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Reduced-rank unscented Kalman filtering using Cholesky-based decomposition

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We consider a reduced-rank square-root unscented Kalman filter based on the Cholesky decomposition of the state-error covariance. The performance of this filter is compared with an analogous filter based on the singular value decomposition. We evaluate the performance of these filters for illustrative linear and non-linear systems.

Keywords: data assimilation; reduced-rank Kalman filter; nonlinear state estimation

1. Introduction

Data assimilation for large-scale systems has gained increasing attention due to non-linear and computationally intensive applications such as weather forecasting (Evensen 2006; Lewis, Lakshmivarahan and Dhall 2006). These problems require algorithms that are computationally tractable despite the enormous dimension of the state. Reduced-order variants of the classical Kalman filter have been developed for computationally demanding applications (Ballabrera-Poy, Busalacchi and Murtugudde 2001; Farrell and Ioannou 2001; Fieguth, Menemenlis and Fukumori 2003; Scherliess, Schunk, Sojka and Thompson 2004), where the classical Kalman filter gain and covariance are modified so as to reduce the computational requirements. A comparison of several techniques is given in Kim, Chandrasekar, Palanthandalam-Madapusi, Ridley and Bernstein (2007).

An alternative technique for reducing the computational requirements of data assimilation for high-dimensional systems is the reduced-rank filter (Verlaan and Heemink 1997; Treebushny and Madsen 2003; Gillijns, Bernstein and Moor 2006). In this method, the error-covariance matrix is factored to obtain a square root, whose rank is then reduced through truncation. The truncated square root is then propagated by the data assimilation algorithm. This technique is closely related to classical decomposition techniques (Morf and Kailath 1975; Bierman 2006), which provide numerical stability and computational efficiency. Factorisation-and-truncation methods have direct application to the problem of generating a reduced ensemble for use in particle filter methods (Anderson 2001; Heemink, Verlaan and Segers 2001).

The primary technique for truncating the error-covariance matrix is the singular value decomposition (SVD), wherein the singular values are used to determine the entries of the error covariance matrix that are most relevant to the accuracy of the state estimates (Verlaan and Heemink 1997; Treebushny and Madsen 2003; Gillijns et al. 2006). Despite the intuitively appealing nature of this approach, the optimality of approximation based on the SVD within the context of recursive state estimation is not guaranteed. The difficulty is due to the fact that optimal approximation depends on the dynamics and measurement maps in addition to the components of the error covariance.

In related work, Chandrasekar, Kim, Bernstein and Ridley (2008) observed that the Kalman filter estimate update depends on the product C_kP_k, where C_k is the measurement map and P_k is the error covariance. Consequently, the approximation technique developed in Chandrasekar et al. (2008) focuses on C_kP_k rather than P_k alone. In particular, it is shown in Chandrasekar et al. (2008) that approximation of C_kP_k leads directly to truncation based on the Cholesky decomposition. Unlike the SVD, however, the Cholesky decomposition does not possess a natural measure of magnitude that is analogous to singular values. Nevertheless, filter reduction based on the Cholesky decomposition provides state-estimation accuracy that is competitive with, and in many cases superior to, that of the SVD. Specifically, examples show that, in special cases, the accuracy of the Cholesky-decomposition-based reduced-rank filter is typically equal to the accuracy of the full-rank filter,

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whereas the SVD-based reduced-rank filter provides arbitrarily poor accuracy.

An additional advantage of using the Cholesky decomposition in place of the SVD for reduced-rank filtering is the fact that the Cholesky decomposition is computationally less expensive than the SVD, specifically, $O(n^3/6)$ versus $O(2n^3)$ (Stewart 1998), and thus an asymptotic computational advantage over SVD by a factor of 12. Furthermore, the entire matrix need not be factored; instead, by arranging the states so that those states that contribute directly to the measurement correspond to the left-most columns of the lower triangular square root, only the leading submatrix of the error covariance must be factored, yielding yet further savings over the SVD. Once the decomposition is performed, the algorithm effectively retains only the initial 'tall' columns of the full Cholesky decomposition and truncates the 'short' columns.

To assimilate data in non-linear systems, particle filters are used to propagate a collection of state estimates from which statistics can be computed. These techniques include the ensemble Kalman filter (EnKF) (Whitaker and Hamill 2002; Evenson 2003), which uses a stochastic construction, as well as the unscented Kalman filter (UKF) (Julier, Uhlmann and Durrant-Whyte 2000; Wan and van der Merwe 2001; Ristic, Arulampalam and Gordon 2004), which deterministically constructs the collection of state estimates by perturbing the nominal state estimate. Specifically, UKF constructs the ensemble members by using the columns of the square root of the error covariance to perturb the nominal state estimate. For a model of order n, the n columns and their negatives (see (5)) result in $2n+1$ ensemble members and thus $2n+1$ model updates.

A straightforward approach to reducing the UKF ensemble size is to use a factorisation-and-truncation method to truncate $n-q$ columns of the square root of the error covariance and construct the ensemble members using the remaining q columns. In Anderson (2001), Heemink et al. (2001) and Tippett, Anderson, Bishop, Hamill and Whitaker (2003), SVD-based decomposition-and-truncation is used to construct reduced-rank approximations of the square root of the error covariance, which are then used to construct the ensemble members resulting in an ensemble of size $2q+1$.

In this paper, we use the Cholesky-based decomposition technique developed in Chandrasekar et al. (2008) to construct the reduced-ensemble members. Specifically, we use the Cholesky decomposition to obtain a square root of the error covariance and select columns of the Cholesky factor to approximate C_kP_k. The retained columns of the Cholesky factor are used to construct the ensemble members. We compare the performance of the Cholesky-decomposition-based reduced-rank UKF and the SVD-based reduced-rank UKF on a linear advection model and a non-linear system with chaotic dynamics.

2. The unscented Kalman filter

We consider the discrete-time system with non-linear dynamics

$$x_{k+1} = f(x_k, u_k, k) + w_k \tag{1}$$

and linearly dependent measurements

$$y_k = C_k x_k + v_k, \tag{2}$$

where $x_k, w_k \in \mathbb{R}^n$, $u_k \in \mathbb{R}^m$, and $y_k, v_k \in \mathbb{R}^p$. The input u_k and output y_k are assumed to be measured, and w_k and v_k are uncorrelated zero-mean white noise processes with covariances Q_k and R_k, respectively. We assume that R_k is positive definite. The objective is to estimate the state x_k using the measurements y_k. When the dynamics (1) are linear, the Kalman filter provides estimates that minimise the mean-square-error (MSE) in the state estimates (Anderson and Moore 2005). However, for non-linear dynamics, we approximate the state error covariance using ensembles that are constructed deterministically according to UKF. The starting point for UKF is a set of sample points, that is, a collection of state estimates that capture the probability distribution of the state (Julier et al. 2000; Wan and van der Merwe 2001; Ristic et al. 2004).

Let $x \in \mathbb{R}^n$, and let $P \in \mathbb{R}^{n\times n}$ be positive semidefinite. The unscented transformation provides $2n+1$ ensembles $X_i \in \mathbb{R}^n$ and corresponding weights $\gamma_i \in \mathbb{R}$, for $0 = 1, \ldots, 2n$, such that the weighted mean and weighted variance of the ensembles are x and P, respectively. Specifically, let $S \in \mathbb{R}^{n\times n}$ satisfy

$$SS^{\mathrm{T}} = P, \tag{3}$$

and, for all $i = 1, \ldots, n$, let $\mathrm{col}_i(S)$ denote the ith column of S. For $\alpha > 0$, the unscented transformation $X = \Psi(x, S, \alpha) \in \mathbb{R}^{n\times(2n+1)}$ of x with covariance $P = SS^{\mathrm{T}}$ is defined by

$$X \triangleq \begin{bmatrix} X_0 & \cdots & X_{2n} \end{bmatrix}, \tag{4}$$

where

$$X_i \triangleq \begin{cases} x, & i = 0, \\ x + \sqrt{\alpha}\,\mathrm{col}_i(S), & i = 1, \ldots, n, \\ x - \sqrt{\alpha}\,\mathrm{col}_{i-n}(S), & i = n+1, \ldots, 2n. \end{cases} \tag{5}$$

The parameter α determines the spread of the ensembles around x. Next, define the weights $\gamma_i \in \mathbb{R}$ by

$$\gamma_0 \triangleq \frac{\alpha - n}{\alpha}, \quad \gamma_i \triangleq \frac{1}{2\alpha}, \quad i = 1, \ldots, 2n. \tag{6}$$

Then,

$$\sum_{i=0}^{2n} \gamma_i X_i = x, \quad \sum_{i=0}^{2n} \gamma_i (X_i - x)(X_i - x)^{\mathrm{T}} = P. \tag{7}$$

UKF uses the unscented transformation to approximate the error covariance and estimate the state x_k. Letting x_0^{f} denote an initial estimate of x_0 with error covariance P_0^{f}, the data assimilation and forecast estimate, x_k^{da} and x_k^{f}, respectively, from UKF are given by the following steps.

UKF data assimilation step:

$$x_k^{\mathrm{da}} = x_k^{\mathrm{f}} + K_k(y_k - y_k^{\mathrm{f}}), \tag{8}$$

$$y_k^{\mathrm{f}} = C_k x_k^{\mathrm{f}}, \tag{9}$$

$$X_k^{\mathrm{da}} = \Psi(x_k^{\mathrm{da}}, S_k^{\mathrm{da}}, \alpha) = \begin{bmatrix} X_{0,k}^{\mathrm{da}} & \cdots & X_{2n,k}^{\mathrm{da}} \end{bmatrix}, \tag{10}$$

$$S_k^{\mathrm{da}} = S_k^{\mathrm{f}} H_k^{\mathrm{f}}, \tag{11}$$

$$K_k = P_k^{\mathrm{f}} C_k^{\mathrm{T}} (C_k P_k^{\mathrm{f}} C_k^{\mathrm{T}} + R_k)^{-1}, \tag{12}$$

where $H_k^{\mathrm{f}} \in \mathbb{R}^{n \times n}$ satisfies

$$H_k^{\mathrm{f}} (H_k^{\mathrm{f}})^{\mathrm{T}} = I_n - (C_k S_k^{\mathrm{f}})^{\mathrm{T}} [C_k S_k^{\mathrm{f}} (C_k S_k^{\mathrm{f}})^{\mathrm{T}} + R_k]^{-1} C_k S_k^{\mathrm{f}} \tag{13}$$

and $S_k^{\mathrm{f}} \in \mathbb{R}^{n \times n}$ satisfies

$$S_k^{\mathrm{f}} (S_k^{\mathrm{f}})^{\mathrm{T}} = P_k^{\mathrm{f}}. \tag{14}$$

UKF forecast step:

$$X_{i,k+1}^{\mathrm{f}} = f(X_{i,k}^{\mathrm{da}}, u_k, k), \quad i = 0, \ldots, 2n, \tag{15}$$

$$x_{k+1}^{\mathrm{f}} = \sum_{i=0}^{2n} \gamma_i X_{i,k+1}^{\mathrm{f}}, \tag{16}$$

$$P_{k+1}^{\mathrm{f}} = \sum_{i=0}^{2n} \gamma_i (X_{i,k+1}^{\mathrm{f}} - x_{k+1}^{\mathrm{f}})(X_{i,k+1}^{\mathrm{f}} - x_{k+1}^{\mathrm{f}})^{\mathrm{T}} + Q_k. \tag{17}$$

In traditional notation, the data assimilation estimate x_k^{da} is denoted by $x_{k|k}$ to indicate that $x_{k|k}$ is the estimate of x_k obtained by using measurements $y_0, \ldots, y_k$, while the optimal forecast x_k^{f} is denoted by $x_{k|k-1}$ to indicate that $x_{k|k-1}$ is the estimate of x_k obtained by using measurements $y_0, \ldots, y_{k-1}$. The notation x_k^{f} and x_k^{da} is motivated by the data assimilation literature (Scherliess et al. 2004).

