Likelihood Gradient Evaluation Using Square-Root Covariance Filters

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Abstract—Using the array form of numerically stable square-root implementation methods for Kalman filtering formulas, we construct a new square-root algorithm for the log-likelihood gradient (score) evaluation. This avoids the use of the conventional Kalman filter with its inherent numerical instabilities and improves the robustness of computations against roundoff errors. The new algorithm is developed in terms of covariance quantities and based on the "condensed form" of the array square-root filter.

Index Terms—identification, maximum likelihood estimation, gradient methods, Kalman filtering, numerical stability.

I. INTRODUCTION

Consider the discrete-time linear stochastic system

\[ x_k = F_k x_{k-1} + G_k w_k, \quad (1) \]
\[ z_k = H_k x_k + v_k, \quad k = 1, \ldots, N, \quad (2) \]

where \( x_k \in \mathbb{R}^n \) and \( z_k \in \mathbb{R}^m \) are, respectively, the state and the measurement vectors; \( k \) is a discrete time, i.e. \( x_k \) means \( x(t_k) \). The noises \( w_k \in \mathbb{R}^q \), \( v_k \in \mathbb{R}^r \) and the initial state \( x_0 \sim \mathcal{N}(\bar{x}_0, P_0) \) are taken from mutually independent Gaussian distributions with zero mean and covariance matrices \( Q_k \) and \( R_k \), respectively, i.e. \( w_k \sim \mathcal{N}(0, Q_k) \), \( v_k \sim \mathcal{N}(0, R_k) \). Additionally, system (1), (2) is parameterized by a vector of unknown system parameters \( \theta \in \mathbb{R}^p \), which needs to be estimated. This means that the entries of the matrices \( F_k, G_k, H_k, Q_k, R_k \) and \( \Pi_0 \) are functions of \( \theta \in \mathbb{R}^p \). However, for the sake of simplicity we will suppress the corresponding notations below, i.e instead of \( (F_k(\theta), G_k(\theta), H_k(\theta), Q_k(\theta), R_k(\theta)) \) and \( \Pi_0(\theta) \) we will write \( F_k, G_k, H_k, Q_k, R_k \) and \( \Pi_0 \).

Solving the parameter estimation problem by the method of maximum likelihood requires the maximization of the likelihood function (LF) with respect to unknown system parameters. It is often done by using a gradient approach where the computation of the likelihood gradient (LG) is necessary. For this case, we will derive the expression for the Log LG evaluation in terms of the square-root covariance variables, i.e. in terms of the one-step predicted error covariance matrix \( \hat{P}_{k|k-1} \) and the one-step predicted error covariance matrix \( \hat{P}_{k|k-1} \).

Straightforward differentiation of the KF equations is a direct approach to the Log LG evaluation, known as a "score". This leads to a set of \( p \) vector equations, known as the filter sensitivity equations, for computing \( \partial x|_{k-1}/\partial \theta \), and a set of \( p \) matrix equations, known as the Riccati-type sensitivity equations, for computing \( \partial P_{k|k-1}/\partial \theta \).

Consequently, the main disadvantage of the standard approach is the problem of numerical instability of the conventional KF, i.e divergence due to the lack of reliability of the numerical algorithm. Solution of the matrix Riccati equation is a major cause of numerical difficulties in the conventional KF implementation, from the standpoint of computational load as well as from the standpoint of computational errors [2].

The alternative approach can be found in, so-called, square-root filtering algorithms. It is well known that numerical solution of the Riccati equation tends to be more robust against roundoff errors if Cholesky factors or modified Cholesky factors (such as the \( L^T DU \)-algorithms) of the covariance matrix are used as the dependent variables. The resulting KF implementation methods are called square-root filters (SRF). They are now generally preferred for practical use [2], [4], [5]. For more insights about numerical properties of different KF implementation methods we refer to the celebrated paper of Verhaegen and Van Dooren [6].

Increasingly, the preferred form for algorithms in many fields is now the array form [7]. Several useful SRF algorithms for KF formulas formulated in the array form have been recently proposed by Park and Kailath [8]. For these implementations the reliability of the filter estimates is expected to be better because of the use of numerically stable orthogonal transformations for each recursion step. Apart from numerical advantages, array SRF algorithms appear to be better suited to parallel and to very large scale integration (VLSI) implementations [8], [9].

The development of numerically stable implementation methods for KF formulas has led to the hope that the Log LG (with respect to unknown system parameters) might be computed more accurately. For this problem, a number of questions arise:

- Is it possible to extend reliable array SRF algorithms to the case of the Log LG evaluation?
- If such methods exist, will they inherit the advantages from the source filtering implementations? In particular, will they improve the robustness of the computations against roundoff errors compared to the conventional KF technique? The question about suitability for parallel implementation is beyond the scope of this paper.

