A Singular Square Root Filter Algorithm for Large Scale Data Assimilation

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ABSTRACT

For systems with a relatively small order the Kalman filter provides an optimal solution to many data assimilation problems. However, for large scale systems that arise from discretizing partial differential equations, the number of computations and the required storage for the Kalman filter become prohibitive. Also numerical difficulties may arise from propagation of errors, due to finite machine precision computations. Often they result in the violation of the requirement that the error covariance matrix should be positive semi-definite. In this paper we will discuss the Singular Square Root Algorithm (SQRT) to compute a Kalman filter gain for large scale systems, which solves in a reasonable manner the problems mentioned above.

KEY WORDS

Data Assimilation, Kalman Filtering, Large Scale Systems, Square Root Algorithm

1 Introduction

Complex processes can be simulated effectively by systems of discretized partial differential equations describing the conservation laws. The discretized system of equations provides a reasonably accurate forecast of the future dynamical behaviour, provided that the initial state of the system and the boundary conditions are known. But in real applications the complete information defining the state of the system at a specific time is rarely available, moreover, both the models and the measured data contain inaccuracies and random noise. Observations of the system measured over an interval of time can be used in combination with the model equations to derive estimates of the expected values of the physical states. The problem of constructing a state-estimator for these systems can be treated by using feedback design techniques from control theory. For very large nonlinear systems, however, traditional control techniques are not directly applicable and data assimilation schemes are used instead to generate accurate sate-estimates.

Hence, the aim of data assimilation is to incorporate measured observations into a dynamical system model to produce optimal estimates of the current and future state variables of the system.

2 Problem Formulation

A discretized linear PDE can be seen as a linear stochastic model state space representation as follows:

$$x_{k+1} = Ax_k + Bu_k + w_k, \tag{1}$$
$$y_k = Cx_k + v_k. \tag{2}$$

where $A \in R^{n\times n}$, $B \in R^{n\times p}$ and $C \in R^{m\times n}$ with $n \gg m, p$. Additionally we have

$$\begin{aligned} E(w_j w_k^T) &= Q\delta_{jk}, \\ E(v_j v_k^T) &= R\delta_{jk}, \\ E(v_j w_k^T) &= 0, \end{aligned} \tag{3}$$

where $E[.]$ denotes expectation, w_k is a white Gaussian system noise process with zero mean and covariance matrix Q which is introduced to take into account model uncertainties, as well as the white Gaussian measurement noise process v_k with zero mean and covariance matrix R to take into account the measurements uncertainties. The initial state x_0 is assumed to be Gaussian with zero mean and covariance matrix P_0. The initial conditions, the system and measurements noise processes are all assumed to be independent of each other.

Moreover, for data assimilation models the probability density function of the states can be determined based on the history of the measurements $y_1, \ldots, y_k$. For the model (2) it can be shown that this conditional density function is Gaussian. Therefore it is completely characterized by its mean and covariance matrix. Furthermore, for a Gaussian distribution, the mean is an optimal estimate in a maximum likelihood sense, via a least squares estimation.

Having defined the general stochastic state space representation of the model (1) and the measurement relation

(2), it is desired to combine the measurements with the information provided by the model to obtain an optimal estimate of the system states, this problem is called a filtering problem. For solving these kind of problems Kalman filtering can be used. Although Kalman filter gives very good results, it is very hard to compute for large scale systems, due to the fact that it has to

3 Discrete Time Kalman Filtering

Since we have assumed an LTI (Linear Time Invariant) system we can compute the discrete-time Kalman filter as follows:

Consider the following state observer

$$\hat{x}_{k+1|k} = A\hat{x}_{k|k-1} + Bu_k + L_k(y_k - C\hat{x}_{k|k-1}), \quad (4)$$

where $L_k \in R^{n\times m}$ is the Kalman gain, and $\hat{x}_{k|k-1}$ the estimate for x_k based on observation up to time $k-1$. Combining equation (4) with (1) and (2) leads to the estimator error equation

$$\begin{aligned} \tilde{x}_{k+1|k} & \quad x_{k+1} - \hat{x}_{k+1|k} & (5) \\ &= (A - L_kC)\tilde{x}_{k|k-1} - L_kv_k + w_k. & (6) \end{aligned}$$

