Score Evaluation Within the Extended Square-Root Information Filter

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Abstract. A newly developed algorithm for evaluating the Log Likelihood Gradient (score) of linear discrete-time dynamic systems is presented, based on the extended Square-Root Information Filter (eSRIF). The new result can be used for efficient calculations in gradient-search algorithms for maximum likelihood estimation of the unknown system parameters. The theoretical results are given with the examples showing the superior performance of this computational approach over the conventional one.

1 Introduction

Consider the discrete-time linear dynamic stochastic system

$$x_{t+1} = F_t x_t + G_t w_t, \quad t = 0, 1, \dots, N \quad (1)$$

$$z_t = H_t x_t + v_t, \quad t = 1, 2, \dots, N \quad (2)$$

with the system state $x_t \in \mathbb{R}^n$, the state disturbance $w_t \in \mathbb{R}^q$, the observed vector $z_t \in \mathbb{R}^m$, and the measurement error $v_t \in \mathbb{R}^m$, such that the initial state x_0 and each w_t, v_t of $\{w_t : t = 0, 1, \dots\}$, $\{v_t : t = 1, 2, \dots\}$ are taken from mutually independent Gaussian distributions with the following expectations:

$$\mathbf{E} \left\{ \begin{bmatrix} x_0 \\ w_t \\ v_t \end{bmatrix} \right\} = \begin{bmatrix} \bar{x}_0 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{E} \left\{ \begin{bmatrix} (x_0 - \bar{x}_0) \\ w_t \\ v_t \end{bmatrix} \begin{bmatrix} (x_0 - \bar{x}_0) \\ w_t \\ v_t \end{bmatrix}^T \right\} = \begin{bmatrix} P_0 & 0 & 0 \\ 0 & Q_t & 0 \\ 0 & 0 & R_t \end{bmatrix}$$

and $\mathbf{E} \{w_t w_{t'}^T\} = 0$, $\mathbf{E} \{v_t v_{t'}^T\} = 0$ if $t \neq t'$. Assume the system is parameterized by a vector $\theta \in \mathbb{R}^p$ of unknown system parameters. This means that all the above characteristics, namely $F_t, G_t, H_t, \bar{x}_0, P_0 \geq 0, Q_t \geq 0$ and $R_t > 0$, can depend upon θ (the corresponding notations $F_t(\theta), G_t(\theta)$ and so on, are suppressed for the sake of simplicity).

Models like (1), (2), together with the associated Kalman filter, have been intensively used in many application fields such as control, communications, and signal/image processing. To apply the Kalman filter/smoothing in the case of parametric uncertainty, it is necessary to identify the model, i. e., to estimate the unknown system parameters (or directly the Kalman filter/smoothing parameters) from the available measurements $Z_1^t = (z_1, z_2, \dots, z_t)$, $t = 1, 2, \dots, N$.

A very general and well known approach to parameter estimation is the maximum likelihood (ML) principle. The ML method for estimating θ requires the maximization of the Log Likelihood Function (LLF) $L_\theta(Z_1^N)$, which is the logarithm of the joint probability density of $z_1, z_2, \dots, z_N$, with respect to θ . It incorporates various gradient-search optimization algorithms. In this context, it is very important to find a means for efficient computation of Log Likelihood Gradient (LLG) known as the “score”.

The first solutions to the problem [1, 2] obtained by the direct differentiating the Kalman filtering equations are time consuming as they require the computation of p vector *filter sensitivity equations* and p matrix *Riccati-type sensitivity equations*, both run recursively in the forward time direction. An alternative approach was developed by Yared [3] who assumed a steady-state Kalman filter and used an adjoint filter, resulting in one additional backward pass in time. It works faster than the forward “differentiated” filter although at the expense of increased storage requirements. Wilson and Kumar simplified Yared’s results [4] by moving from derivatives of Kalman variables to those of the original system matrices. They reduced the problem to solving a time-invariant matrix equation, an algebraic Riccati equation, a time-invariant Kalman filter equation, and the backward adjoint filter equation.

Segal and Weinstein developed LLG formulas for both the discrete and continuous-time systems [5, 6] using Fisher’s identity and employing the Kalman smoother. Their approach enables to compute not only the LLG, but (approximately) the log-likelihood Hessian and the Fisher information matrix of θ as well. The continuous-time formula in [5] uses the Itô integral, which cannot be instrumented. For continuous-time case, Leland developed the improved formulas for the LLG [7, 8] free of this limitation.