When the dynamics in (1) are linear, UKF is equivalent to the Kalman filter (Julier et al. 2000). Define $P_k^{\mathrm{da}} \in \mathbb{R}^{n \times n}$ by

$$P_k^{\mathrm{da}} \triangleq S_k^{\mathrm{da}} (S_k^{\mathrm{da}})^{\mathrm{T}}. \tag{18}$$

In the linear case, P_k^{da} and P_k^{f} are the covariances of the error $x_k - x_k^{\mathrm{da}}$ and $x_k - x_k^{\mathrm{f}}$, respectively. However, in the non-linear case, P_k^{da} and P_k^{f} are pseudo-error covariances and not the covariances of the error $x_k - x_k^{\mathrm{da}}$ and $x_k - x_k^{\mathrm{f}}$, respectively. The case in which the process noise w_k in (1) enters non-linearly is discussed in Wan and van der Merwe (2001), while the case in which the measurements depend non-linearly on the state is discussed in Ristic et al. (2004). Furthermore, although variations of UKF that use fewer ensembles exist (Julier and Uhlmann 2002), the spread of the ensemble members of Julier and Uhlmann (2002) cannot be scaled, and hence some components of the ensemble state may not satisfy physical constraints, for example, states modelling density have to be positive.

Note that H_k^{f} and S_k^{f} satisfying (13) and (14) are not unique. For example, either the SVD or Cholesky decomposition can be used. Moreover, all square H_k^{f} and S_k^{f} satisfying (13) and (14) are related by an orthogonal transformation. Specifically, the following result is given in Bernstein (2005, p. 188).

Lemma 1: *Let $S, \hat{S} \in \mathbb{R}^{n \times n}$. Then, $SS^{\mathrm{T}} = \hat{S}\hat{S}^{\mathrm{T}}$ if and only if there exists an orthogonal matrix $U \in \mathbb{R}^{n \times n}$ such that $\hat{\mathrm{S}} = SU$.*

UKF uses a symmetric positive-negative pairing of the ensemble. Specifically, (5) and (15) imply that, for all $i = 1, \ldots, n$,

$$X_{i,k}^{\mathrm{da}} - x_k^{\mathrm{da}} = -(X_{n+1-i,k}^{\mathrm{da}} - x_k^{\mathrm{da}}), \tag{19}$$

and hence

$$\sum_{i=0}^{2n} \gamma_i X_{i,k}^{\mathrm{da}} = x_k^{\mathrm{da}}. \tag{20}$$

Alternatively, if $\sum_{i=1}^{n} \mathrm{col}_i(S_k^{\mathrm{da}}) = 0$, it can be shown using (5) and (10) that a variation of UKF can be constructed using only $n+1$ ensemble members instead of $2n+1$ without any performance degradation. In Tippett et al. (2003), this ensemble reduction is achieved by choosing H_k^{f} such that $\sum_{i=1}^{n} \mathrm{col}_i(S_k^{\mathrm{f}} H_k^{\mathrm{f}}) = 0$ whenever $\sum_{i=1}^{n} \mathrm{col}_i(S_k^{\mathrm{f}}) = 0$, and since $S_k^{\mathrm{da}} = S_k^{\mathrm{f}} H_k^{\mathrm{f}}$, $\sum_{i=1}^{n} \mathrm{col}_i(S_k^{\mathrm{da}}) = 0$. However, in UKF, $\sum_{i=1}^{n} \mathrm{col}_i(S_k^{\mathrm{f}})$ is not necessarily equal to

zero for all $k \geq 0$, and therefore UKF uses $2n+1$ ensemble members. Finally, for linear dynamics, the performance of UKF is independent of the choice of H_k^{f} and S_k^{f}. However, for non-linear dynamics, the performance of UKF depends on the choice of H_k^{f} and S_k^{f}. The performance of ensemble-based filters for various choices of H_k^{f} is compared in Tippett et al. (2003).

3. Reduced-ensemble unscented Kalman filter

It follows from (15) that UKF involves $2n+1$ model updates, and hence the computational burden of UKF is of the order $(2n+1)n^2 \approx 2n^3$. To define an unscented transformation for a reduced ensemble, let $x \in \mathbb{R}^n$ and $S \in \mathbb{R}^{n \times q}$, where $0 < q \leq n$. The rank-q unscented transformation $X = \Psi_q(x, S, \alpha) \in \mathbb{R}^{n \times (2q+1)}$ of x with covariance $P = SS^{\mathrm{T}}$ is defined by

$$X \triangleq \begin{bmatrix} X_0 & \cdots & X_{2q} \end{bmatrix}, \tag{21}$$

where

$$X_i \triangleq \begin{cases} x, & i = 0, \\ x + \sqrt{\alpha}\,\mathrm{col}_i(S), & i = 1, \ldots, q, \\ x - \sqrt{\alpha}\,\mathrm{col}_{i-q}(S), & i = q+1, \ldots, 2q. \end{cases} \tag{22}$$

Also, defining the weights

$$\gamma_{q,0} \triangleq \frac{\alpha - q}{\alpha}, \quad \gamma_{q,i} \triangleq \frac{1}{2\alpha}, \quad i = i, \ldots, 2q \tag{23}$$

it follows that

$$\sum_{i=0}^{2q} \gamma_{q,i} X_i = x, \quad \sum_{i=0}^{2q} \gamma_{q,i} (X_i - x)(X_i - x)^{\mathrm{T}} = SS^{\mathrm{T}} = P. \tag{24}$$

Next, we show that if the covariance matrix has rank q, then the unscented transformation and rank-q unscented transformation are equivalent. This result is an immediate consequence of (5) and (22).

Lemma 2: *Let $x \in \mathbb{R}^n$, let $P \in \mathbb{R}^{n \times n}$ be positive semidefinite with $\mathrm{rank}(P) \leq q \leq n$, and define $S \triangleq [\hat{S}\, 0_{n \times (n-q)}]$, where $\hat{S} \in \mathbb{R}^{n \times q}$ satisfies $\hat{S}\hat{S}^{\mathrm{T}} = P$. Then $X = \Psi(x, S, \alpha) = [X_0 \quad \cdots \quad X_{2n}]$ satisfies*

$$X_i = x, \quad i = 0, q+1, \ldots, n, n+q+1, \ldots, 2n. \tag{25}$$

Furthermore, $\hat{X} = \Psi_q(x, \hat{S}, \alpha) = \begin{bmatrix} \hat{X}_0 & \cdots & \hat{X}_{2q} \end{bmatrix}$ satisfies

$$\hat{X}_i = \begin{cases} X_i, & i = 0, \ldots, q, \\ X_{n-q+i}, & i = q+1, \ldots, 2q. \end{cases} \tag{26}$$

Proof: Since

$$\mathrm{col}_i(S) = \begin{cases} \mathrm{col}_i(\hat{S}), & \text{if } i = 1, \ldots, q, \\ 0, & \text{if } i = q+1, \ldots, n, \end{cases} \tag{27}$$

(5) and (22) imply (25) and (26), respectively. □

Lemma 3: *Let $P_k^{\mathrm{f}} \in \mathbb{R}^{n \times n}$ be positive semidefinite and let P_k^{da} be given by* (18). *Assume that* $\mathrm{rank}(P_k^{\mathrm{f}}) \leq q \leq n$. *Then*, $\mathrm{rank}(P_k^{\mathrm{da}}) \leq q$.

Proof: See Appendix 1. □

Hence, if P_k^{f} is rank deficient, then P_k^{da} is also rank deficient. The following result shows that the ensemble size can be reduced from $2n+1$ to $2q+1$ without performance degradation whenever $\mathrm{rank}(P_k^{\mathrm{f}}) = q$.

Proposition 1: *Assume* $\mathrm{rank}(P_k^{\mathrm{f}}) \leq q \leq n$, *and define $S_k^{\mathrm{da}} \triangleq [\hat{S}_k^{\mathrm{da}}\, 0_{n \times (n-q)}]$, where $\hat{S}_k^{\mathrm{da}} \in \mathbb{R}^{n \times q}$ satisfies $\hat{S}_k^{\mathrm{da}} (\hat{S}_k^{\mathrm{da}})^{\mathrm{T}} = P_k^{\mathrm{da}}$. Furthermore, define $\hat{X}_k^{\mathrm{da}} \triangleq \Psi_q(x_k^{\mathrm{da}}, \hat{S}_k^{\mathrm{da}}, \alpha) = [\hat{X}_{0,k}^{\mathrm{da}} \quad \cdots \quad \hat{X}_{2q,k}^{\mathrm{da}}]$, and let $\hat{x}_{k+1}^{\mathrm{f}} \in \mathbb{R}^n$ and $\hat{P}_{k+1}^{\mathrm{f}} \in \mathbb{R}^{n \times n}$ be given by*

$$\hat{x}_{k+1}^{\mathrm{f}} = \sum_{i=0}^{2q} \gamma_{q,i} \hat{X}_{i,k+1}^{\mathrm{f}}, \tag{28}$$

$$\hat{P}_{k+1}^{\mathrm{f}} = \sum_{i=0}^{2q} \gamma_{q,i} (\hat{X}_{i,k+1}^{\mathrm{f}} - \hat{x}_{k+1}^{\mathrm{f}})(\hat{X}_{i,k+1}^{\mathrm{f}} - \hat{x}_{k+1}^{\mathrm{f}})^{\mathrm{T}} + Q_k, \tag{29}$$

where $\hat{X}_{i,k+1}^{\mathrm{f}} \in \mathbb{R}^n$ is given by

$$\hat{X}_{i,k+1}^{\mathrm{f}} = f(\hat{X}_{i,k}^{\mathrm{da}}, u_k, k), \quad i = 0, \ldots, 2q. \tag{30}$$

Then, $\hat{x}_{k+1}^{\mathrm{f}} = x_{k+1}^{\mathrm{f}}$ and $\hat{P}_{k+1}^{\mathrm{f}} = P_{k+1}^{\mathrm{f}}$.