The first attempt to answer these questions belongs to Bierman et al. [10]. The authors used the square-root information filter, developed by Dyer and McReynolds [11] and later extended by Bierman [3], as a source filter implementation and constructed the method for score evaluation. The algorithm was developed in the form of measurement and time updates. However, the accuracy of the proposed method has not been investigated.

In contrast to the main result of [10], we focus on the dual class of KF implementation methods (that is the class of covariance-type methods) and discuss the efficient Log LG evaluation in square-root covariance filters. More precisely, we consider the array form of the square-root covariance filter eSRCF introduced in [8]. The purpose of this paper is to design the method for the Log LG evaluation in terms of the square-root covariance variables, i.e. in terms of the quantities that appear naturally in the eSRCF. This avoids the use of the conventional KF with its inherent numerical instabilities and gives us an opportunity to improve the robustness of the Log LG computation against roundoff errors.

II. EXTENDED SQUARE-ROOT COVARIANCE FILTER

To achieve our goal, we are first going to present the extended square-root covariance filter (eSRCF), proposed in [8], and second, we will derive the expression for the Log LG evaluation in terms of the variables that are generated by the eSRCF implementation.

Notations to be used: For the sake of simplicity, we denote the one-step predicted state estimate as \( \hat{x}_k \) and the one-step predicted error covariance matrix as \( \hat{P}_k \). We use Cholesky decomposition of the form \( \hat{P}_k = \hat{P}^{1/2}_k \hat{P}^{1/2}_k \), where \( \hat{P}^{1/2}_k \) is an upper triangular matrix. Similarly, we define \( \hat{R}_k^{1/2}, Q_k^{1/2}, \hat{R}_k^{1/2} \). For convenience we will write

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\( A^{-1/2} = (A^{-1/2})^{-1}, \) \( A^{-T/2} = (A^{-1/2})^T \) and \( \partial \theta_i A \) implies the partial derivative of the matrix \( A \) with respect to the \( i \)th component of \( \theta \), i.e., \( \partial A/\partial \theta_i \).

In this paper, we deal with the "condensed form"\(^1\) of the eSRF [8]: Assume that \( R_k > 0 \). Given \( \Pi^{i/2}_0 \) and \( \Pi^{0/2}_0 \), recursively update \( P^{i/2}_k \) and \( P^{-T/2}_k \bar{\xi}_k \) as follows:

\[
Q_k = \begin{bmatrix} R^{1/2}_k & 0 & -R^{-T/2}_k \bar{\xi}_k \\ P^{1/2}_k H^k & P^{1/2}_k F^k & P^{1/2}_k P^{-T/2}_k \bar{\xi}_k \\ 0 & Q^{1/2}_k G^k & 0 \end{bmatrix} \begin{bmatrix} \partial \theta_i R^{1/2}_k & 0 & \partial \theta_i (P^{1/2}_k H^k) \\ \partial \theta_i (P^{1/2}_k F^k) & \partial \theta_i (P^{1/2}_k P^{-T/2}_k \bar{\xi}_k) & 0 \\ 0 & \partial \theta_i (Q^{1/2}_k G^k) & 0 \end{bmatrix} \begin{bmatrix} \partial \theta_i (-R^{-T/2}_k \bar{\xi}_k) \\ \delta H \end{bmatrix}
\]

(8)

where \( Q_k \) is any orthogonal rotation that upper-triangularizes the first two (block) columns of the matrix on the left-hand side of (3). \( \bar{K}_{p,k} = F_k P_k H^k \) and \( \bar{\xi}_k = R^{-T/2}_k \bar{\xi}_k \).

One can easily obtain the expression for the negative Log LF in terms of the eSRF variables:

\[
L_{\theta} (Z_1^N) = \frac{1}{2} \sum_{k=1}^{N} \left\{ \frac{M}{2} \ln(2\pi) + 2 \ln \left( \text{det} R^{1/2}_{e,k} \right) + e_k^T \bar{\xi}_k \right\}.
\]

(4)

Let \( \theta = [\theta_1, \ldots, \theta_p] \) denote the vector of parameters with respect to which the likelihood function is to be differentiated. Then from (3), we have

\[
\partial \theta_i L_{\theta} (Z_1^N) = \sum_{k=1}^{N} \left\{ \partial \theta_i \ln \left( \text{det} R^{1/2}_{e,k} \right) + \frac{1}{2} \partial \theta_i \left( e^T \bar{\xi}_k \right) \right\}.
\]