Despite this remarkable success it is useful to develop alternative algorithms. The most important reason is that the previously mentioned methods suffer from some limitations mainly stemming from the use of the conventional Kalman filter (KF) implementation. This implementation — in terms of covariance matrices — is particularly sensitive to roundoff errors [12]. As a consequence, any method for evaluating the log-likelihood gradient based on the conventional KF implementation, inherits this drawback and so cannot be considered as numerically stable. The alternative solutions to evaluate the LLG can be found in alternative KF implementation methods developed for dealing with the problem of numerical instability in many papers, for example [9, 10, 11], and described in [12].

In this paper we derive a new algorithm for evaluating the LLG based upon the extended Square-Root Information Filter (eSRIF) recently proposed in [11]. Unlike the Conventional Kalman filter (CKF), the eSRIF avoids numerical

instabilities arising from roundoff errors and has also the added feature of being better suited to parallel and to very large scale integration (VLSI) implementations (see [11]). Thus, inheriting these advantages, we expect our method to outperform the conventional KF mechanization for accuracy. These expectations will be verified by two examples of ill-conditioned problems.

The paper is organized as follows. In Section 2 we present a new algorithm for evaluating the LLG based upon the eSRIF. The comparison of the developed algorithm and the conventional approach in terms of sensitivity to roundoff errors is given in Section 3. Section 4 presents some numerical results and finally, Section 5 concludes the paper.

2 Log Likelihood Gradient Evaluation

The Log Likelihood Function (LLF) of system (1), (2) is given by

$$L_{\theta}(Z_1^N) = -\frac{1}{2} \sum_{t=1}^N \left\{ \frac{m}{2} \ln(2\pi) + \ln(\det(R_{e,t})) + e_t^T R_{e,t}^{-1} e_t \right\}$$

where $Z_1^N = (z_1, z_2, \dots, z_N)$ is N -step measurement history, $e_t \stackrel{\text{def}}{=} z_t - H_t \hat{x}_t$ is the zero-mean innovation sequence whose covariance is determined as $R_{e,t} \stackrel{\text{def}}{=} \mathbf{E} \{e_t e_t^T\} = H_t P_t H_t^T + R_t$. The matrix P_t is the error covariance matrix of the time updated estimate $\hat{x}_t$ of the state vector generated by the Kalman filter.

Let $l_{\theta}(z_t)$ denote the negative LLF for the t -th measurement z_t in system (1), (2), given measurement history $Z_1^{t-1} \stackrel{\text{def}}{=} \{z_1, z_2, \dots, z_{t-1}\}$, then

$$l_{\theta}(z_t) = \frac{1}{2} \left\{ \frac{m}{2} \ln(2\pi) + \ln(\det(R_{e,t})) + e_t^T R_{e,t}^{-1} e_t \right\}. \quad (3)$$

From (3) one can easily obtain the expression for the LLG. Let $R_{e,t} = R_{e,t}^{T/2} R_{e,t}^{1/2}$ where $R_{e,t}^{1/2}$ is a square-root factor of the matrix $R_{e,t}$ and $\bar{e}_t$ are the normalized innovations, i. e. $\bar{e}_t = R_{e,t}^{-T/2} e_t$. Taking into account that the matrix $R_{e,t}^{1/2}$ is triangular, we can write down the expression

$$\frac{\partial}{\partial \theta_i} \left[\ln(\det(R_{e,t}^{1/2})) \right] = \text{tr} \left[R_{e,t}^{-1/2} \frac{\partial (R_{e,t}^{1/2})}{\partial \theta_i} \right]. \quad (4)$$

Hence,

$$\frac{\partial l(z_t)}{\partial \theta_i} = \text{tr} \left[R_{e,t}^{-1/2} \frac{\partial (R_{e,t}^{1/2})}{\partial \theta_i} \right] + \bar{e}_t^T \frac{\partial \bar{e}_t}{\partial \theta_i}, \quad i = 1, 2, \dots, p \quad (5)$$

as it follows directly from (3) and (4).