Proof: See Appendix 1. □

Hence, when $\mathrm{rank}(P_k^{\mathrm{f}}) = q < n$, the ensemble size can be reduced from $2n+1$ to $2q+1$, and thus, using the rank-q unscented transformation instead of the unscented transformation (10), does not degrade the performance of UKF. However, when P_k^{f} has full rank, P_k^{da} generally has full rank. In the following sections, we thus construct rank-q approximations of the pseudo-error covariances and perform estimation using the rank-q unscented transformation based on a square root of the low-rank approximation of the pseudo-error covariance.

4. SVD-based reduced-rank unscented Kalman filter

To reduce the ensemble size, we use a reduced-rank approximation $\hat{P}_{\mathrm{s},k}^{\mathrm{f}}$ of $P_{\mathrm{s},k}^{\mathrm{f}}$. The reduced-rank approximations are chosen such that $\|\hat{P}_{\mathrm{s},k}^{\mathrm{f}} - P_{\mathrm{s},k}^{\mathrm{f}}\|_{\mathrm{F}}$ is minimised subject to $\mathrm{rank}(\hat{P}_{\mathrm{s},k}^{\mathrm{f}}) = q$, where $\|\cdot\|_{\mathrm{F}}$ denotes the

Frobenius norm. Let $P \in \mathbb{R}^{n\times n}$ be positive semidefinite, let $\sigma_1 \geq \cdots \geq \sigma_n \geq 0$ be the singular values of P, and let $u_1, \ldots, u_n \in \mathbb{R}^n$ be the corresponding mutually orthogonal singular vectors. Next, define $U_q \in \mathbb{R}^{n\times q}$ and $\Sigma_q \in \mathbb{R}^{q\times q}$ by

$$U_q \triangleq \begin{bmatrix} u_1 & \cdots & u_q \end{bmatrix}, \quad \Sigma_q \triangleq \operatorname{diag}(\sigma_1, \ldots, \sigma_q). \tag{31}$$

With this notation, the singular value decomposition of P is given by

$$P = U_n \Sigma_n U_n^{\mathrm{T}}, \tag{32}$$

where $U_n \in \mathbb{R}^{n\times n}$ is orthogonal. For $q \leq n$, let $\Phi_{\mathrm{SVD}}(P, q) \in \mathbb{R}^{n\times q}$ denote the SVD-based rank-q approximation of the square root $U_n \Sigma_n^{1/2}$ of P given by

$$\Phi_{\mathrm{SVD}}(P, q) \triangleq U_q \Sigma_q^{1/2}. \tag{33}$$

As noted in Bernstein (2005), $\hat{P} = SS^{\mathrm{T}}$, where $S \triangleq \Phi_{\mathrm{SVD}}(P, q)$, is the best rank-$q$ approximation of P with respect to the Frobenius norm.

Next, we use the SVD at each time step to obtain a reduced-rank approximation of the pseudo-error covariance, and thus a reduced ensemble size. The SVD-based reduced-rank square-root unscented Kalman filter (SVDRRUKF) is given by the following steps.

SVDRRUKF data assimilation step:

$$x_{\mathrm{s},k}^{\mathrm{da}} = x_{\mathrm{s},k}^{\mathrm{f}} + K_{\mathrm{s},k}(y_k - y_{\mathrm{s},k}^{\mathrm{f}}), \tag{34}$$

$$y_{\mathrm{s},k}^{\mathrm{f}} = C_k x_{\mathrm{s},k}^{\mathrm{f}}, \tag{35}$$

$$X_{\mathrm{s},k}^{\mathrm{da}} = \Psi_q(x_{\mathrm{s},k}^{\mathrm{da}}, S_{\mathrm{s},k}^{\mathrm{da}}, \alpha) = \begin{bmatrix} X_{\mathrm{s},0,k}^{\mathrm{da}} & \cdots & X_{\mathrm{s},2q,k}^{\mathrm{da}} \end{bmatrix}, \tag{36}$$

$$S_{\mathrm{s},k}^{\mathrm{da}} = S_{\mathrm{s},k}^{\mathrm{f}} H_{\mathrm{s},k}^{\mathrm{f}}, \tag{37}$$

$$K_{\mathrm{s},k} = S_{\mathrm{s},k}^{\mathrm{f}} (C_k S_{\mathrm{s},k}^{\mathrm{f}})^{\mathrm{T}} [C_k S_{\mathrm{s},k}^{\mathrm{f}} (C_k S_{\mathrm{s},k}^{\mathrm{f}})^{\mathrm{T}} + R_k]^{-1}, \tag{38}$$

where $H_{\mathrm{s},k}^{\mathrm{f}} \in \mathbb{R}^{q\times q}$ satisfies

$$H_{\mathrm{s},k}^{\mathrm{f}} (H_{\mathrm{s},k}^{\mathrm{f}})^{\mathrm{T}} = I_q - (C_k S_{\mathrm{s},k}^{\mathrm{f}})^{\mathrm{T}} [C_k S_{\mathrm{s},k}^{\mathrm{f}} (C_k S_{\mathrm{s},k}^{\mathrm{f}})^{\mathrm{T}} + R_k]^{-1} C_k S_{\mathrm{s},k}^{\mathrm{f}}. \tag{39}$$

SVDRRUKF forecast step:

$$X_{\mathrm{s},i,k+1}^{\mathrm{f}} = f(X_{\mathrm{s},i,k}^{\mathrm{da}}, u_k, k), \quad i = 0, \ldots, 2q, \tag{40}$$

$$x_{\mathrm{s},k+1}^{\mathrm{f}} = \sum_{i=0}^{2q} \gamma_{q,i} X_{\mathrm{s},i,k+1}^{\mathrm{f}}, \tag{41}$$

$$P_{\mathrm{s},k+1}^{\mathrm{f}} = \sum_{i=0}^{2q} \gamma_{q,i} (X_{\mathrm{s},i,k+1}^{\mathrm{f}} - x_{\mathrm{s},k+1}^{\mathrm{f}})(X_{\mathrm{s},i,k+1}^{\mathrm{f}} - x_{\mathrm{s},k+1}^{\mathrm{f}})^{\mathrm{T}} + Q_k, \tag{42}$$

$$S_{\mathrm{s},k+1}^{\mathrm{f}} = \Phi_{\mathrm{SVD}}(P_{\mathrm{s},k+1}^{\mathrm{f}}, q). \tag{43}$$

Next, define $\hat{P}_{\mathrm{s},k}^{\mathrm{f}}, \hat{P}_{\mathrm{s},k}^{\mathrm{da}} \in \mathbb{R}^{n\times n}$ by

$$\hat{P}_{\mathrm{s},k}^{\mathrm{da}} \triangleq S_{\mathrm{s},k}^{\mathrm{f}} - (S_{\mathrm{s},k}^{\mathrm{f}})^{\mathrm{T}}, \quad \hat{P}_{\mathrm{s},k}^{\mathrm{da}} \triangleq S_{\mathrm{s},k}^{\mathrm{da}} (S_{\mathrm{s},k}^{\mathrm{da}})^{\mathrm{T}}. \tag{44}$$

It then follows from (37) and (39) that

$$\hat{P}_{\mathrm{s},k}^{\mathrm{da}} = \hat{P}_{\mathrm{s},k}^{\mathrm{f}} - \hat{P}_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} (C_k \hat{P}_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} + R_k)^{-1} C_k \hat{P}_{\mathrm{s},k}^{\mathrm{f}}. \tag{45}$$

Furthermore, (38) and (15) imply that

$$K_{\mathrm{s},k} = \hat{P}_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} (C_k \hat{P}_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} + R_k)^{-1}. \tag{46}$$

Finally, define $P_{\mathrm{s},k}^{\mathrm{da}} \in \mathbb{R}^{n\times n}$ by

$$P_{\mathrm{s},k}^{\mathrm{da}} \triangleq P_{\mathrm{s},k}^{\mathrm{f}} - P_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} (C_k P_{\mathrm{s},k}^{\mathrm{f}} C_k^{\mathrm{T}} + R_k)^{-1} C_k P_{\mathrm{s},k}^{\mathrm{f}}. \tag{47}$$

Since $\operatorname{rank}(S_{\mathrm{s},k}^{\mathrm{f}}) \leq q$, it follows from (45) that $\operatorname{rank}(\hat{P}_{\mathrm{s},k}^{\mathrm{f}}) \leq q$. Moreover, since $\operatorname{rank}(H_{\mathrm{s},k}^{\mathrm{f}}) \leq q$, (37) implies that $\operatorname{rank}(S_{\mathrm{s},k}^{\mathrm{da}}) \leq q$, and therefore (45) implies that $\operatorname{rank}(\hat{P}_{\mathrm{s},k}^{\mathrm{da}}) \leq q$. Hence, it follows from (46) that the filter gain $K_{\mathrm{s},k}$ depends on $\hat{P}_{\mathrm{s},k}^{\mathrm{f}}$, which is a reduced-rank approximation of $P_{\mathrm{s},k}^{\mathrm{f}}$, while the ensemble $X_{\mathrm{s},k}^{\mathrm{da}}$ depends on $\hat{P}_{\mathrm{s},k}^{\mathrm{da}}$, which is a reduced-rank approximation of $P_{\mathrm{s},k}^{\mathrm{da}}$. Also, as shown in § 2, the matrix $H_{\mathrm{s},k}^{\mathrm{f}}$ satisfying (39) is not unique.

5. Cholesky-decomposition-based reduced-rank unscented Kalman filter

The filter gain K_k of UKF depends on a particular subspace of the forecast error covariance P_k^{f}. Specifically, K_k depends only on the correlation $C_k P_k^{\mathrm{f}}$ between the error in the measured states and unmeasured states. Since $\operatorname{rank}(C_k) = p$, there exists a state space basis with respect to which C_k has the form

$$C_k = \begin{bmatrix} I_p & 0 \end{bmatrix}. \tag{48}$$

Condition (48) is easily satisfied by spatially distributed systems discretised by finite volume methods (see § 6 and 7) when the measurements are confined to a localised region. The following result is given in Chandrasekar et al. (2008).

