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On Ensemble Nonlinear Kalman Filtering with Symmetric Analysis Ensembles

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Abstract. The ensemble square root filter (EnSRF) [1, 2, 3, 4] is a popular method for data assimilation in high dimensional systems (e.g., geophysics models). Essentially the EnSRF is a Monte Carlo implementation of the conventional Kalman filter (KF) [5, 6]. It is mainly different from the KF at the prediction steps, where it is some ensembles, rather than the means and covariance matrices, of the system state that are propagated forward. In doing this, the EnSRF is computationally more efficient than the KF, since propagating a covariance matrix forward in high dimensional systems is prohibitively expensive. In addition, the EnSRF is also very convenient in implementation. By propagating the ensembles of the system state, the EnSRF can be directly applied to nonlinear systems without any change in comparison to the assimilation procedures in linear systems.

However, by adopting the Monte Carlo method, the EnSRF also incurs certain sampling errors. One way to alleviate this problem is to introduce certain symmetry to the ensembles, which can reduce the sampling errors and spurious modes in evaluation of the means and covariances of the ensembles [7]. In this contribution, we present two methods to produce symmetric ensembles. One is based on the unscented transform [8, 9], which leads to the unscented Kalman filter (UKF) [8, 9] and its variant, the ensemble unscented Kalman filter (EnUKF) [7]. The other is based on Stirling's interpolation formula (SIF), which results in the divided difference filter (DDF) [10]. Here we propose a simplified divided difference filter (sDDF) in the context of ensemble filtering. The similarity and difference between the sDDF and the EnUKF will be discussed. Numerical experiments will also be conducted to investigate the performance of the sDDF and the EnUKF, and compare them to a well-established EnSRF, the ensemble transform Kalman filter (ETKF) [2].

Keywords: Data assimilation; Ensemble Kalman filter; Divided difference approximation

PACS: 92.60Wc, 02.50-r

INTRODUCTION

Data assimilation in geoscience often involves high dimensional nonlinear systems. In such practices, one is confronted with two challenging issues: the presence of the nonlinearity in assimilation, and the computational requirement in order to produce timely results. One popular method to tackle these two problems is the ensemble Kalman filter (EnKF) [11], whose main idea is to use an ensemble of the system state to represent the whole state space, and compute the statistics of the system accordingly. In this sense, the EnKF is essentially a Monte Carlo implementation of the conventional Kalman filter (KF) [5, 6]. A variant of the EnKF, under the uniform name of the ensemble square root filter (EnSRF) [3], was also proposed with various implementation forms [1, 2, 4]. It has been shown that the EnSRF has a better performance than the original EnKF in the small sample scenario, since it avoids the sampling errors of perturbing the observations in the original EnKF [4].

Nevertheless, there still exist sampling errors in the EnSRF, since the EnSRF also pertains to the Monte Carlo implementation of the KF. With these sampling errors, there may incur certain biases and spurious modes in the estimations of the sample statistics (e.g., sample mean and sample covariance) of the system state, due to the effect of finite ensemble size [7]. In this work we consider two possible methods to alleviate the effect of finite ensemble size, whose main idea is to introduce symmetry to the analysis ensemble in order to reduce some of the biases and spurious modes in statistical estimations [7]. One method is based on the unscented transform (UT) [8, 9], while the other is via Stirling's interpolation formula (SIF) [10]. Incorporating the UT and the SIF into the prediction step of an EnSRF leads to the unscented Kalman filter (UKF) [8, 9] and the divided difference filter (DDF) [10], respectively. To reduce the computational cost of these two filters in high dimensional systems, we consider a reduced rank version of the UKF, called the ensemble unscented Kalman filter (EnUKF) [7], and a simplified version of the DDF, called the simplified divided difference filter (sDDF) [12]. The focus of this work is to discuss the similarity and difference between the

EnUKF and the sDDF, and compare their performance to a well-established EnSRF, the ensemble transform Kalman filter (ETKF) [2].