According to the goal pursued by this research and stated in Section 1, we consider the eSRIF presented in [11]. For convenience, we reformulate it in the following form: given $P_0^{-T/2}$ and $P_0^{-T/2}\hat{x}_0 = P_0^{-T/2}\bar{x}_0$; calculate

$$O_t \left[\begin{array}{ccc|c} R_t^{-T/2} - R_t^{-T/2} H_t F_t^{-1} & R_t^{-T/2} H_t F_t^{-1} G_t Q_t^{T/2} & -R_t^{-T/2} z_t \\ 0 & P_t^{-T/2} F_t^{-1} & -P_t^{-T/2} F_t^{-1} G_t Q_t^{T/2} & P_t^{-T/2} \hat{x}_t \\ 0 & 0 & I_q & 0 \end{array} \right] = \left[\begin{array}{ccc|c} R_{e,t}^{-T/2} & 0 & 0 & -\bar{e}_t \\ -P_{t+1}^{-T/2} K_{p,t} & P_{t+1}^{-T/2} & 0 & P_{t+1}^{-T/2} \hat{x}_{t+1} \\ * & * & * & * \end{array} \right] \quad (6)$$

where O_t is any orthogonal transformation such that the matrix on the right-hand side of formula (6) is block lower triangular. The matrix $P_t^{1/2}$ is a square-root factor of P_t , i. e. $P_t = P_t^{T/2} P_t^{1/2}$, $P_t^{1/2}$ is upper triangular. Similarly, we define $P_{t+1} = P_{t+1}^{T/2} P_{t+1}^{1/2}$, $R_t = R_t^{T/2} R_t^{1/2}$, $Q_t = Q_t^{T/2} Q_t^{1/2}$ and $R_{e,t} = R_{e,t}^{T/2} R_{e,t}^{1/2}$. For convenience we shall also write $A^{T/2} = (A^{1/2})^T$, $A^{-1/2} = (A^{1/2})^{-1}$ and $A^{-T/2} = (A^{-1/2})^T$. Additionally, $K_{p,t} = F_t P_t H_t^T R_{e,t}^{-1}$.

It is easy to see that the LLG (5) in terms of eSRIF (6) is given by

$$\frac{\partial l(z_t)}{\partial \theta_i} = -\text{tr} \left[R_{e,t}^{1/2} \frac{\partial (R_{e,t}^{-1/2})}{\partial \theta_i} \right] + \bar{e}_t^T \frac{\partial \bar{e}_t}{\partial \theta_i}, \quad i = 1, 2, \dots, p. \quad (7)$$

To establish our algorithm for efficient evaluation of LLG (7) we prove the following result.

Lemma 1. *Let*

$$QA = L \quad (8)$$

where Q is any orthogonal transformation such that the matrix on the right-hand side of formula (8) is lower triangular and A is a nonsingular matrix. If the elements of A are differentiable functions of a parameter θ then the upper triangular matrix U in

$$Q'_\theta Q^T = U^T - U \quad (9)$$

is, in fact, the upper triangular part of the matrix $QA'_\theta L^{-1}$.

Having applied Lemma 1 to eSRIF (6), we obtain the following algorithm for computing LLG (7).

Algorithm LLG-eSRIF

I. For each θ_i , $i = 1, 2, \dots, p$, calculate

$$O_t \begin{bmatrix} \frac{\partial}{\partial \theta_i} (R_t^{-T/2}) & \frac{\partial}{\partial \theta_i} (S_t^{(1)}) & \frac{\partial}{\partial \theta_i} (S_t^{(2)}) & \left| \frac{\partial}{\partial \theta_i} (S_t^{(3)}) \right. \\ 0 & \frac{\partial}{\partial \theta_i} (S_t^{(4)}) & \frac{\partial}{\partial \theta_i} (S_t^{(5)}) & \left| \frac{\partial}{\partial \theta_i} (S_t^{(6)}) \right. \\ 0 & 0 & 0 & \left| 0 \right. \end{bmatrix} = \begin{bmatrix} X_i & Y_i & M_i & \left| L_i \right. \\ N_i & V_i & W_i & \left| K_i \right. \\ * & * & * & \left| * \right. \end{bmatrix}$$

where O_t is the same orthogonal transformation as in (6) and

$$S_t^{(1)} = -R_t^{-T/2} H_t F_t^{-1}, \quad S_t^{(2)} = R_t^{-T/2} H_t F_t^{-1} G_t Q_t^{T/2}, \quad S_t^{(3)} = -R_t^{-T/2} z_t, \\ S_t^{(4)} = P_t^{-T/2} F_t^{-1}, \quad S_t^{(5)} = -P_t^{-T/2} F_t^{-1} G_t Q_t^{T/2}, \quad S_t^{(6)} = P_t^{-T/2} \hat{x}_t.$$

II. For each θ_i , $i = 1, 2, \dots, p$, compute the matrix

$$J_i = \begin{bmatrix} X_i & Y_i & M_i \\ N_i & V_i & W_i \end{bmatrix} \begin{bmatrix} R_{e,t}^{-T/2} & 0 & 0 \\ -P_{t+1}^{-T/2} K_{p,t} & P_{t+1}^{-T/2} & 0 \\ * & * & * \end{bmatrix}^{-1}.$$

III. For each θ_i , $i = 1, 2, \dots, p$, we split the matrices J_i obtained at Step II as follows:

$$J_i = \left[\underbrace{L_i + D_i + U_i}_{m+n} \quad \begin{matrix} m+n+q \\ *** \end{matrix} \right] \quad \Bigg\}_{m+n}$$

where L_i , D_i and U_i are the strictly lower triangular, diagonal and strictly upper triangular parts of matrix J_i , respectively.