Lemma 4: *Partition* P_k^{f} *as*

$$P_k^{\mathrm{f}} = \begin{bmatrix} P_{p,k}^{\mathrm{f}} & (P_{\bar{p}p,k}^{\mathrm{f}})^{\mathrm{T}} \\ P_{\bar{p}p,k}^{\mathrm{f}} & P_{\bar{p},k}^{\mathrm{f}} \end{bmatrix}, \tag{49}$$

where $P_{p,k}^{\mathrm{f}} \in \mathbb{R}^{p\times p}$ *and* $P_{\bar{p},k}^{\mathrm{f}} \in \mathbb{R}^{\bar{p}\times\bar{p}}$, *and assume that* C_k *has the form* (48). *Then*,

$$K_k = \begin{bmatrix} P_{p,k}^{\mathrm{f}} \\ (P_{\bar{p}p,k}^{\mathrm{f}})^{\mathrm{T}} \end{bmatrix} (P_{p,k}^{\mathrm{f}} + R_k)^{-1}. \tag{50}$$

To reduce the ensemble size, we construct a filter that uses a reduced-rank approximation $\hat{P}^{\mathrm{f}}_{\mathrm{c},k}$ of $P^{\mathrm{f}}_{\mathrm{c},k}$ such that $\mathrm{rank}(\hat{P}^{\mathrm{f}}_{\mathrm{c},k}) < n$ and $\|C_k(\hat{P}^{\mathrm{f}}_{\mathrm{c},k} - P^{\mathrm{f}}_{\mathrm{c},k})\|_{\mathrm{F}}$ is minimised. To obtain $\hat{P}^{\mathrm{f}}_{\mathrm{c},k}$, we perform a Cholesky decomposition of the pseudo-error covariance $P^{\mathrm{f}}_{\mathrm{c},k}$ at each time step. Assuming that $P \in \mathbb{R}^{n\times n}$ is positive definite, the Cholesky decomposition of P yields a unique lower triangular Cholesky factor $L \in \mathbb{R}^{n\times n}$ satisfying

$$LL^{\mathrm{T}} = P. \tag{51}$$

Truncating the last $n-q$ columns of $L = [L_1 \quad \dots \quad L_n]$ yields the rank-q Cholesky factor

$$\Phi_{\mathrm{CHOL}}(P,q) \triangleq \begin{bmatrix} L_1 & \cdots & L_q \end{bmatrix} \in \mathbb{R}^{n\times q}. \tag{52}$$

The following result is given in Chandrasekar et al. (2008).

Lemma 5: *Let $P \in \mathbb{R}^{n\times n}$ be positive definite, define $S \triangleq \Phi_{\mathrm{CHOL}}(P,q)$, where $0 \le q \le n$, and partition P and $\hat{P} \triangleq SS^{\mathrm{T}}$ as*

$$P = \begin{bmatrix} P_q & P_{q\bar{q}} \\ (P_{q\bar{q}})^{\mathrm{T}} & P_{\bar{q}} \end{bmatrix}, \quad \hat{P} = \begin{bmatrix} \hat{P}_q & \hat{P}_{q\bar{q}} \\ (\hat{P}_{q\bar{q}})^{\mathrm{T}} & \hat{P}_{\bar{q}} \end{bmatrix}, \tag{53}$$

where $P_q, \hat{P}_q \in \mathbb{R}^{q\times q}$ and $P_{\bar{q}}, \hat{P}_{\bar{q}} \in \mathbb{R}^{\bar{q}\times\bar{q}}$. Then,

$$\begin{bmatrix} \hat{P}_q & \hat{P}_{q\bar{q}} \end{bmatrix} = \begin{bmatrix} P_q & P_{q\bar{q}} \end{bmatrix}. \tag{54}$$

Lemma 5 implies that, if $S = \Phi_{\mathrm{CHOL}}(P,q)$, then the first q columns and rows of SS^{T} and P are equal. Thus, the reduced rank matrix $\hat{P}$ exactly captures a critical portion of P. This result motivates the propagation of a reduced-rank approximation of the pseudo-error covariance using the Cholesky decomposition at each time step, thus reducing the ensemble size. The Cholesky-decomposition-based reduced-rank unscented Kalman filter (CDRRUKF) is summarised as follows.

CDRRUKF data assimilation step:

$$x^{\mathrm{da}}_{\mathrm{c},k} = x^{\mathrm{f}}_{\mathrm{c},k} + K_{\mathrm{c},k}(y_k - y^{\mathrm{f}}_{\mathrm{c},k}), \tag{55}$$

$$y^{\mathrm{f}}_{\mathrm{c},k} = C_k x^{\mathrm{f}}_{\mathrm{c},k}, \tag{56}$$

$$X^{\mathrm{da}}_{\mathrm{c},k} = \Psi_q(x^{\mathrm{da}}_{\mathrm{c},k}, S^{\mathrm{da}}_{\mathrm{c},k}, \alpha), \tag{57}$$

$$S^{\mathrm{da}}_{\mathrm{c},k} = S^{\mathrm{f}}_{\mathrm{c},k} H^{\mathrm{f}}_{\mathrm{c},k}, \tag{58}$$

$$K_{\mathrm{c},k} = S^{\mathrm{f}}_{\mathrm{c},k}(C_k S^{\mathrm{f}}_{\mathrm{c},k})^{\mathrm{T}}[C_k S^{\mathrm{f}}_{\mathrm{c},k}(C_k S^{\mathrm{f}}_{\mathrm{c},k})^{\mathrm{T}} + R_k]^{-1}, \tag{59}$$

where $H^{\mathrm{f}}_{\mathrm{c},k} \in \mathbb{R}^{q\times q}$ satisfies

$$H^{\mathrm{f}}_{\mathrm{c},k}(H^{\mathrm{f}}_{\mathrm{c},k})^{\mathrm{T}} = I_q - (C_k S^{\mathrm{f}}_{\mathrm{c},k})^{\mathrm{T}} \times [C_k S^{\mathrm{f}}_{\mathrm{c},k}(C_k S^{\mathrm{f}}_{\mathrm{c},k})^{\mathrm{T}} + R_k]^{-1} C_k S^{\mathrm{f}}_{\mathrm{c},k}. \tag{60}$$

CDRRUKF forecast step:

$$X^{\mathrm{f}}_{\mathrm{c},i,k+1} = f(X^{\mathrm{da}}_{\mathrm{c},i,k}, u_k, k), \quad i = 0, \dots, 2q \tag{61}$$

$$x^{\mathrm{f}}_{k+1} = \sum_{i=0}^{2q} \gamma_{q,i} X^{\mathrm{f}}_{\mathrm{c},i,k+1}, \tag{62}$$

$$P^{\mathrm{f}}_{\mathrm{c},k+1} = \sum_{i=0}^{2q} \gamma_{q,i}(X^{\mathrm{f}}_{\mathrm{c},i,k+1} - x^{\mathrm{f}}_{\mathrm{c},k+1})(X^{\mathrm{f}}_{\mathrm{c},i,k+1} - x^{\mathrm{f}}_{\mathrm{c},k+1})^{\mathrm{T}} + Q_k, \tag{63}$$

$$S^{\mathrm{f}}_{\mathrm{c},k+1} = \Phi_{\mathrm{CHOL}}(P^{\mathrm{f}}_{\mathrm{c},k+1}, q). \tag{64}$$

It follows from (51), (52), and (64) that the $n\times n$ pseudo-error covariance matrix $P^{\mathrm{f}}_{\mathrm{c},k}$ is constructed at every time-step. Alternatively, partition $P^{\mathrm{f}}_{\mathrm{c},k}$ as

$$P^{\mathrm{f}}_{\mathrm{c},k} = \begin{bmatrix} P^{\mathrm{f}}_{\mathrm{c},k,q} & P^{\mathrm{f}}_{\mathrm{c},k,q\bar{q}} \\ (P^{\mathrm{f}}_{\mathrm{c},k,q\bar{q}})^{\mathrm{T}} & P^{\mathrm{f}}_{\mathrm{c},k,\bar{q}} \end{bmatrix}, \tag{65}$$

where $P^{\mathrm{f}}_{\mathrm{c},k,q} \in \mathbb{R}^{q\times q}$. Furthermore, partition $S^{\mathrm{f}}_{\mathrm{c},k}$ as

$$S^{\mathrm{f}}_{\mathrm{c},k} = \begin{bmatrix} S^{\mathrm{f}}_{\mathrm{c},k,q} \\ S^{\mathrm{f}}_{\mathrm{c},k,\bar{q}} \end{bmatrix}, \tag{66}$$

where $S^{\mathrm{f}}_{\mathrm{c},k,q} \in \mathbb{R}^{q\times q}$. It follows from Lemma 5 that

$$S^{\mathrm{f}}_{\mathrm{c},k,q}(S^{\mathrm{f}}_{\mathrm{c},k,q})^{\mathrm{T}} = P^{\mathrm{f}}_{\mathrm{c},k,q}, \quad S^{\mathrm{f}}_{\mathrm{c},k,\bar{q}} = \begin{bmatrix} \left(S^{\mathrm{f}}_{\mathrm{c},k,q}\right)^{-1} & P^{\mathrm{f}}_{\mathrm{c},k,q\bar{q}} \end{bmatrix}^{\mathrm{T}}. \tag{67}$$

Hence, $S^{\mathrm{f}}_{\mathrm{c},k,q} = \Phi_{\mathrm{CHOL}}(P^{\mathrm{f}}_{\mathrm{c},k,q}, q)$, and therefore (67) implies that only the $n \times q$ submatrix $[P^{\mathrm{f}}_{\mathrm{c},k,q} \;\; P^{\mathrm{f}}_{\mathrm{c},k,q\bar{q}}]^{\mathrm{T}}$ needs to be constructed at every time-step.