It is well known that the Kalman gain L_k minimizes the state error covariance matrix

$$P_{k+1} = E[(\tilde{x}_{k+1|k} - E[\tilde{x}_{k+1|k}]])(\tilde{x}_{k+1|k}... - E[\tilde{x}_{k+1|k}])^T]. \quad (7)$$

Hence, the optimal estimator matrix L_k or Kalman filter gain can be obtained by minimizing

$$L_k = \min_{L_k} \alpha^T P_{k+1}\alpha. \quad (8)$$

As a result, the discrete-time Kalman filter gain is given by

$$L_k = AP_kC^T(R + CP_kC^T)^{-1}, \quad (9)$$

with the error covariance update equation

$$P_{k+1} = AP_kA^T + Q - AP_kC^T(R + CP_kC^T)^{-1}CP_kA^T, \quad (10)$$

which is a Discrete Riccati Difference Equation (DRDE). Now, it can be shown that if the system is observable, and $k \to \infty$, the matrix P_k converges to a steady-state positive semidefinite matrix P, and L_k approaches a constant matrix L, given by

$$L = APC^T(R + CPC^T)^{-1}, \quad (11)$$

and P satisfies the Discrete Algebraic Riccati Equation (DARE)

$$P = APA^T + Q - APC^T(R + CPC^T)^{-1}CPA^T. \quad (12)$$

4 Discrete Riccati Difference Equation (DRDE)

The DRDE equation (10) has to be solved in order to find the Kalman filter gain L_k. This DRDE has several equivalent formulations. In this paper the square root form of the DRDE formulation is used to solve the DRDE more efficiently and accurately, and a two point boundary value problem formulation is used to study the convergence of the algorithm.

In order to derive the square root form of the DRDE, first we note that the Schur complement of (10) (with respect to the (1,1) block) is the matrix:

$$M = \begin{pmatrix} R + CP_KC^T & CP_KA^T \\ AP_KC^T & AP_kA^T + Q \end{pmatrix}. \quad (13)$$

From this one easily derives a factorized form of the Kalman filter algorithm [4]. It is assumed that the Cholesky factorizations of the positive semi-definite matrices R, Q and P_k are given:

$$R \doteq L_RL_R^T, \quad Q \doteq L_QL_Q^T, \quad P_k \doteq S_kS_k^T. \quad (14)$$

M is easily factorized in:

$$M = \begin{pmatrix} L_R & CS_k & 0 \\ 0 & AS_k & L_Q \end{pmatrix} \cdot \begin{pmatrix} L_R^T & 0 \\ S_k^TC^T & S_k^TA^T \\ 0 & L_Q^T \end{pmatrix}. \quad (15)$$

Finally, the so-called square root form of the Riccati difference iteration is obtained from a lower triangular reduction or QR decomposition of the left factor (see [4] for details):

$$\begin{pmatrix} L_R & CS_k & 0 \\ 0 & AS_k & L_Q \end{pmatrix} \cdot U_k = \begin{pmatrix} \hat{F}_k & 0 & 0 \\ \hat{K}_k & S_{k+1} & 0 \end{pmatrix}, \quad (16)$$

where U_k is orthogonal. It will be assumed in this paper that $R > 0$, which implies that $\hat{R}_k \doteq R + C^TP_kC > 0$ as well. As a consequence, a square root factorization of M is obtained as:

$$M = \begin{pmatrix} \hat{F}_k & 0 \\ \hat{K}_k & S_{k+1} \end{pmatrix} \cdot \begin{pmatrix} \hat{F}_k^T & \hat{K}_k^T \\ 0 & S_{k+1}^T \end{pmatrix}, \quad (17)$$

from which it follows that $P_{k+1} = S_{k+1}S_{k+1}^T$. Notice that this holds even if P_{k+1} is not full rank.

