on the model.

8   Parallelism and Performance

G13EAF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

G13EAF 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

For models with time-invariant A, B and C, G13EBF can be used.

The estimate of the state vector $\hat{X}_{i+1|i}$ can be computed from $\hat{X}_{i|i-1}$ by

$$\hat{X}_{i+1|i} = A_i \hat{X}_{i|i-1} + AK_i r_i$$

where

$$r_i = Y_i - C_i \hat{X}_{i|i-1}$$

are the independent one step prediction residuals. The required matrix-vector multiplications can be performed by F06PAF (DGEMV).

If W_i and V_i are independent multivariate Normal variates then the log-likelihood for observations $i = 1, 2, \ldots, t$ is given by

$$l(\theta) = \kappa - \tfrac{1}{2}\sum_{i=1}^{t} ln(\det(H_i)) - \tfrac{1}{2}\sum_{i=1}^{t} \left(Y_i - C_i X_{i|i-1}\right)^{\mathrm{T}} H_i^{-1} \left(Y_i - C_i X_{i|i-1}\right)$$

where κ is a constant.

The Cholesky factors of the covariance matrices can be computed using F07FDF (DPOTRF).

Note that the model

$$X_{i+1} = A_i X_i + W_i, \quad \mathrm{Var}(W_i) = Q_i$$

$$Y_i = C_i X_i + V_i, \qquad \mathrm{Var}(V_i) = R_i$$

can be specified either with B set to the identity matrix and STQ = .FALSE. and the matrix $Q^{1/2}$ input in Q or with STQ = .TRUE. and B set to $Q^{1/2}$.

The algorithm requires $\tfrac{7}{6}n^3 + n^2\left(\tfrac{5}{2}m + l\right) + n\left(\tfrac{1}{2}l^2 + m^2\right)$ operations and is backward stable (see Verhaegen and van Dooren (1986)).

10   Example

This example first inputs the number of updates to be computed and the problem sizes. The initial state vector and state covariance matrix are input followed by the model matrices A_i, B_i, C_i, R_i and optionally Q_i. The Cholesky factors of the covariance matrices can be computed if required. The model matrices can be input at each update or only once at the first step. At each update the observed values are input and the residuals are computed and printed and the estimate of the state vector, $\hat{X}_{i|i-1}$, and the deviance are updated. The deviance is $-2 \times$ log-likelihood ignoring the constant. After the final update the state covariance matrix is computed from S and printed along with final estimate of the state vector and the value of the deviance.

The data is for a two-dimensional time series to which a VARMA$(1, 1)$ has been fitted. For the specification of a VARMA model as a state space model see the G13 Chapter Introduction. The initial value of P, P_0, is the solution to

$$P_0 = A_1 P_0 A_1^T + B_1 Q_1 B_1^T.$$

For convenience, the mean of each series is input before the first update and subtracted from the observations before the measurement update is computed.