Next, define $\hat{P}^{\mathrm{da}}_{\mathrm{c},k}, \hat{P}^{\mathrm{f}}_{\mathrm{c},k} \in \mathbb{R}^{n\times n}$ by

$$\begin{aligned} \hat{P}^{\mathrm{da}}_{\mathrm{c},k} &\triangleq \hat{P}^{\mathrm{f}}_{\mathrm{c},k} - \hat{P}^{\mathrm{f}}_{\mathrm{c},k} C_k^{\mathrm{T}}(C_k \hat{P}^{\mathrm{f}}_{\mathrm{c},k} C_k^{\mathrm{T}} + R_k)^{-1} C_k \hat{P}^{\mathrm{f}}_{\mathrm{c},k}, \\ \hat{P}^{\mathrm{f}}_{\mathrm{c},k} &\triangleq S^{\mathrm{f}}_{\mathrm{c},k}(S^{\mathrm{f}}_{\mathrm{c},k})^{\mathrm{T}}. \end{aligned} \tag{68}$$

It then follows from (58) that $S^{\mathrm{da}}_{\mathrm{c},k}(S^{\mathrm{da}}_{\mathrm{c},k})^{\mathrm{T}} = \hat{P}^{\mathrm{da}}_{\mathrm{c},k}$. Furthermore, (59) and (68) imply that

$$K_{\mathrm{c},k} = \hat{P}^{\mathrm{f}}_{\mathrm{c},k} C_k^{\mathrm{T}}(C_k \hat{P}^{\mathrm{f}}_{\mathrm{c},k} C_k^{\mathrm{T}} + R_k)^{-1}. \tag{69}$$

Hence, like the estimator gain $K_{\mathrm{s},k}$ of SVDRRUKF given by (46), the estimator gain $K_{\mathrm{c},k}$ of CDRRUKF given by (69) depends on a reduced-rank approximation $\hat{P}^{\mathrm{f}}_{\mathrm{c},k}$ of the pseudo-error covariance $P^{\mathrm{f}}_{\mathrm{c},k}$. As discussed in § 2, the matrix $H^{\mathrm{f}}_{\mathrm{c},k}$ satisfying (39) is not unique. Due to the rank-reduction step (64), CDRRUKF is generally not equivalent to UKF. However, we now discuss cases in which the performance of CDRRUKF is close to that of UKF.

5.1 *Basis selection for CDRRUKF*

The following result given in Chandrasekar et al. (2008) shows that the CDRRUKF gain $K_{c,k}$ is identical to the UKF gain K_k for a single time step when C_k has the form (48).

Proposition 2: *Assume that $p \leq n$, $q = p$, and C_k has the structure in* (48). *Let $P_k^f \in \mathbb{R}^{n\times n}$ be positive semidefinite and let K_k be given by* (12). *Furthermore, define $S_{c,k}^f \triangleq \Phi_{CHOL}(P_k^f, q)$ and let $\hat{P}_{c,k}^f$ be given by* (68). *Then, $C_k \hat{P}_{c,k}^f = C_k P_k^f$ and hence, $K_{c,k} = K_k$. Finally, if $x_{c,k}^f = x_k^f$, then $x_{c,k}^{da} = x_k^{da}$.*

If the dynamics (1) are linear and time-invariant, that is, for all $k \geq 0$,

$$x_{k+1} = Ax_k + Bu_k + w_k, \tag{70}$$

$$y_k = Cx_k + v_k, \tag{71}$$

then a basis for the state x can be chosen so that the CDRRUKF gain $K_{c,k}$ is identical to the UKF gain K_k for $r > 0$ time steps, where r is the largest integer not exceeding n/p. To construct such a basis, we define the observability matrix $\mathcal{O}(A, C) \in \mathbb{R}^{pn\times n}$ by

$$\mathcal{O}(A, C) \triangleq \begin{bmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{bmatrix}. \tag{72}$$

The following result is given in Chandrasekar et al. (2008).

Proposition 3: *Assume that $\mathcal{O}(A, C)$ has the form*

$$\mathcal{O}(A, C) = \begin{bmatrix} I_n \\ 0_{(p-1)n\times n} \end{bmatrix}. \tag{73}$$

Let $r = \lfloor n/p \rfloor$, where $\lfloor m \rfloor$ denotes the smallest integer not greater than m, and let $q = pr$. Furthermore, assume that $P_{c,0}^f = P_0^f$. Then, for all $k = 0, \ldots, r$, $K_{c,k} = K_k$. If, in addition, $x_{c,0}^f = x_0^f$, then for all $k = 0, \ldots, r$, $x_{c,k}^f = x_k^f$.

Note that, if (A, C) is observable, then there exists a state space basis with respect to which the observability matrix has the form (73) (see Bernstein (2005). If $u_k = w_k = v_k = 0$, for all $k \geq 0$, then (70)–(72) imply that, for all $k \geq 0$,

$$\begin{bmatrix} y_k \\ \vdots \\ y_{k+n-1} \end{bmatrix} = \mathcal{O}(A, C)x_k. \tag{74}$$

Let x_k have entries

$$x_k = \begin{bmatrix} x_{1,k} & \cdots & x_{n,k} \end{bmatrix}^{\mathrm{T}}. \tag{75}$$

If $\mathcal{O}(A, C)$ has the form (73), then (74) implies that, for every integer $l \geq 0$ such that $pl \leq n$,

$$\begin{bmatrix} y_k \\ \vdots \\ y_{k+l-1} \end{bmatrix} = \begin{bmatrix} x_{1,k} \\ \vdots \\ x_{pl,k} \end{bmatrix}. \tag{76}$$

Therefore, the measurements from time step k to $k+l-1$ depend on only the value of the first pl components of the state vector x_k at time step k.

Next, we consider the non-linear system (1) and assume that the dynamics (1) can be expressed as

$$\begin{aligned} x_{i,k+1} &= f_i(x_{\phi_L(i,b)}, \ldots, x_{\phi_R(i,b)}, u_k, k) + w_{i,k}, \\ &\quad i = 1, \ldots, n, \end{aligned} \tag{77}$$

where $b > 0$ and

$$\phi_L(i, b) \triangleq \max(1, i - b), \quad \phi_R(i, b) \triangleq \min(n, i + b). \tag{78}$$

For example, in systems modelled by finite volume schemes, the next value of a physical variable in a given cell depends only on the present values of the physical variables in the neighbouring cells.

Next, let y_k denote a measurement of a specific component of the state, so that

$$y_k = x_{j,k} + v_k, \tag{79}$$

where $j \in \{1, \ldots, n\}$ and $l > 0$ is an integer such that, $j - lb \geq 1$ and $j + lb \leq n$. It follows from (77) and (79) that, if $w_k = v_k = 0$, for all $k \geq 0$, then

$$\begin{bmatrix} y_k \\ \vdots \\ y_{k+l-1} \end{bmatrix} = \begin{bmatrix} g_1(x_{j-b,k}, \ldots, x_{j+b,k}, u_k, k) \\ \vdots \\ g_r(x_{j-lb,k}, \ldots, x_{j+lb,k}, u_k, k) \end{bmatrix}. \tag{80}$$

Hence, (80) can be expressed as

$$\begin{bmatrix} y_k \\ \vdots \\ y_{k+l-1} \end{bmatrix} = g(x_{j-lb,k}, \ldots, x_{j+lb,k}, u_k, k). \tag{81}$$

Now define $\tilde{x}_k \in \mathbb{R}^n$ by

$$\tilde{x}_k = \begin{bmatrix} x_{j,k} & x_{j-1,k} & x_{j+1,k} & x_{j-2,k} & x_{j+2,k} & \cdots \end{bmatrix}. \tag{82}$$

Then, (81) implies that $y_k, \ldots, y_{k+l-1}$ depends on only the first $2lb$ components of the state vector $\tilde{x}_k$ at time step k. Hence, a state space basis can be chosen such

that the outputs $y_k, \ldots, y_{k+l-1}$ depend on only the first few components of the state vector.

6. Linear advection model

Consider a linear advection model (Evensen 2006) with n cells, and let $x_{i,k}$ be the energy in the ith cell at time k. The energy flow satisfies

$$x_{i,k+1} = \begin{cases} x_{i-1,k} & \text{if } i = 2, \ldots, n, \\ x_{n,k} & \text{if } i = 1. \end{cases} \tag{83}$$

Hence, energy in the ith cell flows to the $(i+1)$th cell, while the periodic boundary condition ensures that the energy circulates continually. We choose $n = 100$ and assume that the disturbance w_k enters selected cells, where $w_k \in \mathbb{R}^n$ is a white noise process with covariance $Q_k = Q$ for all $k \geq 0$, and $Q \in \mathbb{R}^{n \times n}$ is diagonal with entries

$$Q_{i,i} = \begin{cases} 1 & \text{if } i \in \{10, 20, \ldots, 100\}, \\ 0 & \text{else.} \end{cases} \tag{84}$$

It follows from (83) that the energy flow can be expressed as

$$x_{k+1} = Ax_k + w_k, \tag{85}$$

where $A \in \mathbb{R}^{n \times n}$ has entries

$$A_{i,j} = \begin{cases} 1 & \text{if } j = i - 1 \text{ for } i = 2, \ldots, n, \\ 1 & \text{if } (i,j) = (1,n), \\ 0 & \text{else.} \end{cases} \tag{86}$$

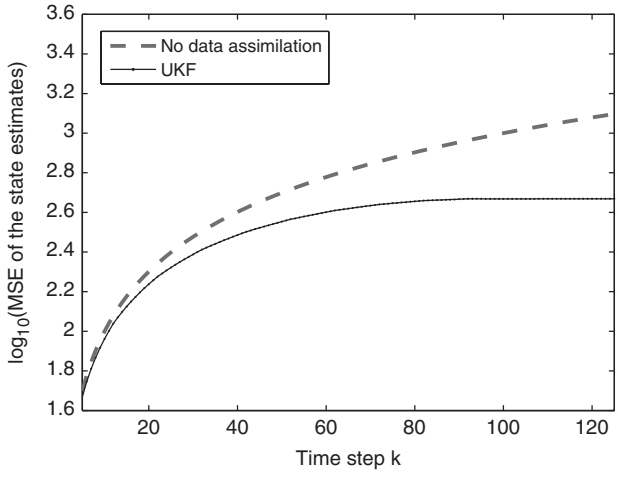

Figure 1. MSE of the state estimates obtained from UKF. Since the dynamics are linear, UKF is equivalent to the Kalman filter. The MSE of state estimates based on data-free simulation, that is, from (1) with $w_k = 0$ for all $k \geq 0$, is shown for comparison.

Note that the eigenvalues of A are simple and lie on the unit circle, and hence (85) is Lyapunov stable but not asymptotically stable. Next, we assume that measurements of the energy in cells 50 and 51 are available so that

$$y_k = \begin{bmatrix} x_{50,k} \\ x_{51,k} \end{bmatrix} + v_k, \tag{87}$$

where v_k is white noise process with covariance $R_k = 0.1I_2$. Note that (87) can be expressed as (2).

