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DEPARTMENT OF ECONOMETRICS, FACULTY OF ECONOMICS AND POLITICS

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# Kalman Filtering with Partially Diffuse Initial Conditions

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June, 1988

## Abstract

In this paper a square root algorithm is proposed for estimating linear state space models. A particular feature of the approach is that it contains special provisions for nonstationary time series with incompletely specified initial conditions. It differs from earlier approaches to the problem in that an additional property of the covariance matrix of the state estimation error vector is exploited to further reduce storage requirements and computational loads in computer implementations.

*Keywords:* Kalman filtering; state space models; time series; square root algorithm.

## 1 Introduction

It is widely accepted that Kalman filtering has a pivotal place in time series analysis eg. see Harrison and Stevens (1976), Harvey and Phillips (1979), Harvey and Peirse (1984), Harvey (1984), Ansley and Kohn (1985a). Much effort has been devoted to the computational aspects of this method, including the development of more accurate square root filters as outlined in Kaminsky, Bryson and Schmidt (1971). In this paper it is argued that one aspect still warrants further consideration: the issue of initializing such filters with diffuse and partially diffuse prior probability distributions.

The Kalman filter is used to estimate statistical models which conform to the so-called state space framework. The latter presupposes that the key characteristics of the process under consideration can be summarized in typical period  $t$  by a random  $q$ -vector  $x(t)$  called the *state vector*. The process

is assumed to evolve over time according to the *transition equation*

$$x(t) = Fx(t-1) + v(t) \quad (1a)$$

where  $F$  is a fixed  $q \times q$  *transition matrix* and the  $v(t)$  are statistically independent, normally distributed, zero mean random  $q$ -vectors with a common variance matrix  $Q$ . Each  $v(t)$  is statistically independent of the state vector  $x(t-1)$  from the previous period.

Only  $p$  of the  $q$  states can be directly observed where  $p \leq q$ . To facilitate matters, but without loss of generality, it is assumed that the observable states, denoted by a random  $p$ -vector  $y(t)$ , are placed at the top of the state vector  $x(t)$ . In other words

$$y(t) = Hx(t) \quad (1b)$$

where  $H = [ I \ O ]$ ,  $I$  and  $O$  being the identity and null matrices which, in this context, are of order  $p \times p$  and  $p \times (q-p)$  respectively.

It is conventional to seed the Kalman filter with the mean and variance of a marginal distribution of the initial state vector  $x(0)$ . These quantities are usually derived from the transition equation (1a) on the assumption that the process has operated over an infinite time span prior to the first measurement period. To ensure that the framework accommodates nonstationary as well as stationary time series, it can be established that the initial state vector  $x(0)$  must have a variance matrix  $S$  with the general form

$$S = \kappa S^{[1]} + S^{[0]} \quad (2)$$

where  $\kappa$  is an arbitrarily large number, and  $S^{[1]}$  and  $S^{[0]}$  are  $q \times q$  matrices, both of which are independent of  $\kappa$ . Equation (2) encompasses the variance of *diffuse* priors when  $S^{[1]}$  has full rank, *partially diffuse* priors when it is rank deficient, and non-diffuse priors associated with stationary processes when it is null.

It is no simple matter to implement the Kalman filter for the diffuse and partially diffuse cases. A common practice, given the finite precision of computers, was to treat  $\kappa$  as a large rather than an infinite number in the conventional filter. However, it was argued in Ansley and Kohn (1985a) that this practice can be an unnecessary source of numerical errors and that it is possible to devise an alternative strategy which completely avoids the explicit use of the big- $\kappa$  and the associated errors. This strategy, which has been restated in simpler terms in a later paper by Ansley and Kohn (1985b), together with its square root counterpart in Snyder (1988), are both effective, in the sense that they solve the basic problem. However, neither are particularly efficient. Not only are they more complicated than their traditional counterparts, but they also require approximately double the storage space and double the calculations in computer implementations

during the initial 'run-in' phase while the distributions of the errors of the estimates of the state vectors remain partially diffuse.