PROBLEM STATEMENT AND SOLUTIONS

We study the state estimation problem in the following system:

$$\mathbf{x}_k = \mathcal{M}_{k,k-1}(\mathbf{x}_{k-1}) + \mathbf{u}_k, \quad (1a)$$

$$\mathbf{y}_k = \mathcal{H}_k(\mathbf{x}_k) + \mathbf{v}_k. \quad (1b)$$

Eqs. (1a) and (1b) represent the m_x -dimensional dynamical system and m_y -dimensional observation system, respectively. $\mathcal{M}_{k,k-1} : \mathbb{R}^{m_x} \rightarrow \mathbb{R}^{m_x}$ is the transition operator, while $\mathcal{H}_k : \mathbb{R}^{m_x} \rightarrow \mathbb{R}^{m_y}$ represents the observation operator. We assume that the model error in the dynamical system Eq. (1a) is characterized by a white Gaussian random process \mathbf{u}_k with zero mean and covariance \mathbf{Q}_k (denoted by $\mathbf{u}_k \sim N(\mathbf{u}_k : \mathbf{0}, \mathbf{Q}_k)$), while the observation error in Eq. (1b) is described by another white Gaussian process \mathbf{v}_k with zero mean and covariance \mathbf{R}_k ($\mathbf{v}_k \sim N(\mathbf{v}_k : \mathbf{0}, \mathbf{R}_k)$). In addition, \mathbf{u}_i and \mathbf{v}_j are independent from each other for all indices i and j .

The EnUKF as the solution

Suppose that at the $(i-1)$ th cycle, there exists an analysis ensemble $\{\mathcal{X}_{i-1,j}^a, j=0, \dots, 2l_{i-1}\}$, associated with a set of weights $\{W_{i-1,j}, j=0, \dots, 2l_{i-1}\}$. At the next cycle i , we need to evaluate the analysis mean $\hat{\mathbf{x}}_i^a$ and covariance $\hat{\mathbf{P}}_i^a$, and generate a new analysis ensemble $\{\mathcal{X}_{i,j}^a, j=0, \dots, 2l_i\}$ and the associated weights accordingly. The procedures of the EnUKF at the i th cycle are outlined as follows, while readers are referred to [7, 13] for more details.

Prediction step:

$$\mathbf{x}_{i,j}^b = \mathcal{M}_{i,i-1}(\mathcal{X}_{i-1,j}^a) + \eta_{i,j}, \quad j=0, \dots, 2l_{i-1}; \quad \hat{\mathbf{x}}_i^b = \sum_{j=0}^{2l_{i-1}} W_{i-1,j} \mathbf{x}_{i,j}^b; \quad \hat{\mathbf{y}}_i^b = \sum_{j=0}^{2l_{i-1}} W_{i-1,j} \mathcal{H}_i(\mathbf{x}_{i,j}^b), \quad (2a)$$

$$\mathbf{S}_i^{xb} = \left[\sqrt{W_{i-1,0} + \beta} (\mathbf{x}_{i,0}^b - \hat{\mathbf{x}}_i^b), \sqrt{W_{i-1,1}} (\mathbf{x}_{i,1}^b - \hat{\mathbf{x}}_i^b), \dots, \sqrt{W_{i-1,2l_{i-1}}} (\mathbf{x}_{i,2l_{i-1}}^b - \hat{\mathbf{x}}_i^b) \right], \quad (2b)$$

$$\mathbf{S}_i^h = \left[\sqrt{W_{i-1,0} + \beta} (\mathcal{H}_i(\mathbf{x}_{i,0}^b) - \hat{\mathbf{y}}_i), \sqrt{W_{i-1,1}} (\mathcal{H}_i(\mathbf{x}_{i,1}^b) - \hat{\mathbf{y}}_i), \dots, \sqrt{W_{i-1,2l_{i-1}}} (\mathcal{H}_i(\mathbf{x}_{i,2l_{i-1}}^b) - \hat{\mathbf{y}}_i) \right], \quad (2c)$$

$$\hat{\mathbf{P}}_i^b = \mathbf{S}_i^{xb} (\mathbf{S}_i^{xb})^T, \quad (2d)$$

$$\hat{\mathbf{K}}_i = \mathbf{S}_i^{xb} (\mathbf{S}_i^h)^T \left(\mathbf{S}_i^h (\mathbf{S}_i^h)^T + \mathbf{R}_i \right)^{-1}. \quad (2e)$$

Here $\eta_{i,j}$ is a realization of the dynamical noise \mathbf{u}_i , and β is an intrinsic filter parameter. In this work we set $\beta = 2$.