(5)

Taking into account that the matrix \( R^{1/2}_{e,k} \) is upper triangular, we derive

\[
\partial \theta_i \ln \left( \text{det} R^{1/2}_{e,k} \right) = \partial \theta_i \sum_{j=1}^{m} \ln \left( r^{ij}_{e,k} \right) = \sum_{j=1}^{m} \frac{1}{r^{ij}_{e,k}} \partial \theta_i r^{ij}_{e,k}
\]

where \( r^{ij}_{e,k}, j = 1, \ldots, m \) denote the diagonal elements of the matrix \( R^{1/2}_{e,k} \). Substitution of (6) into (5) yields the result that we are looking for

\[
\partial \theta_i L_{\theta} (Z_1^N) = \sum_{k=1}^{N} \left\{ \text{tr} \left( R^{-1/2}_{e,k} \partial \theta_i R^{1/2}_{e,k} + e_k^T \bar{\xi}_k \right) \right\}.
\]

(7)

Ultimately, our problem is to compute Log LF (7) by using the eSRF equation (3). Before we come to the main result of this paper, there are a few points to be considered. As can be seen from (7), the elements \( e_k \) and \( R^{1/2}_{e,k} \) involved in the Log LF evaluation are obtained from the underlying filtering algorithm directly, i.e., from (3). No additional computations are needed. Hence, our aim is to explain how the last two terms in the Log LF expression, \( \partial \theta_i e_k \) and \( \partial \theta_i R^{-T/2}_k \bar{\xi}_k \), can be computed using quantities available from eSRF [3].

III. SUGGESTED SQUARE-ROOT METHOD FOR SCORE
EVALUATION

We can now prove the following result.

Theorem 1: Let the entries of the matrices \( F_k, G_k, H_k, Q_k, R_k, \) \( \Pi_0 \) describing the linear discrete-time stochastic system (1), (2) be differentiable functions of a parameter \( \theta \in \mathbb{R}^P \). Then in order to compute the Log LF and its gradient (with respect to unknown system parameter \( \theta \)) the eSRF, which is used to filter the data, needs to be extended as follows. Assume that \( R_k > 0 \). Given the initial values \( \Pi^{i/2}_0, \Pi^{0/2}_0, \bar{\xi}_0, \) and \( \partial \theta_i \Pi^{i/2}_0, \) \( \partial \theta_i (\Pi^{0/2}_0) \), recursively update \( P^{i/2}_k, P^{-T/2}_k \bar{\xi}_k \) and \( \partial \theta_i P^{i/2}_k, \partial \theta_i (P^{-T/2}_k \bar{\xi}_k) \) as follows:

I. Replace the eSRF equation (3) by (8) where \( Q_k \) is any orthogonal rotation that upper-triangularizes the first two (block) columns of the matrix on the left-hand side of (5).

II. Having computed the elements of the right-hand side matrix in (8), calculate for each \( \theta_i \):

\[
\begin{bmatrix} \partial \theta_i R^{1/2}_{e,k} & \partial \theta_i R^{-T/2}_{p,k} \\ 0 & \partial \theta_i P^{1/2}_{k+1} \end{bmatrix} = \begin{bmatrix} L^T_i - L_i & -e_k \\ 0 & P^{1/2}_{k+1} \end{bmatrix},
\]

(9)

where \( L_i, D_i, \) and \( U_i \) are strictly triangular, diagonal and strictly upper triangular parts of the following matrix product:

\[
X_i Y_i \begin{bmatrix} R^{-1/2}_{e,k} & -R^{-1/2}_{e,k} K^T \bar{\xi}_k P^{-1/2}_{k+1} \\ N_i V_i & 0 \end{bmatrix} = L_i + D_i + U_i.
\]

(11)

III. Having determined \( e_k, R^{1/2}_{e,k} \) and \( \partial \theta_i e_k, \partial \theta_i R^{1/2}_{e,k} \) compute Log LF (4) and Log LG (7).

Proof: As discussed earlier, the main difficulty in score evaluation (7) is to define \( \partial \theta_i R^{1/2}_{e,k} \) and \( \partial \theta_i \bar{\xi}_k \) from the underlying filter, i.e., from (3). We divide the proof into two parts, first proving (9) for the \( \partial \theta_i R^{1/2}_{e,k} \) evaluation and then validating (10) for \( \partial \theta_i \bar{\xi}_k \).