In this paper a reasonably conventional square root filter is initially specified. Utilizing a special property of the covariance matrix of the state estimates error vector, it is then established that this filter requires only minor changes to accommodate the diffuse and partially diffuse cases provided some extensions are made to the formulae for the orthogonalization procedure used to derive the required square-root decompositions. It is also shown that the resulting algorithm requires less storage space and has lower computational loads during the run-in phase than the earlier modified square root filter in Snyder (1988).

## 2 The Kalman Filter

Models conforming to the state space framework can be estimated recursively with the Kalman filter. In the following description  $x(t|n)$  denotes the estimate of the state vector  $x(t)$  from a sample of size  $n$ , while  $S(t|n)$  is used to represent the variance of its error  $x(t) - x(t|n)$ . Each pass of the the algorithm involves the following steps:

### Covariance Filter

#### Time Advance Stage

1.  $x(n|n-1) = Fx(n-1|n-1)$
2.  $S(n|n-1) = FS(n-1|n-1)F' + Q$

#### Measurement Update Stage

1.  $G(n) = S(n|n-1)H'[HS(n|n-1)H']^{-1}$
2.  $x(n|n) = x(n|n-1) + G(n)[y(n) - Hx(n|n-1)]$
3.  $S(n|n) = [I - G(n)H]S(n|n-1)[I - G(n)H]'$

It can be established that by choosing the so-called Kalman gain matrix  $G(n)$  according to step 1 of the measurement update stage,  $x(n|n)$  is a linear, minimum variance estimate of  $x(n)$ .

Special structural features of the problem can be exploited to reduce the computational loads. Consider the partitions:

$$x(s|t) = \begin{bmatrix} x_1(s|t) \\ x_2(s|t) \end{bmatrix}$$

where the  $x_1(s|t)$  and  $x_2(s|t)$  are  $p$  and  $(q-p)$  subvectors respectively;

$$S(s|t) = \begin{bmatrix} S_{11}(s|t) & S_{12}(s|t) \\ S_{12}(s|t)' & S_{22}(s|t) \end{bmatrix} \quad (3)$$

where the submatrices are  $p \times p$ ,  $p \times (q-p)$  and  $(q-p) \times (q-p)$  respectively; and

$$G(n) = \begin{bmatrix} G_1(n) \\ G_2(n) \end{bmatrix}$$

where the submatrices are  $p \times p$  and  $(q-p) \times p$  respectively.

It can be established that  $G_1(n) = I$ ,  $x_1(n|n) = y(n)$ , so that the vector of estimation errors is  $[O, x_2(n) - x_2(n|n)]'$  with a corresponding variance matrix

$$S(n|n) = \begin{bmatrix} O & O \\ O & S_{22}(n|n) \end{bmatrix}.$$

The measurement update stage of the covariance filter can therefore be streamlined to:

#### Measurement Update Stage (revised)

1.  $G_2(n) = S_{12}(n|n-1)'S_{11}^{-1}$
2.  $x_2(n|n) = x_2(n|n-1) + G_2(n)[y(n) - x_1(n|n-1)]$
3.  $S_{22}(n|n) = S_{22}(n|n-1) - G_2(n)S_{12}(n|n-1)$

The accuracy of the Kalman filter can be doubled by using square root methods as outlined in Kaminsky, Bryson and Schmidt (1971). Assume that the  $q \times q$  unit upper triangular matrix  $U$  and  $q \times q$  diagonal matrix  $D$  of the decomposition  $Q = U'DU$  is available, obtained where necessary by the Cholesky procedure. Also assume that the  $q \times q$  matrix  $R(n|n-1)$  and the  $q \times q$  diagonal matrix  $\Lambda(n|n-1)$  of the decomposition  $S(n|n-1) = R(n|n-1)\Lambda(n|n-1)R(n|n-1)$  are available from the previous iteration of the algorithm. Each iteration of the square root filter then involves the following steps:

#### Square Root Filter

##### Time Advance Stage

1.  $x(n|n-1) = Fx(n-1|n-1)$

2. Form the matrices

$$Z(n) = \begin{bmatrix} U \\ R(n-1|n-1)F' \end{bmatrix} \text{ and } W(n) = \begin{bmatrix} D & O \\ O & \Lambda(n-1|n-1) \end{bmatrix}.$$

Then apply an orthogonalization procedure to  $Z(n)$  relative to  $W(n)$  to give the unit upper triangular matrix  $R(n|n-1)$  and diagonal matrix  $\Lambda(n|n-1)$  of the square root decomposition  $S(n|n-1) = R(n|n-1)' \Lambda(n|n-1) R(n|n-1)$ .

### Measurement Update Stage

1.  $G(n) = R(n|n-1)' H [H R(n|n-1) H']^{-1}$
2.  $x(n|n) = x(n|n-1) + G(n) [y(n) - H x(n|n-1)]$
3.  $R(n|n) = R(n|n-1) [I - G(n) H']'$  and  $\Lambda(n|n) = \Lambda(n|n-1)$   
where  $S(n|n) = R(n|n)' \Lambda(n|n) R(n|n)$ .

The efficiency of this algorithm can also be improved. Consider the partitions:

$$R(s|t) = \begin{bmatrix} R_{11}(s|t) & R_{12}(s|t) \\ O & R_{22}(s|t) \end{bmatrix}$$

$$\Lambda(s|t) = \begin{bmatrix} \Lambda_1(s|t) & O \\ O & \Lambda_2(s|t) \end{bmatrix}$$

where the submatrices of  $R(s|t)$  and  $\Lambda(s|t)$  are conformable with the submatrices of  $S(s|t)$  above. The measurement update stage of the square root algorithm can also be altered to a more efficient form.

### Measurement Update Stage (revised)

1.  $G_2(n) = R_{12}(n|n-1)' R_{11}(n|n-1)^{-1}$
2.  $x_2(n|n) = x_2(n|n-1) + G_2(n) [y(n) - x_1(n|n-1)]$
3.  $R(n|n) = R(n|n-1)$  and  $\Lambda(n|n) = \begin{bmatrix} O & O \\ O & \Lambda_{22}(n|n-1) \end{bmatrix}$ .

When initializing the Kalman filter it is conventional to let  $S_{22}(0|0) = S_{22}$  where  $S_{22}$  is the variance of  $x_2(0)$ . The latter is found from the transition equation (1a), on the assumption of an infinite past prior to the first measurement period. Assuming that it is nonsingular, it must have the general form, (possibly after permuting the rows):

$$S_{22} = \kappa \begin{bmatrix} \Sigma_{11}^{[1]} & O \\ O & O \end{bmatrix} + \begin{bmatrix} \Sigma_{11}^{[0]} & \Sigma_{12}^{[0]} \\ \Sigma_{12}^{[0]} & \Sigma_{22}^{[0]} \end{bmatrix} \quad (4)$$

where  $\Sigma_{11}^{[1]}$  and  $\Sigma_{22}^{[0]}$  are non-singular submatrices, both of which are independent of  $\kappa$ . The corresponding information matrix  $I_f$  obtained by inverting  $S_{22}$  using partitioned inverse theory and then taking the limit with respect to  $\kappa$  is



$$I_f = \begin{bmatrix} O & O \\ O & \Sigma_{22}^{[0]-1} \end{bmatrix}$$

and this is independent of all the submatrices in (4) except  $\Sigma_{22}^{[0]}$ . Since any information filter seeded with  $I_f$  should yield the same results as the corresponding Kalman filter,  $\Sigma_{12}^{[0]}$  and  $\Sigma_{22}^{[0]}$  can be selected arbitrarily. Furthermore,  $\Sigma_{11}^{[1]}$  can be an arbitrary nonsingular matrix. Hence  $S_{22}$  can be more conveniently written in the form

$$S_{22} = \begin{bmatrix} \kappa I & O \\ O & \Sigma_{22}^{[0]} \end{bmatrix}.$$

The Cholesky decomposition of  $S$  is therefore

$$S = R' \Lambda R, \quad (5a)$$

$\Lambda$  being a diagonal matrix with the general form

$$\Lambda = \kappa \Lambda^{[1]} + \Lambda^{[0]} \quad (5b)$$

where the unit upper triangular matrix  $R$  and the diagonal matrices  $\Lambda^{[1]}$  and  $\Lambda^{[0]}$  are all independent of  $\kappa$ .