Filtering step:

$$\hat{\mathbf{x}}_i^a = \hat{\mathbf{x}}_i^b + \hat{\mathbf{K}}_i \left(\mathbf{y}_i - \mathcal{H}_i(\hat{\mathbf{x}}_i^b) \right), \quad (3a)$$

$$\mathbf{S}_i^{xa} = \mathbf{S}_i^{xb} \mathbf{T}_i, \quad (3b)$$

$$\hat{\mathbf{P}}_i^a = \mathbf{S}_i^{xa} (\mathbf{S}_i^{xa})^T. \quad (3c)$$

Here \mathbf{T}_i is the transform matrix at the i th assimilation cycle as defined in [2].

Analysis scheme:

$$\begin{aligned}\mathcal{X}_{i,0}^a &= \hat{\mathbf{x}}_i^a, \\ \mathcal{X}_{i,j}^a &= \hat{\mathbf{x}}_i^a + \sqrt{\sigma_{i,j}(l_i + \lambda)} \mathbf{e}_{i,j}, \quad j = 1, 2, \dots, l_i, \\ \mathcal{X}_{i,j}^a &= \hat{\mathbf{x}}_i^a - \sqrt{\sigma_{i,j-l_i}(l_i + \lambda)} \mathbf{e}_{i,j-l_i}, \quad j = l_i + 1, l_i + 2, \dots, 2l_i.\end{aligned}\quad (4)$$

Here λ is another intrinsic filter parameter and is set to be -2 in this work. $\sigma_{k,j}$ ($j = 1, 2, \dots, l_i$) are the first l_i leading eigenvalues of $\hat{\mathbf{P}}_i^a$, with the corresponding eigenvectors $\mathbf{e}_{k,j}$. The determination of l_i was discussed in [7].

Associated weights:

$$W_{i,0} = \frac{\lambda}{l_i + \lambda}; \quad W_{i,j} = \frac{1}{2(l_i + \lambda)}, \quad j = 1, 2, \dots, 2l_i. \quad (5)$$

The sDDF as the solution

Suppose that at the $(i-1)$ th cycle, we have the analysis mean $\hat{\mathbf{x}}_{i-1}^a$ and an associated square root matrix $\hat{\mathbf{S}}_{i-1}^a$ of the analysis covariance $\hat{\mathbf{P}}_{i-1}^a$. We construct a set of sigma points $\mathbf{X}_{k-1}^a \equiv \{\mathcal{X}_{k-1,i}^a : i = 0, \dots, 2n\}$ with $2n + 1$ members in the following manner

$$\begin{aligned}\mathcal{X}_{i-1,0}^a &= \hat{\mathbf{x}}_{i-1}^a, \\ \mathcal{X}_{i-1,j}^a &= \hat{\mathbf{x}}_{i-1}^a + h_{i-1} (\hat{\mathbf{S}}_{i-1}^a)_j, \quad i = j, 2, \dots, n, \\ \mathcal{X}_{i-1,j}^a &= \hat{\mathbf{x}}_{i-1}^a - h_{i-1} (\hat{\mathbf{S}}_{i-1}^a)_{j-n}, \quad j = n + 1, n + 2, \dots, 2n,\end{aligned}\quad (6)$$

where $(\hat{\mathbf{S}}_{i-1}^a)_j$ is the j th column of $\hat{\mathbf{S}}_{i-1}^a$, and h_{i-1} is an intrinsic parameter, called *the length of interpolation interval* at $i-1$ ($h_i = 3$ for all i in this work). For convenience, we say that sigma points \mathbf{X}_{i-1}^a are generated with respect to the triplet $(h_{i-1}, \hat{\mathbf{x}}_{i-1}^a, \hat{\mathbf{S}}_{i-1}^a)$. Note that, different from the situation in the EnUKF, here n is a constant independent of the time index i .