Part I. Our goal is to express \( \partial \theta_i R^{-T/2}_k \bar{\xi}_k \) in terms of the variables that appear naturally in the eSRF implementation. First, we can note that the eSRF transformation in (3) has a form

\[
Q A = B
\]

where \( A \) is a rectangular matrix, and \( Q \) is an orthogonal transformation that block upper-triangularizes \( B \). If matrix \( A \) is square and

1The "condensed form" of filtering algorithms refers to the case when implementation method for the KF formulas is not divided into the measurement and time updates.
invertible, then given the matrix of derivatives $A'_\theta = \frac{da_{ij}}{d\theta}$ we can compute $B'_\theta$ as follows [10]:

$$B'_\theta = \begin{pmatrix} L^T + D + U \end{pmatrix} B \quad (12)$$

where $L$, $D$ and $U$ are, respectively, strictly lower triangular, diagonal and strictly upper triangular parts of the matrix $QA'_\theta B^{-1}$.

However, this idea cannot be applied to the eSRCF because the matrix to be triangularized, i.e. the first two (block) columns of the matrix on the left-hand side of (3), is not square and, hence, not invertible. By using the pseudoinverse (Moore-Penrose) inversion we avoid this obstacle and generalize the scheme of computations [12] to the case of eSRCF [5].

To begin constructing the method for score evaluation, we augment the matrix to be triangularized by $q$ columns of zeros. Hence, we obtain

$$Q_k \begin{bmatrix} R_k^{1/2} & 0 & 0 \\ P_k^{1/2} H_k & P_k^{1/2} F_k & 0 \\ Q_k^{1/2} G_k & 0 & 0 \end{bmatrix} = \begin{bmatrix} R_k^{1/2} & \tilde{K}_k^{T} & 0 \\ 0 & P_k^{1/2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (13)$$

The matrices in (13) have dimensions $(m+n+q) \times (m+n+q)$. For the sake of simplicity, we denote the left-hand side and the right-hand side matrices of (13) as $A_k$ and $B_k$, respectively. Then, by differentiating (13) with respect to the components of $\theta$, we obtain

$$\partial_\theta Q_k \cdot A_k + Q_k \cdot \partial_\theta A_k = \partial_\theta B_k \quad (14)$$

Multiplication both sides of (14) by the pseudoinverse matrix $B^+_k$ yields

$$\partial_\theta B_k \cdot B^+_k = \partial_\theta Q_k \left( A_k B^+_k \right) + Q_k \cdot \partial_\theta A_k \cdot B^+_k = \partial_\theta Q_k \left( Q_k^T B_k B^+_k \right) + \left( Q_k \cdot \partial_\theta A_k \right) B^+_k \quad (15)$$

One can easily obtain the explicit expression for $B^+_k$:

$$B^+_k = \begin{bmatrix} R_k^{1/2} - R_k^{1/2} K_p^{1/2} P_k^{1/2} & 0 \\ 0 & P_k^{1/2} \\ 0 & 0 & 0 \end{bmatrix} \quad (16)$$

By using (8), we replace $Q_k \cdot \partial_\theta A_k$ in (15) by the quantities already computed. Then, taking into account (16), we derive the equation for the $(m+n) \times (m+n)$ main block of the matrix $B_k$:

$$\begin{bmatrix} \partial_\theta R_k^{1/2} & \partial_\theta \tilde{K}_k^{T} \\ 0 & \partial_\theta P_k^{1/2} \end{bmatrix} \begin{bmatrix} R_k^{1/2} K_k^{1/2} & 0 \\ 0 & P_k^{1/2} \end{bmatrix}^{-1} = \begin{bmatrix} \partial_\theta Q_k \cdot Q_k^T & 0 \\ 0 & 0 \end{bmatrix} \quad (17)$$

where $\partial_\theta Q_k \cdot Q_k^T_{m+n}$ denotes the $(m+n) \times (m+n)$ main block of the matrix $\partial_\theta Q_k \cdot Q_k^T$.

As discussed in [10], the matrix $\partial_\theta Q_k \cdot Q_k^T$ is skew symmetric, and hence, can be represented in the form $L^T - L$ where $L$ is strictly lower triangular.