10.1 Program Text

```
      Program g13eafe

!     G13EAF Example Program Text

!     Mark 26 Release. NAG Copyright 2016.

!     .. Use Statements ..
      Use nag_library, Only: daxpy, ddot, dgemv, dpotrf, dtrmv, dtrsv, g13eaf, &
                             nag_wp, x04caf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Real (Kind=nag_wp), Parameter    :: one = 1.0_nag_wp
      Real (Kind=nag_wp), Parameter    :: zero = 0.0_nag_wp
      Integer, Parameter               :: inc1 = 1, nin = 5, nout = 6
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: dev, tol
      Integer                          :: i, ifail, info, istep, l, ldm, ldq, &
                                          lds, lwk, m, n, ncall, tdq
      Logical                          :: full, is_const, read_matrix, stq
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: a(:,:), ax(:), b(:,:), c(:,:),       &
                                          h(:,:), k(:,:), p(:,:), q(:,:),      &
                                          r(:,:), s(:,:), wk(:), x(:), y(:),   &
                                          ymean(:)
      Integer, Allocatable             :: iwk(:)
!     .. Intrinsic Procedures ..
      Intrinsic                        :: log
!     .. Executable Statements ..
      Write (nout,*) 'G13EAF Example Program Results'
      Write (nout,*)

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

!     Read in the problem size
      Read (nin,*) n, m, l, stq, is_const

      lds = n
      If (.Not. stq) Then
        ldq = l
        tdq = l
      Else
        ldq = 1
        tdq = 1
      End If
      ldm = m
      lwk = (n+m)*(n+m+l)
      Allocate (a(lds,n),b(lds,l),q(ldq,tdq),c(ldm,n),r(ldm,m),s(lds,n),       &
        k(lds,m),h(ldm,m),iwk(m),wk(lwk),x(n),ymean(m),y(m),ax(n),p(lds,n))

!     Read in the state covariance matrix, S
      Read (nin,*)(s(i,1:n),i=1,n)

!     Read in flag indicating whether S is the full matrix, or its
!     Cholesky decomposition
      Read (nin,*) full

!     If required (full), perform the Cholesky decomposition on S
      If (full) Then
!       The NAG name equivalent of dpotrf is f07fdf
```

```
            Call dpotrf('L',n,s,lds,info)
            If (info>0) Then
              Write (nout,*) ' S not positive definite'
              Go To 100
            End If
          End If

!     Read in initial state vector
          Read (nin,*) x(1:n)

!     Read in mean of the series
          Read (nin,*) ymean(1:m)

!     Read in control parameter
          Read (nin,*) ncall, tol

!     Display titles
          Write (nout,*) '          Residuals'
          Write (nout,*)

!     Initialize variables
          dev = zero
          read_matrix = .True.

!     Loop through data
          Do istep = 1, ncall
!       Read in the various matrices. If the series is constant
!       then this only happens at the first call
            If (read_matrix) Then

!         Read in transition matrix, A
              Read (nin,*)(a(i,1:n),i=1,n)
!         Read in noise coefficient matrix, B
              Read (nin,*)(b(i,1:l),i=1,n)
!         Read in measurement coefficient matrix, C
              Read (nin,*)(c(i,1:n),i=1,m)

!         Read in measurement noise covariance matrix, R
              Read (nin,*)(r(i,1:m),i=1,m)
!         Read in flag indicating whether R is the full matrix, or its
!         Cholesky decomposition
              Read (nin,*) full
!         If required (full), perform the Cholesky decomposition on R
              If (full) Then
!           The NAG name equivalent of dpotrf is f07fdf
                Call dpotrf('L',m,r,ldm,info)
                If (info>0) Then
                  Write (nout,*) ' R not positive definite'
                  Go To 100
                End If
              End If

!         Read in state noise matrix Q, if not assume to be identity matrix
              If (.Not. stq) Then
                Read (nin,*)(q(i,1:l),i=1,l)
!           Read in flag indicating whether Q is the full matrix, or its
!           Cholesky decomposition
                Read (nin,*) full
!           Perform Cholesky factorization on Q, if full matrix is supplied
                If (full) Then
!             The NAG name equivalent of dpotrf is f07fdf
                  Call dpotrf('L',l,q,ldq,info)
                  If (info>0) Then
                    Write (nout,*) ' Q not positive definite'
                    Go To 100
                  End If
                End If
              End If

!         If series is constant set flag to false
              read_matrix = .Not. is_const
```

```
          End If

!         Read in observed values
          Read (nin,*) y(1:m)

!         Call G13EAF
          ifail = 0
          Call g13eaf(n,m,l,a,lds,b,stq,q,ldq,c,ldm,r,s,k,h,tol,iwk,wk,ifail)

!         Subtract the mean y:= y-ymean
!         The NAG name equivalent of daxpy is f06ecf
          Call daxpy(m,-one,ymean,inc1,y,inc1)

!         Perform time and measurement update x <= Ax + K(y-Cx)
!         The NAG name equivalent of dgemv is f06paf
          Call dgemv('N',m,n,-one,c,ldm,x,inc1,one,y,1)
          Call dgemv('N',n,n,one,a,lds,x,inc1,zero,ax,1)
          Call dgemv('N',n,m,one,k,lds,y,inc1,one,ax,1)
          x(1:n) = ax(1:n)

!         Display the residuals
          Write (nout,99999) y(1:m)

!         Update log-likelihood.
!         The NAG name equivalent of dtrsv is f06pjf
          Call dtrsv('L','N','N',m,h,ldm,y,1)
!         The NAG name equivalent of ddot is f06eaf
          dev = dev + ddot(m,y,1,y,1)
          Do i = 1, m
            dev = dev + 2.0_nag_wp*log(h(i,i))
          End Do
        End Do

!       Compute P from S
!       The NAG name equivalent of dtrmv is f06pff
        Do i = 1, n
          p(1:i,i) = s(i,1:i)
          Call dtrmv('L','N','N',i,s,lds,p(1,i),inc1)
          p(i,1:i-1) = p(1:i-1,i)
        End Do

!     Display final results
      Write (nout,*)
      Write (nout,*) ' Final X(I+1:I) '
      Write (nout,*)
      Write (nout,99999) x(1:n)
      Write (nout,*)
      Flush (nout)
      ifail = 0
      Call x04caf('Lower','Non-Diag',n,n,p,lds,'Final Value of P',ifail)
      Write (nout,*)
      Write (nout,99998) ' Deviance = ', dev

100   Continue

99999 Format (6F12.4)
99998 Format (A,E13.4)
    End Program g13eafe
```