First, we use the measurements y_k to estimate the energy in the remaining cells using UKF. In all three cases, the initial estimates $x_0^{\mathrm{f}}, x_{\mathrm{s},0}^{\mathrm{f}}$, and $x_{\mathrm{c},0}^{\mathrm{f}}$ are not equal to the initial state x_0. Moreover, we choose $P_0^{\mathrm{f}} = P_{\mathrm{s},0}^{\mathrm{f}} = P_{\mathrm{c},0}^{\mathrm{f}} = 0.1I_n$. Finally, we choose $\alpha = 0.6$ for all three filters. Note that, since the dynamics in (83) are linear, UKF is equivalent to the Kalman filter and hence UKF provides optimal estimates of the state x_k that minimise the MSE. The MSE of state estimates from UKF is shown in Figure 1. The MSE based on data-free simulation, that is, estimates from (1) with $w_k = 0$, that is,

$$x_{k+1}^{\mathrm{f}} = f(x_k^{\mathrm{f}}, u_k, k), \tag{88}$$

is shown for comparison.

Next, as shown in Figures 2 and 3, data assimilation is performed using SVDRRUKF and CDRRUKF for several values of q between 5 and 100. Note that SVDRRUKF and CDRRUKF use $2q+1$ ensemble members, whereas UKF uses $2n+1$ ensemble members. It can be seen that the performance

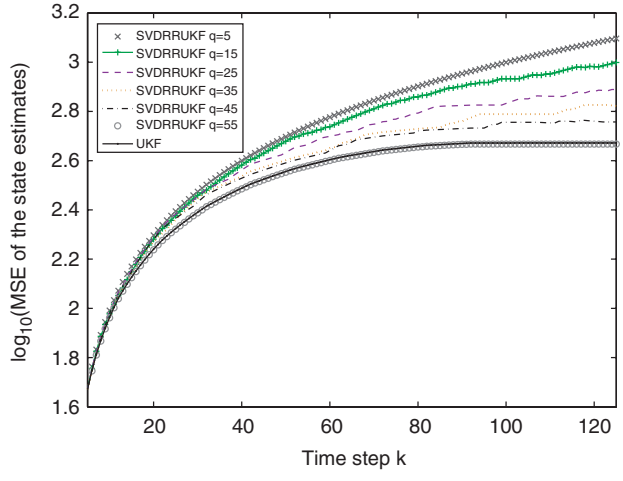

Figure 2. MSE of the state estimates obtained from SVDRRUKF for several values of q. SVDRRUKF with $q = 5$ is unstable, while the performance of SVDRRUKF with $q = 55$ is close to the performance of full-order UKF. Note that SVDRRUKF with $q = 55$ uses 111 ensemble members, whereas UKF uses 201 ensemble members.

of SVDRRUKF with 111 ensemble members ($q = 55$) is close to optimal, whereas the performance of CDRRUKF is close to optimal with 11 ensemble members ($q = 5$). The steady-state MSE of state estimates for various values of q is plotted in Figures 4 and 5. The performance of SVDRRUKF is poor when $q < 55$, and close to optimal when $q \geq 55$. Thus the ensemble size can be reduced from 201 to 111 with negligible change in the performance. Finally, note that even with $q = 5$, the performance of CDRRUKF is close to optimal. Hence, the ensemble size can be reduced from 211 to 11 with negligible performance deterioration.

Next, we repeat the same procedure except with a poor estimate of the process noise covariance for data assimilation. Specifically, we replace Q_k in (42) and (63) by $\hat{Q}_k$, where $\hat{Q}_k = I$ for all $k \geq 0$. The steady-state MSE of state estimates for different choices of q is plotted in Figure 4 and Figure 5. SVDRRUKF with a poor estimate of the error covariance is unstable for all $q \leq 95$ (indicated by the X's). However, Figure 5 shows that even with $q = 5$ and a poor estimate of the process noise covariance, the steady-state performance of CDRRUKF is close to optimal.

Finally, we replace Q_k in (64) with $\hat{Q}_k$, where $\hat{Q}_k = \alpha I$ for all $k \geq 0$, and perform state estimation using CDRRUKF. The steady-state MSE of the state estimates is shown in Figure 6 for several values of α. The performance degradation for small values of α is less when the ensemble size is large. However, for all three cases $q = 5$, $q = 15$, and $q = 15$, the performance of CDRRUKF is close to optimal when $\alpha \geq 1$. This suggests that it is advantageous to overestimate

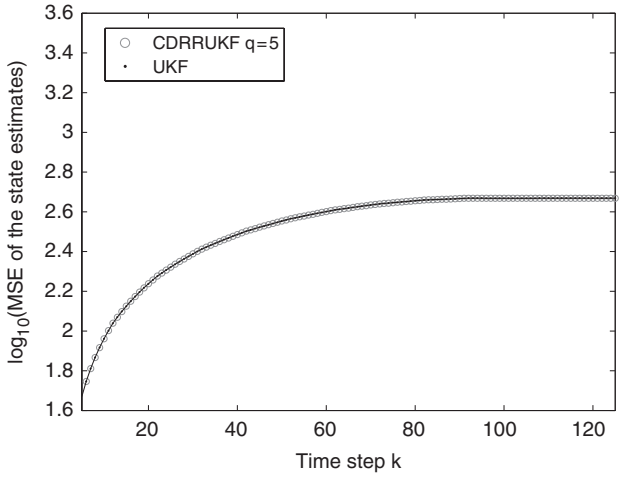

Figure 3. MSE of the state estimates obtained from CDRRUKF with $q = 5$. The performance of CDRRUKF with $q = 5$ is close to the full-order UKF performance. Note that CDRRUKF with $q = 5$ uses 11 ensemble members, while UKF uses 201 ensemble members.

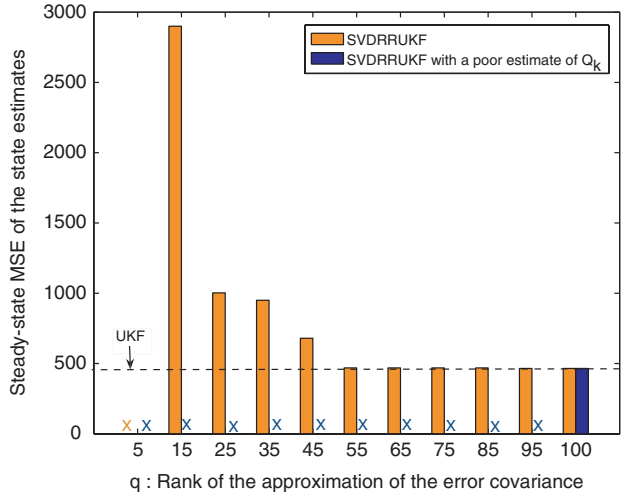

Figure 4. Steady-state performance of SVDRRUKF for several values of q between 5 and 100. For each value of q, we perform data assimilation with the true value of the process noise covariance and with a poor estimate of the process noise covariance. Specifically, we replace Q_k by $\hat{Q}_k$ in (42), where $\hat{Q}_k = I$ for all $k \geq 0$. The performance of UKF is shown for comparison. The X's indicate cases in which the filter is unstable. SVDRRUKF is unstable when $q = 5$, irrespective of the value of the process noise covariance used for data assimilation. When the true value of the process noise covariance is used for data assimilation, the performance of SVDRRUKF is poor when $q < 55$ and close to optimal for $q > 55$. However, when a poor estimate of the process noise covariance is used for data assimilation, SVDRRUKF is unstable for all $q = 5, \ldots, 95$. These results indicate that SVDRRUKF is sensitive to uncertainties in the estimate of the process noise covariance.

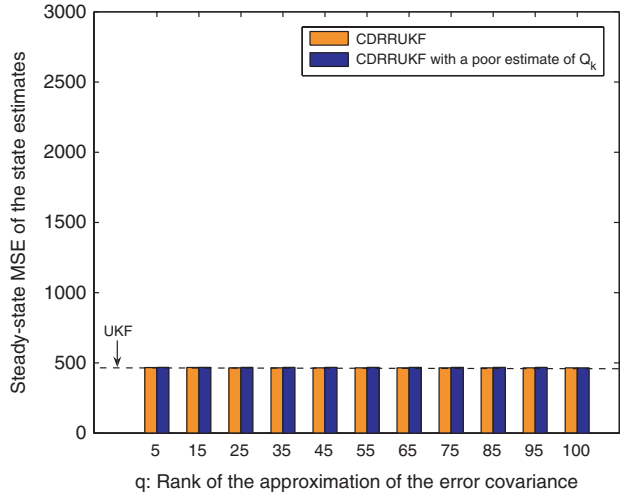

Figure 5. Steady-state performance of CDRRUKF for values of q between 5 and 100. We first perform data assimilation using the true value of the process noise covariance, and then perform data assimilation with a poor estimate of the process noise covariance, that is, we replace Q_k in (63) by $\hat{Q}_k$, where $\hat{Q}_k = I$ for all $k \geq 0$. Note that, for $q = 5$, the performance of CDRRUKF is close to optimal, irrespective of the value of the process noise covariance used for data assimilation.

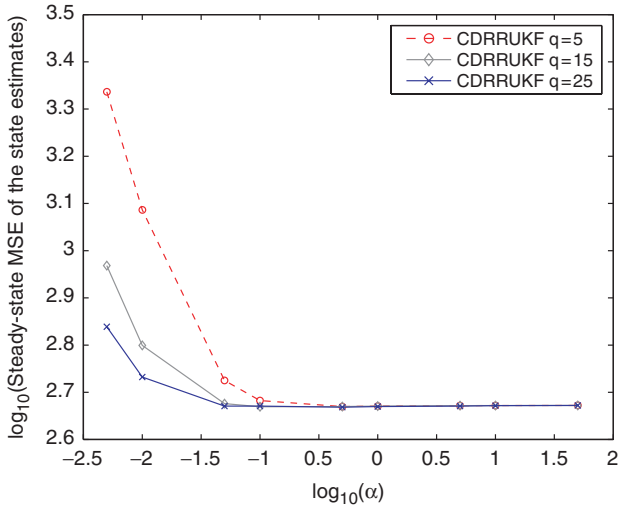

Figure 6. Steady-state performance of CDRRUKF with $q = 5, 15, 25$. In all three cases, we use a poor estimate of the process noise covariance for data assimilation, that is, we replace Q_k in (63) by $\hat{Q}_k$, where $\hat{Q}_k = \alpha I$ for all $k \geq 0$. In spite of the presence of an error in the process noise covariance, CDRRUKF is stable and thus robust to uncertainty in the process noise covariance. For a fixed level of uncertainty in the process noise covariance, the performance of CDRRUKF improves when the ensemble size increases. Moreover, for a specific choice of q, the performance improves as α increases. These results suggest that it is advantageous to overestimate the process noise covariance. The performance of SVDRRUKF is not shown since SVDRRUKF is unstable for all values of α and $q = 5, 15, 25$.

the process noise covariance. In contrast to these results, SVDRRUKF with $q = 5$, 15, 25 is unstable for all choices of $\alpha = 0.005, \ldots, 50$. Hence, these simulations suggest that CDRRUKF is more robust than SVDRRUKF with respect to uncertainties in the process noise covariance. All of the results for CDRRUKF in Figures 1–6 are obtained using a state space basis with respect to which the observability matrix has the form (73).