Another formulation of equation (10) follows from the underlying two point boundary value problem [1]:

$$\begin{pmatrix} A^T & 0 \\ -Q & I \end{pmatrix} \begin{pmatrix} X_{k+1} \\ Y_{k+1} \end{pmatrix} = \begin{pmatrix} I_n & C^TR^{-1}C \\ 0 & A^T \end{pmatrix} \begin{pmatrix} X_k \\ Y_k \end{pmatrix}, \quad (18)$$

where $P_k = Y_kX_k^{-1}$ implies $P_{k+1} = Y_{k+1}X_{k+1}^{-1}$ and vice versa (this implies that both X_k and X_{k+1} must be invertible).

Hence, the convergence of the DRDE is a subspace iteration as in

$$\begin{pmatrix} X_{k+1} \\ Y_{k+1} \end{pmatrix} = M_1^{-1} M_2 \begin{pmatrix} X_k \\ Y_k \end{pmatrix}, \tag{19}$$

with

$$M_1 = \begin{pmatrix} A^T & 0 \\ -Q & I \end{pmatrix}, \quad M_2 = \begin{pmatrix} I_n & C^T R^{-1} C \\ 0 & A \end{pmatrix}, \tag{20}$$

with M_1 invertible.
Let λ_k be an eigenvalue of $M_1^{-1}M_2$ and assume they are ordered by decreasing magnitude $|\lambda_k|$. If $|\lambda_n|$ is strictly larger than $|\lambda_{n+1}|$ then this recurrence is known to converge for almost all initial conditions X_0, Y_0, to the so-called dominant invariant subspace of $M_1^{-1}M_2$ (power method see details in [2]). If, on the other hand, $|\lambda_n| = |\lambda_{n+1}|$ then the iteration almost never converges: there exist fixed points but they correspond to very special initial conditions [2]. It turns out that $M_1^{-1}M_2$ is simplectic and therefore has a special eigenvalue pattern: the eigenvalues which are not on the unit circle come in pairs that are mirror images of each other with respect to the unit circle. Therefore the condition $|\lambda_n| > |\lambda_{n+1}|$ is satisfied iff $M_1^{-1}M_2$ has no eigenvalues on the unit circle. This assumption is made in the rest of the paper. This is a classical assumption in the DRE literature since it is closely linked to the existence of stabilizing solutions of the corresponding feedback problem [2]. (for more details on DRDE convergence, we refer to [7]).

Finally, the following theorem has to be fulfilled to guarantee the existence of a stabilizing solution P_k of the DRDE.

Theorem [6]
A stabilizing solution P_k of the DRDE exists and is unique if and only if either of the following two conditions is satisfied

1. (A, C) is detectable and (A, Q) has no unobservable eigenvalue on the unit circle

2. (A, C) is detectable and the pencil $\lambda M_1 - M_2$ has no generalized eigenvalue on the unit circle.

From this consideration, it is clear that the calculation of the Kalman filter gain is prohibitive for large scale system, Therefore we will introduce an algorithm that we call SSQRTKF Singular Square Root Kalman Filter, which is able to compute a sort of suboptimal Kalman filter gain very efficiently, assuming the covariance process noise $Q = 0$, as will be shown below. Afterwards, the well known Reduced Rank Square Root algorithm (RRSQRT) [5] will be introduced and compared to SSQRTKF and Kalman filtering.

5 SSQRT Kalman Filter (SSQRTKF) algorithm

The Singular Square Root algorithm (SSQRT) of this paper is based on the DRDE with $Q = 0$ which implies that the variance of the process noise is zero. In the previous section we showed that the DRDE equation converges under very mild conditions to the stabilizing solution P_k, providing that the corresponding pencil $\lambda M_1 - M2$ has no unit circle eigenvalues. For $Q = 0$ this pencil has a spectrum that is the union of the spectrum of A and that of A^{-1} since

$$\lambda M_1 - M_2 = \lambda \begin{pmatrix} A^T & 0 \\ 0 & I_n \end{pmatrix} - \begin{pmatrix} I_n & C^T R^{-1} C \\ 0 & A \end{pmatrix}. \tag{21}$$