Many common cases such as the various versions of exponential smoothing and ARIMA processes have initial variance matrices conforming to the structure of (4).

### Example

A variation of exponential smoothing with a damped trend is outlined in Gardner and McKenzie (1985). It involves an observable random variable  $y(t)$  which depends on a local level  $\mu(t)$ , a local growth rate  $\beta(t)$ , a dampening factor  $\phi$ , smoothing parameters  $\alpha_1$  and  $\alpha_2$ , and a disturbance  $\epsilon(t)$  as follows:

$$y(t) = \mu(t-1) + \beta(t-1) + \epsilon(t) \quad (6a)$$

$$\mu(t) = \mu(t-1) + \beta(t-1) + \alpha_1 \epsilon(t) \quad (6b)$$

$$\beta(t) = \phi \beta(t-1) + \alpha_2 \epsilon(t). \quad (6c)$$

When the dampening factor lies in the range  $0 < \phi < 1$  then it is readily established from (6c) that the recurrence relationship governing the variance of the growth rate is stable and that the variances converge to a constant value. From a combination of (6b) and (6c) a similar result can be obtained for the covariance between the local level and growth rates. However, (6a) indicates that recurrence relationship for the variance of the local level is unstable and fails to yield bounded results. Accordingly, it can be shown that the seed variance matrix takes the form:

$$S_{22} = \begin{bmatrix} \kappa & (\alpha_1 + \alpha_2 \phi / (1 - \phi^2)) / (1 - \phi) \\ (\alpha_1 + \alpha_2 \phi / (1 - \phi^2)) / (1 - \phi) & \alpha_2^2 / (1 - \phi^2) \end{bmatrix}.$$

This conforms to the structure of (4) and is an example of a process with a partially diffuse prior distribution. Given the above results, the off-diagonal terms are redundant and can be set to zero.  $S_{22}$  then has a form which can be decomposed according to (5).

When the square root filter is initialized with the decomposition (5) of  $S$  all the quantities in it become functions of  $\kappa$ . Given the result in the next section about the effect of  $\kappa$  on the orthogonal triangular procedures, the following theorem can readily be established by induction.

**Theorem 1** *If the square root filter is initialized with  $R$  and  $\Lambda$  of the Cholesky factorization (5) then at typical stage  $n$  the key quantities are, apart from an error term  $O(1/\kappa)$  which disappears as  $\kappa$  becomes arbitrarily large, either constant or linear functions of  $\kappa$  ie.*

$$x(t|n) = x^{[0]}(t|n) + O(1/\kappa)$$

$$R(t|n) = R^{[0]}(t|n) + O(1/\kappa)$$

$$\Lambda(t|n) = \kappa\Lambda^{[1]}(t|n) + \Lambda^{[0]}(t|n) + O(1/\kappa)$$

for  $t = n, n + 1$  where the vectors and matrices with superscripts are all independent of  $\kappa$ .

This suggests that provided special provisions are made to store the  $\Lambda^{[1]}(t|n)$  in addition to the  $\Lambda^{[0]}(t|n)$  then the basic structure of the square root filter remains unchanged.