10.2 Program Data

```
G13EAF Example Program Data
4 2 2 F T                           :: N,M,L,STQ,IS_CONST
 8.2068  2.0599  1.4807  0.3627
 2.0599  7.9645  0.9703  0.2136
 1.4807  0.9703  0.9253  0.2236
 0.3627  0.2136  0.2236  0.0542     :: End of S
 T                                  :: FULL flag for S
 0.000  0.000  0.000  0.000         :: X
 4.404  7.991                       :: YMEAN
```

```
48 0.0                                  :: NCALL,TOL
0.607 -0.033  1.000  0.000
0.000  0.543  0.000  1.000
0.000  0.000  0.000  0.000
0.000  0.000  0.000  0.000        :: End of A
1.000  0.000
0.000  1.000
0.543  0.125
0.134  0.026                      :: End of B
1.000  0.000  0.000  0.000
0.000  1.000  0.000  0.000        :: End of C
0.000  0.000
0.000  0.000                      :: End of R
 F                                :: FULL flag for R
2.598  0.560
0.560  5.330                      :: End of Q
 T                                :: FULL flag for Q
-1.490  7.340
-1.620  6.350
 5.200  6.960
 6.230  8.540
 6.210  6.620
 5.860  4.970
 4.090  4.550
 3.180  4.810
 2.620  4.750
 1.490  4.760
 1.170 10.880
 0.850 10.010
-0.350 11.620
 0.240 10.360
 2.440  6.400
 2.580  6.240
 2.040  7.930
 0.400  4.040
 2.260  3.730
 3.340  5.600
 5.090  5.350
 5.000  6.810
 4.780  8.270
 4.110  7.680
 3.450  6.650
 1.650  6.080
 1.290 10.250
 4.090  9.140
 6.320 17.750
 7.500 13.300
 3.890  9.630
 1.580  6.800
 5.210  4.080
 5.250  5.060
 4.930  4.940
 7.380  6.650
 5.870  7.940
 5.810 10.760
 9.680 11.890
 9.070  5.850
 7.290  9.010
 7.840  7.500
 7.550 10.020
 7.320 10.380
 7.970  8.150
 7.760  8.370
 7.000 10.730
 8.350 12.140                     : End of Y
```

10.3 Program Results

```
G13EAF Example Program Results

        Residuals

    -5.8940      -0.6510
    -1.4710      -1.0407
     5.1658       0.0447
    -1.3280       0.4580
     1.3652      -1.5066
    -0.2337      -2.4192
    -0.8685      -1.7065
    -0.4624      -1.1519
    -0.7510      -1.4218
    -1.3526      -1.3335
    -0.6707       4.8593
    -1.7389       0.4138
    -1.6376       2.7549
    -0.6137       0.5463
     0.9067      -2.8093
    -0.8255      -0.9355
    -0.7494       1.0247
    -2.2922      -3.8441
     1.8812      -1.7085
    -0.7112      -0.2849
     1.6747      -1.2400
    -0.6619       0.0609
     0.3271       1.0074
    -0.8165      -0.5325
    -0.2759      -1.0489
    -1.9383      -1.1186
    -0.3131       3.5855
     1.3726      -0.1289
     1.4153       8.9545
     0.3672      -0.4126
    -2.3659      -1.2823
    -1.0130      -1.7306
     3.2472      -3.0836
    -1.1501      -1.1623
     0.6855      -1.2751
     2.3432       0.2570
    -1.6892       0.3565
     1.3871       3.0138
     3.3840       2.1312
    -0.5118      -4.7670
     0.8569       2.3741
     0.9558      -1.2209
     0.6778       2.1993
     0.4304       1.1393
     1.4987      -1.2255
     0.5361       0.1237
     0.2649       2.4582
     2.0095       2.5623

  Final X(I+1:I)

     3.6698       2.5888       0.0000       0.0000

Final Value of P
             1            2            3            4
 1      2.5980
 2      0.5600       5.3300
 3      1.4807       0.9703       0.9253
 4      0.3627       0.2136       0.2236       0.0542

Deviance =     0.2229E+03
```