is a upper block triangular.
Therefore the suboptimal Kalman filter gain L_{ks} generated in the limit moves the eigenvalues of A, $\lambda > 1$ to their unit circle mirror images, $1/\lambda$ and leaves the eigenvalues $\lambda < 1$ unchanged. As a special case of the square root form of DRDE, the QR decomposition of (16)

$$\begin{pmatrix} L_R & CS_k \\ 0 & AS_k \end{pmatrix} U_k = \begin{pmatrix} \hat{F}_k & 0 \\ \hat{K}_k & S_{k+1} \end{pmatrix}, \tag{22}$$

where U_k is orthogonal and the dimension of S_k is $n \times l$, the same as S_0, with $l \geq \#\{|\lambda(A)| > 1\}$ Note that the QR decomposition is computed for a small matrix with size $(p + l) \times p$ making it very cheap to compute. On the other hand the Kalman filter gain can be computed at any time from $\hat{F}_k$ and $\hat{K}_k$ as follows:

$$L_k = \hat{K}_k \hat{F}_k^{-1}, \tag{23}$$

provided that F_k is invertible. But we have to take into account that the matrix F_k is diagonally dominant as a result of the QR decomoposition, therefore instead of inverting F_k, we just need to invert its diagonal elements, making even cheaper the computations.

Moreover, if A and C are sparse, the construction of the left factor in the left hand side of equation (22) is cheap as well, because of the matrix multiplication of A and C with S_k (see [6]).

6 Reduced Rank Square Root Filter (RRSQRT) [5]

In the RRSQRT algorithm the square root factors are based on an eigendecomposition. Let $P_{k|k} = V_k \Lambda_k V_k^T$ be the eigendecomposition of the error covariance matrix $P_{k|k}$, then $S_{k|k} = V_k \Lambda_k^{1/2}$ is a square root factor of $P_{k|k}$. The error covariance matrix is now approximated by using q leading eigenvalues only. If the eigenvalues are ordered, i.e. $\lambda_1 \geq \ldots \geq \lambda_n \geq 0$, then the approximation can be accomplished by truncating after the first q columns of the square root factor $S_{k|k}$ The three main steps are the "time-step" the "reduction-step" and the "measurement-step".

a. Time-step: The "time-step" performs the time propagation of the state estimate and error covariance and are equivalent to the Kalman filter equations, hence

$$\begin{aligned} \hat{x}_{k+1|k} &= A\hat{x}_{k|k-1} + Bu_k + L_k(y_k - \hat{(y)}_{k|k)} \\ S_{k|k} &= [AS_{k|k-1}\ BQ^{1/2}], \end{aligned} \quad (24)$$

where $S_{k|k}$ is the $n \times q$ estimate square root of the error covariance $P_{k|k}$.

b. Reduction-step: The addition of rows, $BQ^{1/2}$ in equation (24), for the system noise every time-step would quickly increase the computation time. Therefore the number of columns is reduced to q after every "time-step". The idea for this approximation is to use only the first q leading eigenvalues and eigenvectors of the error covariance matrix $S_{k|k}S_{k|k}^T$. In order to compute this efficiently, first the eigendecomposition of the matrix $S_{k|k}^T S_{k|k}$ is determined:

$$S_{k|k}^T S_{k|k} = V_k \Lambda_k V_k^T. \quad (25)$$

It can easily be shown that

$$(S_{k|k} V_k \Lambda_k^{-1/2}) \Lambda_k (S_{k|k} V_k \Lambda_k^{-1/2})^T \quad (26)$$

is the eigendecomposition of $S_{k|k}S_{k|k}^T$ and thus

$$S_{k|k}^* = [S_{k|k} V_k]_{1:n,1:q} \quad (27)$$

is the square root of the optimal rank q approximation of $S_{k|k}S_{k|k}^T$.