### 3 Orthogonal Triangularization

In principle any suitable orthogonalization procedure can be applied in the square root algorithm to obtain the required decomposition: the modified Gram-Schmidt or Householder transformations are possibilities. However, in this paper Givens transformations are used because, as it transpires, the impact of a partially diffuse prior on the associated formulae is more easily determined. Like all orthogonal triangularization methods, the basic idea is to apply transformations to a 'data' matrix  $Z$  relative to a 'weight' matrix  $W$  to obtain a unit upper triangular matrix  $R$  and a diagonal matrix  $\Lambda$  such that  $Z'WZ = R'\Lambda R$ . An excellent introduction to the theory of Givens transformations is presented in Golub and van Loan (1983). However, in this paper, the version from Gentleman (1973) is employed where  $Z$  and  $W$  are implicitly assumed to have the general form

$$Z = \begin{bmatrix} U \\ Z \end{bmatrix} \text{ and } W = \begin{bmatrix} D & O \\ O & W \end{bmatrix}$$

where  $U$  is unit upper triangular,  $D$  and  $W$  are diagonal, and  $Z$  is rectangular. <sup>1</sup> The algorithm is initialized with  $R = U$  and  $\Lambda = D$  and is then applied to each successive row  $z$  of  $Z$  with corresponding weight  $w$  from  $W$ .

### Givens Transformations

```

FOR  $k = 1, \dots, q$  REPEAT
   $\bar{\lambda}_k = \lambda_k + wz_k^2$ 
   $c = \lambda_k / \bar{\lambda}_k$ 
   $\bar{w} = wc$ 
   $s = wz_k / \bar{\lambda}_k$ 
  FOR  $j = k + 1, \dots, q$  REPEAT
     $\bar{r}_{kj} = cr_{kj} + sz_j$ 
     $\bar{z}_j = z_j - z_k r_{kj}$ 

```

Note that at the end of each pass through these six steps, the old quantities are replaced by their corresponding new values designated with a bar.

When the square root filter is seeded with a partially diffuse prior distribution, the quantities in the Givens transformations formulae also become dependent on  $\kappa$ . The following results can be established by induction:

$$\lambda_k = \kappa \lambda_k^{[1]} + \lambda_k^{[0]} + O(1/\kappa)$$

$$w = \kappa w^{[1]} + w^{[0]} + O(1/\kappa)$$

$$r_{kj} = r_{kj}^{[0]} + O(1/\kappa)$$

$$z_j = z_j^{[0]} + O(1/\kappa)$$

where the superscripted quantities are all independent of  $\kappa$ . In the process it also can be shown that successive values of the superscripted quantities are related by the formulae in the following algorithm which can be applied to each successive row of  $Z$ :

<sup>1</sup>In regression applications it is normal to set  $U = I$  and  $D = O$  so that  $Z'WZ = Z'WZ$  where  $Z$  and  $W$  are the data and weight matrices respectively.

## Modified Givens Transformations

FOR  $k = 1, \dots, q$  REPEAT

IF ( $\lambda_k^{[1]} = 0$  and  $w^{[1]} = 0$ ) THEN

$$\bar{\lambda}_k^{[0]} = \lambda_k^{[0]} + w^{[0]} z_k^{[0]2}$$

$$c = \lambda_k^{[0]} / \bar{\lambda}_k^{[0]}$$

$$\bar{w}^{[0]} = w^{[0]} c$$

$$s = w^{[0]} z_k^{[0]} / \bar{\lambda}_k^{[0]}$$

IF ( $\lambda_k^{[1]} > 0$  or  $w^{[1]} > 0$ ) THEN

$$\bar{\lambda}_k^{[1]} = \lambda_k^{[1]} + w^{[1]} z_k^{[0]2}$$

$$\bar{\lambda}_k^{[0]} = \lambda_k^{[0]} + w^{[0]} z_k^{[0]2}$$

$$c = \lambda_k^{[1]} / \bar{\lambda}_k^{[1]}$$

$$\bar{w}^{[1]} = w^{[1]} c$$

$$\bar{w}^{[0]} = w^{[1]} \lambda_k^{[0]} / \bar{\lambda}_k^{[1]} + w^{[0]} \lambda_k^{[1]} / \bar{\lambda}_k^{[1]} - w^{[1]} \lambda_k^{[1]} \bar{\lambda}_k^{[0]} / \bar{\lambda}_k^{[1]2}$$

$$s = w^{[1]} z_k^{[0]} / \bar{\lambda}_k^{[1]}$$

FOR  $j = k + 1, \dots, q$  REPEAT

$$\bar{r}_{kj}^{[0]} = c r_{kj}^{[0]} + s z_j^{[0]}$$

$$\bar{z}_j^{[0]} = z_j^{[0]} - z_k^{[0]} r_{kj}^{[0]}$$

This modified version of the Givens transformations can be used in conjunction with the square root filter in the previous section to accommodate partially diffuse priors without the explicit use of the big- $\kappa$ .