7. L96 model

Next, we compare the performance of SVDRRUKF and CDRRUKF on a non-linear model that exhibits chaotic dynamics. The L96 model mimics the propagation of an unspecified meteorological quantity along a latitude circle (Lorenz 2006). The L96 model is commonly used to compare the performance of various ensemble-based data assimilation schemes (see Anderson (2001) and Whitaker and Hamill (2002)). The dynamics are governed by

$$\frac{\mathrm{d}}{\mathrm{d}t} x_i(t) = (x_{i+1}(t) - x_{i-2}(t))x_{i-1}(t) - x_i(t) + u_i(t), \tag{89}$$

where $x_i(t) \in \mathbb{R}$ denotes the meteorological quantity at the ith grid point at time t, $u_i \in \mathbb{R}$ denotes an external forcing term, and w_i denotes unknown disturbances affecting the ith grid point. For all $t \geq 0$, the boundary conditions are defined by

$$x_0(t) = x_n(t), \quad x_{-1}(t) = x_{n-1}(t), \quad x_{n+1}(t) = x_1(t). \tag{90}$$

We choose $u_i(t) = 8$ for all $i = 1, \ldots, n$ and all $t \geq 0$. Using fourth-order Runge–Kutta discretisation with a sampling time of 0.05 s, we obtain a discrete-time model of (89) that can be expressed as (1). Furthermore, we assume that the discretised model is corrupted by an unknown external disturbance that affects specified cells. We choose $n = 40$, and assume that w_k is a white noise process with covariance $Q_k = Q$ for all $k \geq 0$, where $Q \in \mathbb{R}^{n \times n}$ is diagonal with entries

$$Q_{i,i} = \begin{cases} 0.1 & \text{if } i \in \{5, 15, 25, 35\}, \\ 0 & \text{else.} \end{cases} \tag{91}$$

Next, we assume that measurements from cells 20 and 23 are available so that

$$y_k = \begin{bmatrix} x_{20,k} \\ x_{23,k} \end{bmatrix} + v_k, \tag{92}$$

where v_k is white noise process with covariance $R_k = 0.01 I_2$. Hence, (92) can be expressed as (2) with $C_k = C \in \mathbb{R}^{2 \times 40}$.

We use the measurements y_k to estimate the state in the cells where measurements are not available. The estimates of $x_{20}(t)$ and $x_{23}(t)$ obtained using UKF are shown in Figure 7. The MSE of state estimates obtained using UKF is shown in Figure 8. The error in the state estimates based on data-free simulation with $w_k = 0$ for all $k \geq 0$ is shown for comparison. Since $n = 40$, UKF uses 81 ensembles.

Next, as shown in Figures 9 and 10, we reduce the ensemble size and use SVDRRUKF and CDRRUKF with $q = 10, 20, 30$. Although the number of ensembles in SVDRRUKF and CDRRUKF is the same for each value of q, it can be seen that the performance of SVDRRUKF is poor compared to the performance of CDRRUKF for both $q = 20$ and $q = 30$. Moreover, the performance of CDRRUKF with 61 ($q = 30$) ensemble members is close to the performance of UKF with 81 ensemble members. Figure 11 shows the difference in the MSE of state estimates between data-free simulation and the reduced-rank filters with $q = 10$ from $t = 25$ sec to $t = 30$ sec. Positive values indicate the cells and time instants at which estimates from the reduced-rank filters are better than the

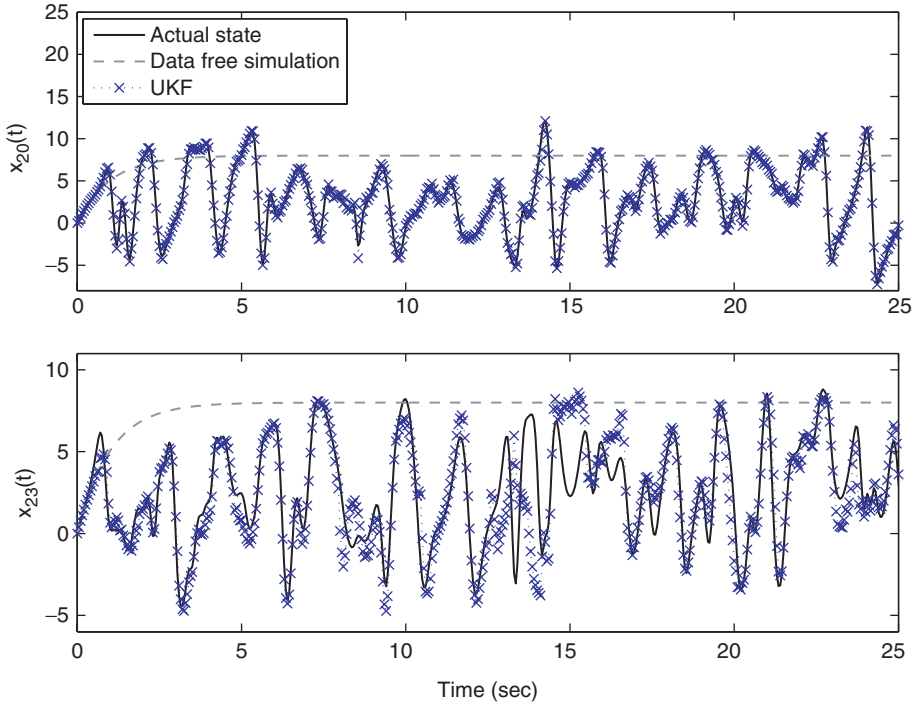

Figure 7. Estimates of $x_{20}(t)$ and $x_{23}(t)$ when measurements of $x_{20}(t)$ and $x_{23}(t)$ are used by UKF. The results of data-free simulation with $w_k = 0$ for all $k \geq 0$ are shown for comparison. In both UKF and data-free simulation, all of the intial states are set to zero.

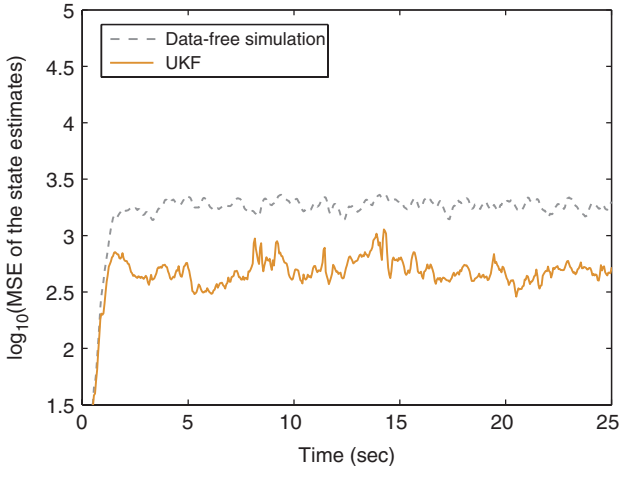

Figure 8. MSE of the state estimates obtained using UKF when the exact value of the process noise covarianace is used. The MSE of the state estimates obtained from data-free simulation with $w_k = 0$ for all $k \geq 0$, is also shown for comparison.

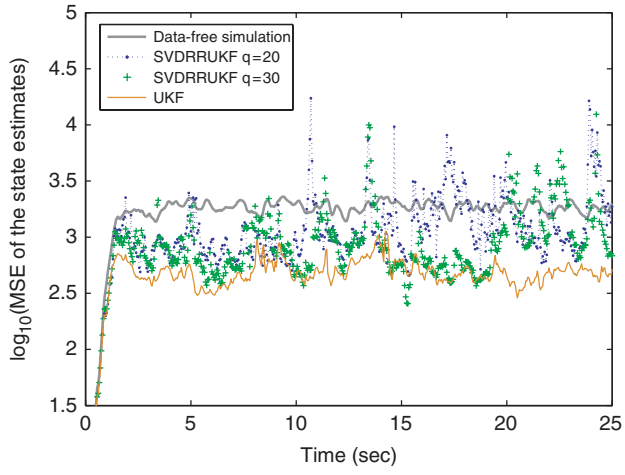

Figure 9. MSE of the state estimates obtained using SVDRRUKF with $q = 20, 30$. The error in state estimates based on UKF and data-free simulation is shown for comparison. The performance of SVDRRUKF with $q = 20$ and $q = 30$ is poor. In fact, SVDRRUKF with $q = 20$ and $q = 30$ sometimes yields estimates that are worse than estimates based on data-free simulation.

estimates obtained when data assimilation is not performed, while negative values indicate the cells and time instants at which estimates from the reduced-rank filters are worse than the estimates obtained from data-free simulation.

Next, since the process noise covariance Q_k is often unknown, we assume that the estimate of the process noise covariance is poor. Specifically, we replace Q_k in (42) and (63) by $\hat{Q}_k$, where

$\hat{Q}_k = \alpha I$ for all $k \geq 0$. Figure 12 shows the time-averaged MSE of state estimates obtained using SVDRRUKF and CDRRUKF with $q = 10$ and $q = 20$ for several values of α between 0.001 and 100. The errors in state estimates are averaged

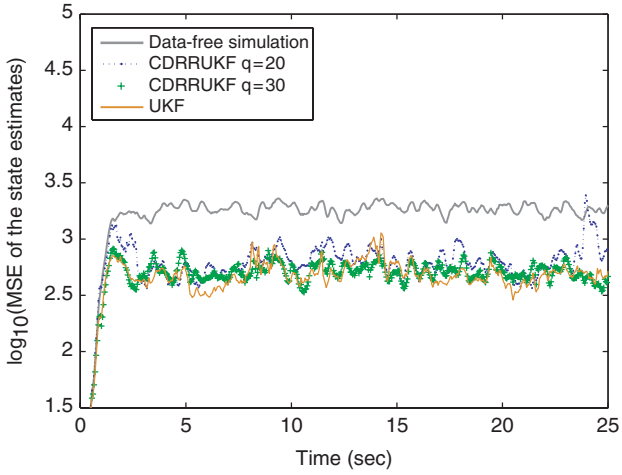

Figure 10. Performance of CDRRUKF with $n = 40$ and $q = 20, 30$. Note that the performance of CDRRUKF with $q = 20$ is better than the performance of SVDRRUKF with $q = 30$.