IV. For each θ_i , $i = 1, 2, \dots, p$, compute the following quantities:

$$\begin{bmatrix} \frac{\partial R_{e,t}^{-T/2}}{\partial \theta_i} & 0 \\ -\frac{\partial (\tilde{P}_{t+1}^{-T/2} K_{p,t})}{\partial \theta_i} & \frac{\partial \tilde{P}_{t+1}^{-T/2}}{\partial \theta_i} \end{bmatrix} = [L_i + D_i + U_i^T] \begin{bmatrix} R_{e,t}^{-T/2} & 0 \\ -\tilde{P}_{t+1}^{-T/2} K_{p,t} & \tilde{P}_{t+1}^{-T/2} \end{bmatrix} \\ \frac{\partial \bar{e}_t}{\partial \theta_i} = \left[\frac{\partial R_{e,t}^{-T/2}}{\partial \theta_i} - X_i \right] R_{e,t}^{T/2} \bar{e}_t + Y_i F_t \hat{x}_t - L_i,$$

$$\frac{\partial S_{t+1}^{(6)}}{\partial \theta_i} = \left[\frac{\partial (\tilde{P}_{t+1}^{-T/2} K_{p,t})}{\partial \theta_i} + N_i \right] R_{e,t}^{T/2} \bar{e}_t + \left[\frac{\partial \tilde{P}_{t+1}^{-T/2}}{\partial \theta_i} - V_i \right] F_t \hat{x}_t + K_i.$$

Table 1. Comparison of Rounded Solutions to Problem 1 evaluated at the point $\theta = 1$

Filter Implementation	Solution	
	Exact Answer	Rounded Answer
“differentiated” Conventional Covariance Filter	$(P_1)'_{\theta} _{\theta=1} = \begin{bmatrix} \frac{e^2}{1+e^2} & 0 \\ 0 & 1 \end{bmatrix}$	$(P_1)'_{\theta} _{\theta=1} \stackrel{r}{=} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$
“differentiated” Conventional Information Filter	$(P_1^{-1})'_{\theta} _{\theta=1} = - \begin{bmatrix} \frac{1+e^2}{e^2} & 0 \\ 0 & 1 \end{bmatrix}$	$(P_1^{-1})'_{\theta} _{\theta=1} \stackrel{r}{=} - \begin{bmatrix} \frac{1}{e^2} & 0 \\ 0 & 1 \end{bmatrix}$
Algorithm LLG- eSRIF	$(P_1^{-1/2})'_{\theta} _{\theta=1} = -\frac{1}{2} \begin{bmatrix} \frac{\sqrt{1+e^2}}{e} & 0 \\ 0 & 1 \end{bmatrix}$	$(P_1^{-1/2})'_{\theta} _{\theta=1} \stackrel{r}{=} -\frac{1}{2} \begin{bmatrix} \frac{1}{e} & 0 \\ 0 & 1 \end{bmatrix}$

V. Finally, compute the LLG according to (7).

Remark 1. Since, the matrices in (7) are triangular, only the diagonal elements of $R_{e,t}^{1/2}$ and $\frac{\partial(R_{e,t}^{-1/2})}{\partial\theta_i}$ need to be computed. Hence, the Algorithm LLG-eSRIF allows the $m \times m$ -matrix inversion of $R_{e,t}$ to be avoided in the evaluation of LLG.

3 Ill-Conditioned Example Problems and Comparison

To illustrate and compare the performance of the presented Algorithm LLG-eSRIF and the conventional approach, i.e. a straightforward differentiation of the KF (“differentiated” KF), two simple test problems have been constructed.

Problem 1. Given:

$$P_0 = \begin{bmatrix} \theta & 0 \\ 0 & \theta \end{bmatrix}, H = [1, 0], R = e^2\theta \quad \text{and} \quad F = I_2, Q = 0, G = [0, 0]^T$$

where θ is an unknown parameter, I_2 is an identity 2×2 matrix, $0 < e \ll 1$; to simulate roundoff we assume $e + 1 \neq 1$ but $e^2 + 1 \stackrel{r}{=} 1$.