Now, let us consider matrix equation (17). As can be seen, the matrix on the left-hand side of (17) is block upper triangular. Thus, the strictly lower triangular part of the matrix $\partial_\theta Q_k \cdot Q_k^T_{m+n}$ must exactly cancel the strictly lower triangular part of the second term on the right-hand side of (17). In other words, if

$$\begin{bmatrix} X_i Y_i \\ N_i V_i \end{bmatrix} \begin{bmatrix} R_k^{1/2} & 0 \\ 0 & P_k^{1/2} \end{bmatrix}^{-1} = \tilde{L}_i + D_i + \tilde{U}_i,$$

then

$$\partial_\theta Q_k \cdot Q_k^T_{m+n} = \tilde{L}_i - \tilde{L}_i. \quad (18)$$

Substitution of (18) into (17) leads to

$$\begin{bmatrix} \partial_\theta R_k^{1/2} & \partial_\theta \tilde{K}_k^{T} \\ 0 & \partial_\theta P_k^{1/2} \end{bmatrix} \begin{bmatrix} R_k^{1/2} & \tilde{K}_k^{T} \\ 0 & P_k^{1/2} \end{bmatrix}^{-1} = \begin{bmatrix} \tilde{L}_i^T + D_i + \tilde{U}_i \end{bmatrix} \quad (19)$$

Formulas (19) and (18) are, in fact, equations (9) and (11) of the proposed method for score evaluation. The theorem is half proved. Part II. We need to verify (10). By differentiating the last equation of the eSRCF with respect to the components of $\theta$

$$\begin{bmatrix} -R_k^{1/2}/z_k \\ P_k^{1/2} x_k + 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -\tilde{e}_k \\ P_k^{1/2} x_k + 1 \end{bmatrix}$$

we obtain

$$\begin{bmatrix} -\partial_\theta \tilde{e}_k \\ \partial_\theta \tilde{e}_k \end{bmatrix} \begin{bmatrix} P_k^{1/2} x_k + 1 \\ 0 \end{bmatrix} = \partial_\theta Q_k \cdot Q_k^T \quad (20)$$

Next, we replace the last term in (20) with the quantities already computed and collected in the right-hand side matrix of (8). Furthermore, it is useful to note that the element $\partial_\theta \gamma_k$ is of no interest here. These two steps give us

$$\begin{bmatrix} \partial_\theta \tilde{e}_k \\ \partial_\theta \tilde{e}_k \end{bmatrix} \begin{bmatrix} P_k^{1/2} x_k + 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \partial_\theta Q_k \cdot Q_k^T \\ \partial_\theta Q_k \cdot Q_k^T \end{bmatrix} \quad (21)$$

where \(\partial_\theta Q_k \cdot Q_k^T\) stands for the $(m+n) \times q$ matrix composed of the entries that are located at the intersections of the last $q$ columns with the first $m+n$ rows of $\partial_\theta Q_k \cdot Q_k^T$.

Taking into account (15), from the equation above we obtain

$$\begin{bmatrix} \partial_\theta \tilde{e}_k \\ \partial_\theta \tilde{e}_k \end{bmatrix} \begin{bmatrix} P_k^{1/2} x_k + 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \tilde{L}_i^T - \tilde{L}_i \\ 0 \end{bmatrix} \quad (22)$$

where $\tilde{L}_i$ is strictly lower triangular part of the matrix in (11).

Since $\partial_\theta Q_k \cdot Q_k^T$ is skew symmetric, we can write down

$$\begin{bmatrix} \partial_\theta Q_k \cdot Q_k^T \\ \partial_\theta Q_k \cdot Q_k^T \end{bmatrix} \quad (23)$$

where \(\partial_\theta Q_k \cdot Q_k^T\) stands for the $q \times (m+n)$ matrix composed of the entries that are located at the intersections of the last $q$ rows with the first $(m+n)$ columns of $\partial_\theta Q_k \cdot Q_k^T$.

To evaluate the right-hand side of (23), we return to (13) and write it in the matrix form:

$$\begin{bmatrix} \partial_\theta R_k^{1/2} & \partial_\theta \tilde{K}_k^{T} \\ 0 & \partial_\theta P_k^{1/2} \end{bmatrix} \begin{bmatrix} R_k^{1/2} & \tilde{K}_k^{T} \quad 0 \\ 0 & P_k^{1/2} \end{bmatrix} = \begin{bmatrix} \partial_\theta Q_k \cdot Q_k^T \\ \partial_\theta Q_k \cdot Q_k^T \end{bmatrix} \quad (24)$$
As can be seen, the last (block) row of the left-hand side matrix in (24) is zero. Thus, the last (block) row of the matrix \( \partial_{\hat{\theta}_i} Q_k \cdot Q_k^T \) must exactly cancel the last (block) row of the second term in (24):

\[
\begin{bmatrix}
\partial_{\hat{\theta}_i} Q_k \cdot Q_k^T \\
\end{bmatrix}_{\text{row: last q}}_{\text{col: 1:m+n}} = - \begin{bmatrix} B_i & K_i \end{bmatrix} \begin{bmatrix} R_{k+1}^{1/2} & K_{k+1}^T \\
0 & P_{k+1}^{1/2} \\
\end{bmatrix}^{-1}.
\]