The above procedure is much faster than eigenvalue computations on the matrix $S_{k|k}S_{k|k}^T$ or singular value computations on $S_{k|k}$, which could also accomplish the task of reduction. This is caused by the fact that the matrix $S_{k|k}^T S_{k|k}$ is a $q+m$ by $q+m$ matrix and $q, m \ll n$.

c. Measurement-step: The measurements update for scalar measurements $p = 1$ is given by

$$\begin{aligned} H_k &= S_{k|k}^{*T} C^T \\ \gamma_k &= (H_k^T H_k + R)^{-1} \\ L_{k+1} &= S_{k|k}^* H_k \gamma_k \\ S_{k+1|k} &= S_{k|k}^* - L_{k+1} H_k^T [1 + (\gamma_k R)^{1/2}]^{-1}, \end{aligned} \quad (28)$$

with L_{k+1} the approximated (suboptimal) Kalman filter gain. If there is more than one measurement, these can be processed one at a time.

The number of computations required in the time propagation of the error in the covariance, which is a major fraction of the total number, is reduced by a factor n/q with respect to the original Kalman filter algorithm. It can be shown that for $q = n$ the RRSQRT algorithm is exact in the sense that it is equivalent to the Kalman filter equations. The parameter q controls the accuracy of the approximation. The price for greater accuracy is as always a larger computational burden.

7 SSQRTKF in Data Assimilation

In this section, the performance of the SSQRTKF algorithm will be compared to the Kalman and RRSQRT filtering algorithms in a data assimilation problem.

The SSQRTKF algorithm described in section (5) is an approach to compute the suboptimal Kalman filter gain L_{ks} such that,

$$\lambda(A - L_{ks}C) = \begin{pmatrix} |\lambda(A)| < 1 & 0 \\ 0 & \frac{1}{|\lambda(A)| > 1} \end{pmatrix}$$

This guarantees that the state estimation will converge. Moreover, this estimator is optimal -in the sense of least squares- for the case when the covariance matrix Q is zero.

On the other hand, the matrix A of a discretized PDE system (equation (1)) is stable in most of the cases, therefore, in order to compute the Kalman filter gain with the SSQRT algorithm, the discretized PDE system has to be manipulated such that the most dominant eigenvalues will be located outside the unit circle, as is required for the SSQRTKF algorithm in order to obtain a good performance of the filter. This can be done by scaling the matrix A by A/r if there exists a $r < 1$ such that the number of eigenvalues of A with absolute value not less than r is very small. This scaling value r can be used as a filter design parameter, in addition, it is used to accelerate both the stabilization and convergence of the SSQRTKF algorithm.

As an example, a heat transfer system in an finite insulated bar will be taken. The PDE which describes such a system [3] is given by

$$\frac{\partial T(t,x)}{\partial t} = \alpha \frac{\partial^2 T(t,x)}{\partial x^2} + u(x,t), \quad (29)$$

where $T(x,t)$, $u(x,t)$, and α are the temperature distribution, the heat input, and the heat transfer coefficient of the bar, respectively. In this example the PDE is discretized using finite differences, with the bart length $L = 1m$, and $\alpha = 1 \times 10^{-4} W/^oCm^2$, with the following boundary and initial conditions

$$T(x,0) = 0, \;\; T(0,t) = 150e^{-t/5000}+30, \;\; u(L,t) = 100,$$

and the heat input

$$u(x,t) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-x_0(t))^2}{2\sigma^2}} \tag{30}$$

where $x_0(t)$ is the mean value that changes with time, and $\sigma = 0.07$ the standard deviation. The system is discretized in 101 points equally spaced by $\Delta x = 0.01$ for $0 < x < 1$, with a sampling time $\Delta_t = 0.36 sec$, this in order to keep the discretized system stable. For simulation purposes it is assumed that the inputs and outputs are measured in the same points p_i as shown is figure (1). Here we show how the A matrix looks like

$$A = \begin{pmatrix} 1-2z & z & 0 & 0 & \dots & 0 \\ z & 1-2z & z & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & z & 1-2z \end{pmatrix}, \tag{31}$$

with $z = \alpha\Delta t/\Delta x^2$, where we have to assure $z \leq 1/2$ to keep the system stable.