Calculate: $(P_1)'_{\theta}$ at the point $\theta = 1$.

For the $\theta = 1$, this example illustrates the initialization problems that result when $H_t P_t H_t^T + R_t$ is rounded to $H_t P_t H_t^T$ (see, for example, [9]). The exact answer and the rounded answer, using $e^2 + 1 \stackrel{r}{=} 1$ in all calculations, are given for the “differentiated” CKF, “differentiated” Conventional Information filter (CIF) and the new Algorithm LLG-eSRIF developed in this paper (see Table 1).

Table 2. Comparison of Rounded Solutions to Problem 2 evaluated at the point $\theta = 1$

Filter Implement.	Solution	
	Exact Answer	Rounded Answer
“diff.” CKF	$(P_1)'_{\theta} _{\theta=1} = \frac{1}{2+e^2} \begin{bmatrix} 1+e^2 & -1 \\ -1 & 1+e^2 \end{bmatrix}$	$(P_1)'_{\theta} _{\theta=1} \stackrel{r}{=} \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$
“diff.” CIF	$(P_1^{-1})'_{\theta} _{\theta=1} = -\frac{1}{e^2} \begin{bmatrix} 1+e^2 & 1 \\ 1 & 1+e^2 \end{bmatrix}$	$(P_1^{-1})'_{\theta} _{\theta=1} \stackrel{r}{=} -\frac{1}{e^2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$
Algorithm LLG- eSRIF	$(P_1^{-1/2})'_{\theta} _{\theta=1} = -\frac{1}{2} \begin{bmatrix} \sqrt{\frac{2+e^2}{1+e^2}} & \frac{1}{e\sqrt{1+e^2}} \\ 0 & \frac{\sqrt{1+e^2}}{e} \end{bmatrix}$	$\stackrel{r}{=} -\frac{1}{2} \begin{bmatrix} \sqrt{2} & \frac{1}{e} \\ 0 & \frac{1}{e} \end{bmatrix}$

It can be seen that all algorithms except the “differentiated” CKF give the nonsingular result. A singular answer will lead to a zero gain if a second measurement of the same type is processed.

Problem 2. Given: same as Problem 1, but $H = [1, 1]$.

Find: $(P_1)'_{\theta}$ at the point $\theta = 1$.

The exact solution and the rounded one for Problem 2 are summarized in Table 2. With this more general type of ill-conditioning, only Algorithm LLG-eSRIF gives a nonsingular result.

4 Numerical Results

To substantiate the above theoretical result experimentally, we consider the example taken from [10]. Our simulation experiments are broken down into the following steps. Step 1 is planned to compute the negative LLF; in so doing, we compare our simulation results with those produced by the Conventional Information Filter (CIF). Step 2 is intended to compute the LLG; in this case, we compare the result generated by the Algorithm LLG-eSRIF with those produced by the “differentiated” CIF.

Example 1. Let the test system (1), (2) be defined as follows:

$$x_{t+1} = \begin{bmatrix} 1 & \Delta t \\ 0 & e^{-\Delta t/\tau} \end{bmatrix} x_t + \begin{bmatrix} 0 \\ 1 \end{bmatrix} w_t,$$

$$z_t = \begin{bmatrix} 1 & 0 \end{bmatrix} x_t + v_t$$

where τ is a parameter which needs to be estimated.

Fig. 1. The negative LLF and LLG calculated by the Conventional Information Filter, the extended Square-Root Information Filter, the “differentiated” Conventional Information Filter and Algorithm LLG-eSRIF, respectively.

The results of Step 1 and Step 2 are shown in Fig. 1. For the test problem, $\tau^* = 15$ was chosen as the true value of parameter τ . As can be seen, all two algorithms for evaluating the LLG produce exactly the same result and give the same zero point. Besides, it is readily seen that the estimate $\hat{\tau}_{\min}$ minimizing the negative LLF coincides with the estimate $\hat{\tau}_{\text{grad}}$ at which the LLG is zero. Moreover, all estimates fit the true value of parameter τ , i.e. $\tau^* = 15$.

5 Conclusion

In this paper, the new algorithm for evaluating the Log Likelihood Gradient (score) of linear discrete-time dynamic systems has been developed. The necessary theory has been given and substantiated by the computational experiments. Two ill-conditioned example problems have been constructed to show the superior performance of the Algorithm LLG-eSRIF over the conventional approach.

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