By substituting (25) into (24), we obtain

\[
\begin{bmatrix}
\partial_{\hat{\theta}_i} Q_k \cdot Q_k^T \\
\end{bmatrix}_{\text{row: last q}}_{\text{col: 1:m+n}} = \begin{bmatrix} R_{k+1}^{1/2} & K_{k+1}^T \\
0 & P_{k+1}^{1/2} \\
\end{bmatrix}^{-T} \begin{bmatrix} B_i \end{bmatrix}.
\]

Final substitution of (26) into (22) validates (10) of the proposed method for the Log LG evaluation. This completes the proof.

Remark 1: The method for score evaluation introduced above has been derived from the eSRCF implementation. As a consequence, the proposed method is of covariance-type.

Remark 2: The new square-root algorithm for score evaluation naturally extends the eSRCF filter and, hence, consists of two parts. They are the "filtered" and "differentiated" parts. This structure allows the Log LF and its gradient to be computed simultaneously. Thus, the method is ideal for simultaneous state estimation and parameter identification.

Remark 3: In the KF formulation of the Log LG evaluation, it is necessary to run the "differentiated" KF for each of the parameters \( \theta_i \) to be estimated. As in [10], in the eSRCF formulation this "bank" of filters is replaced with the augmented arrays to which orthogonal transformations are applied.

IV. NUMERICAL RESULTS

First, we would like to check our theoretical derivations. To do so, we apply the square-root algorithm introduced in Theorem 1 to the following simple test problem.

Example 1: Consider the special case of the system (1), (2) being

\[
x_k = \begin{bmatrix} d_k \\ s_k \end{bmatrix} = \begin{bmatrix} 1 & \Delta t \\ 0 & e^{-\Delta t / \tau} \end{bmatrix} x_{k-1} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} w_k, \quad z_k = \begin{bmatrix} 1 & 0 \end{bmatrix} x_k + v_k
\]

where \( w_k \sim N(0, I_2) \), \( v_k \sim N(0, I_2) \), \( I_n \) denotes the \( n \times n \) identity matrix and \( \tau \) is a parameter which needs to be estimated.

In our simulation experiment, we compute the negative Log LF and its gradient by the proposed square-root method and, then, compare the results to those produced by the conventional KF approach. The outcomes of this experiments are illustrated by Fig. 1 and 2.

As can be seen from Fig. 3 all algorithms for score evaluation produce exactly the same result and give the same zero point that further coincides with the minimum point of the negative Log LF (see Fig. 1). All these evidences substantiate the theoretical derivations of Section III.

Next, we wish to answer the second question posed in this paper: does the algorithm for score evaluation derived from numerically stable square-root implementation method improve the robustness of computations against roundoff errors? The previously obtained results (Example 1) indicate that both methods, i.e. the conventional KF technique and the new square-root algorithm, produce exactly the same answer for the Log LF and Log LG evaluation. However, numerically they no longer agree. We are now going to explore the accuracy of the numerical algorithms.

To begin designing the ill-conditioned test problem we, first, stress the type of the proposed method. As discussed in Remark 1 the new square-root algorithm belongs to the class of covariance-type methods. From Verhaegen and Van Dooren’s celebrated paper [6], we know that the condition number of the innovation covariance matrix \( K(R_{\theta,k}) \) is the key parameter determining the numerical behavior of the covariance algorithms. Taking into account these two important facts, we construct the following ill-conditioned test problem.

Example 2: Consider the problem with the measurement sensitivity matrix

\[
H_k = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 + \delta \end{bmatrix}
\]

and \( F_k = I_3, G_k = 0, Q_k = I_1, R_k = \delta^2 \theta I_2 \)

with \( x_0 \sim N(0, \theta I_2) \), where \( \theta \) is an unknown system parameter. To simulate roundoff we assume that \( \delta^2 < \epsilon_{\text{roundoff}} \) but \( \delta > \epsilon_{\text{roundoff}} \) where \( \epsilon_{\text{roundoff}} \) denotes the unit roundoff error.

When \( \theta = 1 \), Example 2 coincides with well-known ill-conditioned filtering problem (see, for instance, [2]) and demonstrates how a problem that is well-conditioned, as posed, can be made ill-conditioned by the filter implementation. The difficulty to be explored is in matrix inversion. As can be seen, although \( \text{rank } H = 2 \), the matrix \( R_{\theta,3} \) is singular in machine precision that yields the failure of the conventional KF implementation. We introduced an unknown system parameter \( \theta \) making sure that the same problem is applied to the matrix \( (R_{\theta,k})^{1/2} \) for each value of \( \theta \). Thus, both parts of the method for score evaluation, that are the "filtered" and "differentiated" parts, fail after processing the first measurement. From the discussion above we understand that Example 2 demonstrates the difficulty only for the covariance-type methods.