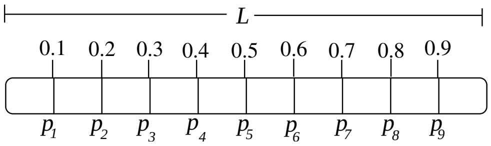

Figure 1. Measurement points on the insulated bar.

In figure (2) we see how the eigenvalues of A are scaled by $r = max|\lambda(A)|/1.06$, and a comparison between the resulting eigenvalues of the $(A-L_kC)$ matrix to the $(A-L_{ks}C)$ matrix, where L_k gain matrix is the optimal Kalman filter gain, and L_{ks} is the suboptimal SSQRTKF filter gain, figure (3) is a zoom into the most dominant eigenvalues. General speaking, the smallest eigenvalues of the A, $(A - L_kC)$, and $(A - L_{ks}C)$ matrices are quite equal, while the biggest eigenvalues are the most affected as is expected, due to the fact that these are the dominant ones.

Figure (3) shows a comparison between the previous eigenvalues and the ones of the $(A - L_{kr}C)$ matrix resulting from the RRSQRT filter.

Another important feature of the SSQRTKF algorithm is its low computation cost as can be seen in table (1) below,

	Kalman Filter	RRSQRT	SSQRTKF
flops	$6n^3 + (8m+1)n^2$	$2n^2q$	$2n^2l$

Table 1. Comparison of the computation complexity between Kalman filter, RRSQRT filter, and SSQRTKF algorithm for $n \gg m, l, q, p$.

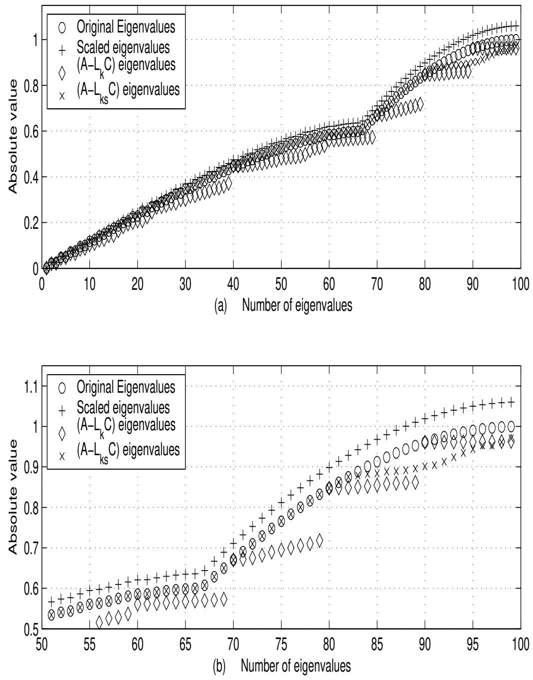

Figure 2. Figure (a) shows how the eigenvalues of A are scaled by $r = max|\lambda(A)|/1.06$, and a comparison between the eigenvalues of the $(A-L_kC)$ to the $(A-L_{ks}C)$, where L_k is the optimal Kalman filter gain, and L_{ks} is the suboptimal SSQRTKF Kalman filter gain. Observe that the smallest eigenvalues are no moved, while the most dominant eigenvalues change in all the cases. In figure (b) a zoom into the area of the most dominant eigenvalues is done.

Furthermore, the performance of the SSQRTKF filter is quite close to the others as shown below in figures (4), and (5). Figure (4) shows a comparison between the RMSE of the three algorithm and how they converge to zero. The remaining bias error is due to the fact that the boundary conditions are not estimated correctly because the system is not sampled in that area. Finally, figure (5) shows a comparison between the real output to the Kalman Filtering, RRSQRT, and SSQRTKF estimations.