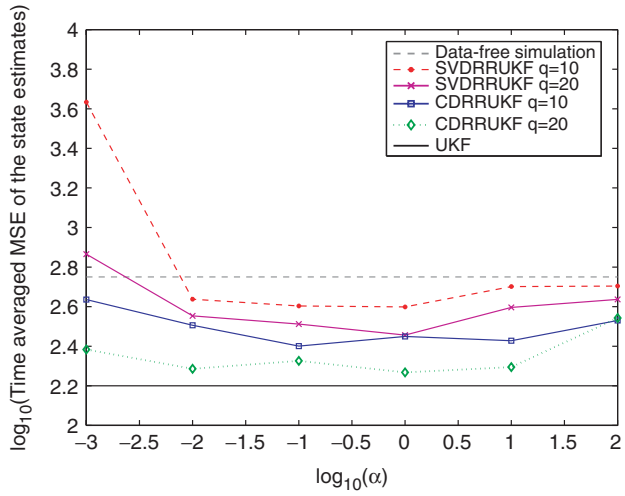

Figure 12. Time-averaged MSE of state estimates between 35 s and 50 s. The state estimates are obtained using SVDRRUKF and CDRRUKF with $q = 10$ and $q = 20$, and a poor estimate of the process noise covariance. Specifically, we replace Q_k in (42) and (63) by $\hat{Q}_k$, where $\hat{Q}_k = \alpha I$ for all $k \geq 0$. The MSE of the state estimates based on data-free simulation with $w_k = 0$ for all $k \geq 0$ and UKF is shown for comparison. For all values of α, the performance of CDRRUKF is better than the performance of SVDRRUKF. Furthermore, CDRRUF is more robust to uncertainties in the estimate of the process noise covariance.

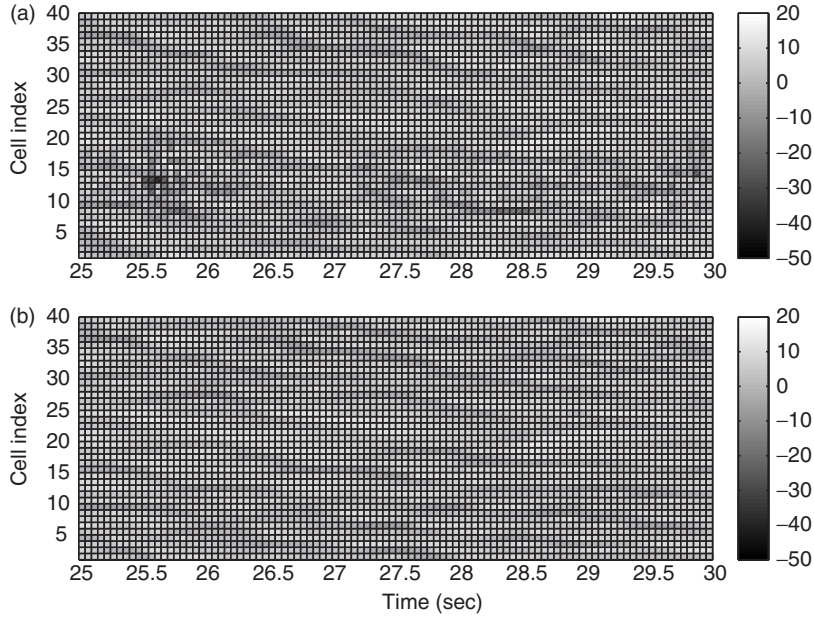

Figure 11. Time history of the difference in the MSE of estimates of the state in cells $1, \ldots, 40$, based-on data-free simulation and SVDRRUKF in (a) and CDRRUKF in (b). We use measurements from cells 20 and 21 for data assimilation. For both SVDRRUKF and CDRRUKF, we choose $q = 10$ so that the ensemble size is 21. Regions with positive values indicate the cells and time instants at which the estimates from the reduced-rank filters are better than the estimates obtained when data assimilation is not performed. Alternatively, negative values indicate time instants at which the estimates from SVDRRUKF and CDRRUKF are worse than the estimates obtained from data-free simulation. Note that CDRRUKF with 21 ensembles improves the estimates in most of the cells. However, the estimates from SVDRRUKF are extremely poor in certain cells, for example, in cells $10, \ldots, 15$ between 25.5 s and 26 s.

between 35 snd 50 s. It can be seen that, for all values of α, the performance of CDRRUKF is superior to the performance of SVDRRUKF. In fact, CDRRUKF with 21 ensemble members ($q=10$) consistently outperforms SVDRRUKF with 41 ensemble members ($q=20$). The Cholesky decomposition is used to obtain H_k^{f} and S_k^{f} in UKF, and to obtain $H_{\mathrm{s},k}^{\mathrm{f}}$ and $H_{\mathrm{c},k}^{\mathrm{f}}$ in SVDRRUKF and CDRRUKF, respectively. Moreover, the performance is similar when the singular value decomposition is used to obtain H_k^{f}, S_k^{f}, $H_{\mathrm{s},k}^{\mathrm{f}}$ and $H_{\mathrm{c},k}^{\mathrm{f}}$. Finally, note that (89) can be expressed as (77) with $b=1$. Moreover, in analogy with Proposition 3, simulation results indicate that the performance of CDRRUKF improves significantly when a state space basis is selected according to § 5.1. Hence, all of the results for CDRRUKF in Figures 8–12 are obtained using the state space basis discussed in § 5.1.

8. Conclusions

We developed a reduced-rank square-root unscented Kalman filter based on the Cholesky decomposition of the pseudo-error covariance. We compared the performance of the Cholesky-based filter with an analogous filter that uses the singular value decomposition for a linear advection model and a non-linear system that exhibits chaotic behaviour. The ensemble size of both the Cholesky-based and SVD-based reduced-rank unscented Kalman filter is less than that of the unscented Kalman filter. Although the computational requirement of the Cholesky-based reduced-rank filter is less than that of the SVD-based reduced-rank filter, the results presented here suggest that the estimation accuracy of the Cholesky-based reduced-rank filter is significantly better than that of the SVD-based reduced-rank filter. Moreover, simulation results suggest that the Cholesky-based reduced-rank filter is more robust to uncertainties in the process noise covariance than the SVD-based reduced-rank filter.

Acknowledgements

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Appendix 1: Proofs

Proof of Lemma 3: Since rank $(P_k^{\mathrm{f}}) \leq q$, it follows that there exists $S_k^{\mathrm{f}} \in \mathbb{R}^{n\times q}$ satisfying

$$S_k^{\mathrm{f}}(S_k^{\mathrm{f}})^{\mathrm{T}} = P_k^{\mathrm{f}}. \tag{A1}$$

In fact, $S_k^{\mathrm{f}} = \Phi_{\mathrm{SVD}}(P_k^{\mathrm{f}}, q)$ satisfies (A1). Therefore, (11) implies that P_k^{da} can be expressed as

$$P_k^{\mathrm{da}} = S_k^{\mathrm{f}}[I - (C_k S_k^{\mathrm{f}})^{\mathrm{T}}(C_k S_k^{\mathrm{f}}(C_k S_k^{\mathrm{f}})^{\mathrm{T}} + R_k)^{-1} C_k S_k^{\mathrm{f}}](S_k^{\mathrm{f}})^{\mathrm{T}}. \tag{A2}$$

Hence, (A2) implies that $\mathrm{rank}(P_k^{\mathrm{da}}) \leq q$.

Proof of Proposition 1: It follows from Lemma 3 that $\mathrm{rank}(P_k^{\mathrm{da}}) \leq q$. Hence, there exists $\hat{S}_k^{\mathrm{da}} \in \mathbb{R}^{n\times q}$ such that $\hat{S}_k^{\mathrm{da}}(\hat{S}_k^{\mathrm{da}})^{\mathrm{T}} = P_k^{\mathrm{da}}$. Therefore, Lemma 2 implies that $X_{i,k}^{\mathrm{da}} = x_k^{\mathrm{da}}$, for all $i = 0, q+1, \ldots, n, n = q = 1, \ldots, 2n$. Hence, (15) implies that $X_{i,k+1}^{\mathrm{f}} = X_{0,k+1}^{\mathrm{f}}$, for all $i = q+1, \ldots, n, n+q+1, \ldots, 2n$. Therefore,

$$\frac{\alpha - n}{\alpha} X_{0,k+1}^{\mathrm{f}} + \frac{1}{2\alpha}\left[\sum_{i=q+1}^{n} X_{i,k+1}^{\mathrm{f}} + \sum_{i=n+q+1}^{2n} X_{i,k+1}^{\mathrm{f}}\right] = \frac{\alpha - q}{\alpha} X_{0,k+1}^{\mathrm{f}}, \tag{A3}$$

and it follows from (6) and (16) that

$$x_{k+1}^{\mathrm{f}} = \frac{\alpha - q}{\alpha} X_{0,k+1}^{\mathrm{f}} + \frac{1}{2\alpha}\left[\sum_{i=1}^{q} X_{i,k+1}^{\mathrm{f}} + \sum_{i=n+1}^{n+q} X_{i,k+1}^{\mathrm{f}}\right]. \tag{A4}$$

Hence, (23) and Lemma 2 imply that $\hat{x}_{k+1}^{\mathrm{f}} = x_{k+1}^{\mathrm{f}}$. Similarly, (6) and (17) imply that

$$\begin{aligned} P_{k+1}^{\mathrm{f}} = {} & \frac{\alpha - q}{\alpha}[X_{0,k+1}^{\mathrm{f}} - x_{k+1}^{\mathrm{f}}][X_{0,k+1}^{\mathrm{f}} - x_{k+1}^{\mathrm{f}}]^{\mathrm{T}} \\ & + \frac{1}{2\alpha}\sum_{i=1}^{q}[X_{i,k+1}^{\mathrm{f}} - x_{k+1}^{\mathrm{f}}][X_{i,k+1}^{\mathrm{f}} - x_{k+1}^{\mathrm{f}}]^{\mathrm{T}} \\ & + \frac{1}{2\alpha}\sum_{i=n+1}^{n+q}[X_{i,k+1}^{\mathrm{f}} - x_{k+1}^{\mathrm{f}}][X_{i,k+1}^{\mathrm{f}} - x_{k+1}^{\mathrm{f}}]^{\mathrm{T}}. \end{aligned} \tag{A5}$$

Since $\hat{x}_{k+1}^{\mathrm{f}} = x_{k+1}^{\mathrm{f}}$, it follows from (23) and Lemma 2 that $\hat{P}_{k+1}^{\mathrm{f}} = P_{k+1}^{\mathrm{f}}$.