Our simulation experiments presented below are organized as follows. All methods were implemented in the same precision (64-bit floating-point arithmetic).
floating point) in MatLab where the unit roundoff error is $2^{-53} \approx 1.11 \cdot 10^{-16}$. The MatLab function \( \text{eps} \) is twice the unit roundoff error and \( \delta = \text{eps}^{2/3} \) satisfies the conditions \( \delta^2 < \epsilon_{\text{roundoff}} \) and \( \delta > \epsilon_{\text{roundoff}} \) from Example 2. We provide the computations for different values of \( \delta \), say \( \delta \in [10^{-9}, \text{eps}^{2/3}, 10^9 \text{eps}^{2/3}] \). This means that we consider a set of test problems from Example 2. The unknown system parameter \( \theta \) is fixed, say \( \theta = 2 \). The exact answers are produced by the Symbolic Math Toolbox of MatLab.

**Experiment 1:** In this experiment we are going to use the performance profile technique to compare the conventional KF approach for score evaluation with the square-root algorithm introduced in this paper. The performance profile method was developed by Dolan and Moré [12] to answer a common question in scientific computing: how to compare several competing methods on a set of test problem. Now, it can be found in textbooks (see, for instance, [13]).

In our simulation experiments we consider a set \( A \) of \( n = 2 \) algorithms, mentioned above. The performance measure, \( \tau_a(p) \), is a measure of accuracy. More precisely, \( \tau_a(p) \) is the maximum absolute error in Log LG computed for 7 different values of \( \delta \). Thus, we consider a set \( P \) of \( m = 7 \) test problems from Example 2, \( \delta \in [10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}, 10^{-8}] \). According to the performance profile technique, we compute the performance ratio

\[
r_{p,a} = \frac{\tau_a(p)}{\min\{\tau_a(p) : \sigma \in A\}} \geq 1,
\]

which is the performance of algorithm \( a \) on problem \( p \) divided by the best performance of all the methods (we mean a particular implementation method for score evaluation) on this problem. The performance profile of algorithm \( a \) is the function

\[
\phi_a(\mu) = \frac{1}{m} \times \text{number of } p \in P \text{ such that } r_{p,a} \leq \mu,
\]

which is monotonically increasing. Thus, \( \phi_a(\mu) \) is the probability that the performance of algorithm \( a \) is within a factor \( \mu \) of the best performance over all implementations on the given set of problems.

The results of this experiment are illustrated by Fig. 3. For each method, \( \mu \) is plotted against the performance profile \( \phi_a(\mu) \), for \( \mu \in [0, 3] \). We are now going to explain Fig. 3.

Let us consider the left-hand side of Fig. 3 where \( \mu = 1 \). We can say that the new square-root algorithm proposed in this paper is the most accurate implementation on \( \approx 71\% \) of the problems, with the conventional KF being accurate on \( 30\% \) of the problems. Next, we consider the middle of the plot, looking where the curve first hit probability 1. We conclude that the suggested square-root method is within a factor \( \mu \approx 1.3 \) of being the most accurate implementation on every test problem. However, the conventional KF approach for score evaluation will never manage all 7 problems (as \( \delta \to \epsilon_{\text{roundoff}} \), the machine precision limit, the test problems become ill-conditioned). We need to increase \( \mu \) to \( \approx 2.7 \) to be able to say that for \( \approx 58\% \) of the test problems the conventional KF provides an accurate Log LG evaluation within a factor \( \mu \approx 2.7 \).

Thus, the performance profiles clearly indicate that on the set of the test problems from Example 2 the new square-root algorithm derived in this paper provides more accurate evaluation of the Log LG compared with the conventional KF approach.

**Experiment 2:** In this experiment we use the conventional KF technique and the proposed square-root method to compute the maximum absolute error in Log LF, denoted as \( \Delta \text{LogLF} \), and its gradient, denoted as \( \Delta \text{LogLG} \). The results of this experiment are summarized in Table I. We also present the maximum absolute error among elements in matrices \( P_L \) and \( (P_L)^T \) (denoted as \( \Delta P_L \) and \( \Delta P_L^T \), respectively) to explore the numerical behavior of the "filtered" and "differentiated" parts of the methods for score evaluation.