8 Conclusions

In this paper a new algorithm to compute a suboptimal Kalman filter (SSQRTKF) has been introduced. This algorithm has shown to be very cheap to compute compare to other algorithms of the same structure, RRSQRT for instance. It has been tested and compared with the optimal Kalman filtering as well as the suboptimal RRSQRT filtering with excellent results in performance. As a result, SSQRTKF algorithm suits very well to Data Assimilation problems because of its low computation cost and good estimation performance.

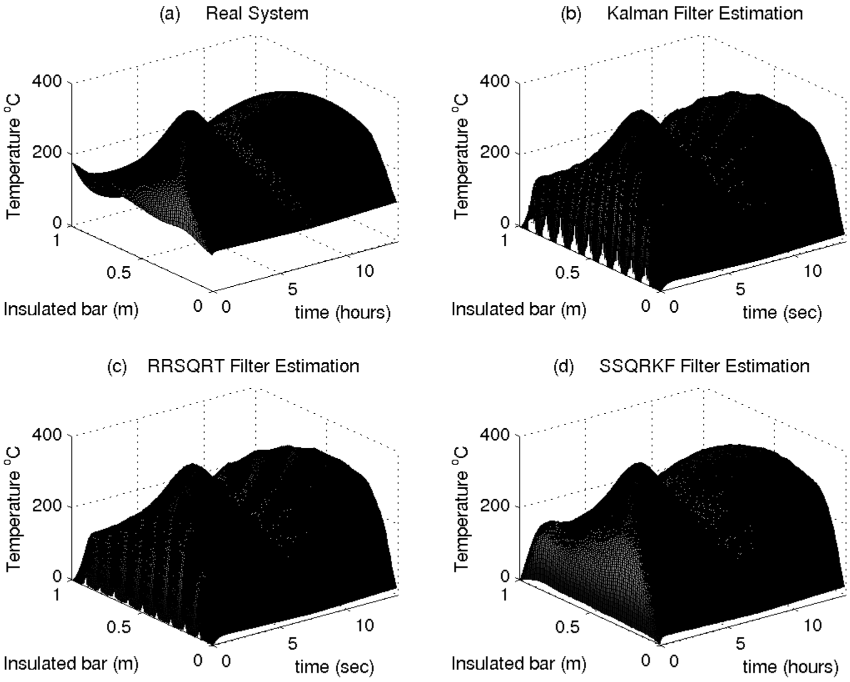

Figure 5. comparison between the real output to the Kalman Filtering, RRSQRT, and SSQRTKF estimations.

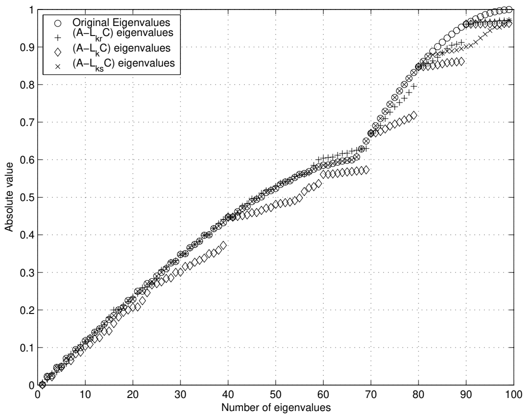

Figure 3. Comparison between the eigenvalues of the $(A - L_kC)$, $(A - L_{ks}C)$, $(A - L_{kr}C)$. Here can be seen that the most dominant eigenvalues are the ones which are most affected by the filter gains.

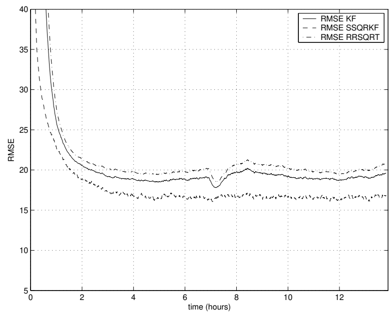

Figure 4. Comparison of performance between Kalman Filtering, RRSQRT, and SSQRTKF algorithms based on the RMSE (Root Mean Square Error). Here is observed that SSQRTKF performance is as good as Kalman Filtering and RRSQRT

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