## 4 Concluding Remarks

During the "run-in" period, the modified Kalman filter in Ansley and Kohn (1985b) is based on the proposition that the variance matrix of the estimation errors can be written in the form:

$$S(t|n) = \kappa S^{[1]}(t|n) + S^{[0]}(t|n) + O(1/\kappa)$$

where  $S^{[1]}(t|n)$  and  $S^{[0]}(t|n)$  are square symmetric matrices. In contrast to the conventional Kalman filter, it is necessary to revise two symmetric matrices instead of one with consequent increases in computational loads and the demand for storage space. The situation is essentially the same for the earlier square root algorithm in Snyder (1988) except that it relies on the triangular and diagonal counterparts of the component matrices above. In contrast, the algorithm in this paper is different, in that it is based on the observation that the error variance matrix can be written as:

$$S(t|n) = R^{[0]}(t|n)' [\kappa \Lambda^{[1]}(t|n) + \Lambda^{[0]}(t|n)] R^{[0]}(t|n) + O(1/\kappa).$$

Hence it is only necessary to contend with the  $q$  diagonal elements of the additional diagonal matrix  $\Lambda^{[1]}(t|n)$  rather than an entire symmetric matrix  $S^{[1]}(t|n)$ . Furthermore, given that each pass of the modified Givens transformations involves only a few additional calculations, the modifications to the conventional square root filter can be implemented with only a moderate increase in computational loads.

Another approach outlined in Rosenberg (1973) for the case of a diffuse prior distribution and extended in de Jong (1988) to accommodate arbitrary priors, involves the following steps:

1. apply to the data a Kalman filter initialized with a null mean vector and a null variance matrix to give biased estimates of the state vector;
2. also apply certain auxiliary transformations in parallel with step 1;
3. regress the one-step ahead prediction errors obtained from step 1 against the transformed data to estimate the initial state  $x(0)$ ;
4. utilize the result from step 3 to eliminate the bias in the estimates of the state vector from step 1.

Although any square root version of this algorithm should yield the same results as the method proposed in this paper, the auxiliary transformations at step 2 require substantial additional computations and storage space. The proposed algorithm is therefore better.

The state space model considered in this paper is time invariant in the sense that both  $F$  and  $Q$  are independent of  $t$ . The effect of this is to limit the methodology to mainly time series applications. However, the results can be generalized quite substantially without any substantive changes by subscripting these matrices with  $t$ . Such cases as conventional multiple regression can then be accommodated within the framework.

Considerable computational savings can also be made by exploiting special structural features in the problems under consideration. Usually, the transition matrix  $F$  is quite sparse and substantial reductions can be achieved by using sparse matrix arithmetic in those parts of the algorithm where it occurs. Furthermore, in applications to such areas as regression analysis, exponential smoothing and mixed autoregressive-moving average processes, all of which conform to the special case of state space framework described in Snyder (1985), all but one of the diagonal elements of  $D$  equal zero. Since  $\Lambda(n|n-1)$  is initially set equal to  $D$  in step 2 of the time advance stage of the square root filter, substantial computational savings can also be

achieved by employing a special case of the Givens formulae obtained after the substitution of  $\lambda_k = 0$ . The details can be readily determined by the reader.

Finally, it should be noted that the framework can readily accommodate missing values. By setting equal to  $\kappa$  the diagonal elements of  $D$  corresponding to the missing values, the algorithm automatically reverts to the required form.

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