As can be seen from Table I, the square-root implementation of the Riccati-type sensitivity equation degrades more slowly than the conventional Riccati-type sensitivity recursion as \( \delta \to \epsilon_{\text{roundoff}} \). The machine precision limit (see columns denoted as \( \Delta P_L^T \)). For instance, the "filtered" (columns \( \Delta P_L \)) and "differentiated" (columns \( \Delta P_L^T \)) parts of the proposed square-root method for score evaluation maintain about 7 and 8 digits of accuracy, respectively, at \( \delta = 10^{-9} \). The conventional KF technique provides essentially no correct digits in both computed solutions. Besides, it seems that the roundoff errors tend to accumulate and degrade the accuracies of the Log LF and Log LG faster than the accuracies of \( \Delta P_L \) and \( \Delta P_L^T \). Indeed, for the same \( \delta = 10^{-9} \) we obtain no correct digits in the computed solutions for all methods. In MatLab, the term "NaN" stands for "Not a Number" that actually means the failure of the numerical algorithm.

**Remark 4:** The results of Experiment 2 indicate that the new square-root algorithm provides more accurate computation of the sensitivity matrix \( (P_L)^T \) compared to the conventional KF. Hence, it can be successfully used in all applications where this quantity is required.

### Table I

| Problem conditioning | Conventional KF technique | Suggested square-root method |
|----------------------|---------------------------|-----------------------------|
| \( K(\text{Ric}) \)  | \( \Delta P_L \) \( \Delta P_L^T \) \( \Delta \text{LogLF} \) \( \Delta \text{LogLG} \) | \( \Delta P_L \) \( \Delta P_L^T \) \( \Delta \text{LogLF} \) \( \Delta \text{LogLG} \) |
| \( 10^{-2} \)        | 1.0 \( \times 10^{-13} \) 1.0 \( \times 10^{-10} \) 2.0 \( \times 10^{-13} \) 1.0 \( \times 10^{-13} \) | 4.0 \( \times 10^{-15} \) 7.0 \( \times 10^{-16} \) 1.0 \( \times 10^{-13} \) 9.0 \( \times 10^{-14} \) |
| \( 10^{-4} \)        | 5.0 \( \times 10^{-10} \) 9.0 \( \times 10^{-4} \) 4.0 \( \times 10^{-9} \) 1.0 \( \times 10^{-9} \) | 4.0 \( \times 10^{-13} \) 7.0 \( \times 10^{-14} \) 6.0 \( \times 10^{-10} \) 7.0 \( \times 10^{-10} \) |
| \( 10^{-6} \)        | 2.0 \( \times 10^{-6} \) 2.0 \( \times 10^{-1} \) 2.0 \( \times 10^{-5} \) 6.0 \( \times 10^{-6} \) | 3.0 \( \times 10^{-11} \) 1.0 \( \times 10^{-11} \) 9.0 \( \times 10^{-6} \) 4.0 \( \times 10^{-6} \) |
| \( 10^{-8} \)        | 3.0 \( \times 10^{-3} \) 3.0 \( \times 10^{-1} \) 3.0 \( \times 10^{-1} \) 2.0 \( \times 10^{-2} \) | 3.0 \( \times 10^{-10} \) 2.0 \( \times 10^{-10} \) 2.0 \( \times 10^{-1} \) 9.0 \( \times 10^{-3} \) |
| \( 10^{-9} \)        | 3.0 \( \times 10^{-1} \) NaN NaN NaN NaN | 2.0 \( \times 10^{-8} \) 7.0 \( \times 10^{-9} \) 1.0 \( \times 10^{1} \) 5.0 \( \times 10^{1} \) |

Note: NaN stands for Not a Number.
V. CONCLUDING REMARKS

In this paper, a numerically stable square-root implementation method for KF formulas, the eSRCF, has been extended in order to compute the Log LG for linear discrete-time stochastic systems. The preliminary analysis indicates that the new algorithm for score evaluation provides more accurate computations compared with the conventional KF approach. The new result can be used for efficient calculations in sensitivity analysis and in gradient-search optimization algorithms for the maximum likelihood estimation of unknown system parameters.

As an extension of the eSRCF, the new method for score evaluation is expected to inherit its benefits. However, the question about suitability for parallel implementation is still open.

It can be mentioned that another approach to construct numerically stable implementation method for score evaluation is to use the UD filter [3]. Being the modification of the square-root implementations, the UD-type algorithms improve the robustness of computations against roundoff errors, but compared with SRF, the UD filter reduces the computational cost (see [3], [6], [5]). As mentioned in [10] and as far as this author knows, it is still not known how to use the UD filter to compute the score.

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