Prediction step:

$$\mathbf{x}_{i,j}^b = \mathcal{M}_{i,i-1}(\mathcal{X}_{i-1,j}^a) + \eta_{i,j}, \quad j = 0, \dots, 2n; \quad \hat{\mathbf{x}}_i^b = \frac{h_{i-1}^2 - n}{h_{i-1}^2} \mathbf{x}_{i,0}^b + \frac{1}{2h_{i-1}^2} \sum_{j=1}^{2n} \mathbf{x}_{i,j}^b, \quad (7a)$$

$$\mathbf{S}_i^{xb} = \frac{1}{2h_{i-1}} \left[\mathbf{x}_{i,1}^b - \mathbf{x}_{i,n+1}^b, \mathbf{x}_{i,2}^b - \mathbf{x}_{i,n+2}^b, \dots, \mathbf{x}_{i,n}^b - \mathbf{x}_{i,2n}^b \right], \quad (7b)$$

$$\mathbf{X}_i^b \equiv \{\mathcal{X}_{i,j}^b : \mathcal{X}_{i,j}^b \in \sigma(d_i, \hat{\mathbf{x}}_i^b, \mathbf{S}_i^{xb}), j = 0, \dots, 2n\} \quad (7c)$$

$$\mathbf{S}_i^h = \frac{1}{2d_i} \left[\mathcal{H}_i(\mathcal{X}_{i,1}^b) - \mathcal{H}_i(\mathcal{X}_{i,n+1}^b), \mathcal{H}_i(\mathcal{X}_{i,2}^b) - \mathcal{H}_i(\mathcal{X}_{i,n+2}^b), \dots, \mathcal{H}_i(\mathcal{X}_{i,n}^b) - \mathcal{H}_i(\mathcal{X}_{i,2n}^b) \right], \quad (7d)$$

$$\hat{\mathbf{K}}_i = \mathbf{S}_i^{xb} (\mathbf{S}_i^h)^T \left(\mathbf{S}_i^h (\mathbf{S}_i^h)^T + \mathbf{R}_i \right)^{-1}. \quad (7e)$$

Eq. (7c) means that the set $\mathbf{X}_i^b = \{\mathcal{X}_{i,j}^b, j = 0, \dots, 2n\}$ of sigma points is generated with respect to $(d_i, \hat{\mathbf{x}}_i^b, \mathbf{S}_i^{xb})$, with d_i being the length of interpolation interval of \mathcal{H}_i .

Filtering step:

$$\hat{\mathbf{x}}_i^a = \hat{\mathbf{x}}_i^b + \hat{\mathbf{K}}_i \left(\mathbf{y}_i - \mathcal{H}_i(\hat{\mathbf{x}}_i^b) \right), \quad (8a)$$

$$\mathbf{S}_i^{xa} = \mathbf{S}_i^{xb} \mathbf{T}_i. \quad (8b)$$

TABLE 1. Minimum RMSEs $\hat{\epsilon}_{min}$ of the ensemble filters with various ensemble sizes.

| Ensemble size | $\hat{\epsilon}_{min}$ | | | Parameter values |
|---------------|------------------------|--------|--------|---|
| | sDDF | EnUKF | ETKF | |
| 11 | 0.7537 | 0.7190 | 0.6879 | $\delta \in \{0 : 1 : 8\}; l_c \in \{40 : 40 : 320\}$ |
| 21 | 0.5525 | 0.5757 | 0.2599 | $\delta \in \{0 : 0.5 : 5\}; l_c \in \{40 : 40 : 320\}$ |
| 41 | 0.2456 | 0.2339 | 0.2230 | $\delta \in \{0 : 0.5 : 5\}; l_c \in \{40 : 40 : 320\}$ |
| 81 | 0.2059 | 0.2044 | 0.2375 | $\delta \in \{0 : 0.05 : 0.3\}; l_c \in \{100 : 200 : 900\}$ |
| 161 | 0.2048 | – | 0.2389 | $\delta \in \{0 : 0.02 : 0.1\}; l_c \in \{100 : 200 : 900\}$ |
| 321 | 0.2069 | – | 0.2628 | $\delta \in \{0 : 0.02 : 0.1\}; l_c \in \{100 : 200 : 900\}$ |
| 641 | 0.2046 | – | 0.2797 | $\delta \in \{0 : 0.01 : 0.05\}; l_c \in \{100 : 200 : 900\}$ |

Analysis scheme:

$$\mathbf{X}_i^a \equiv \{\mathcal{X}_{i,j}^a : \mathcal{X}_{i,j}^a \in \sigma(h_i, \hat{\mathbf{x}}_i^a, \mathbf{S}_i^{xa}), j = 0, \dots, 2n\}. \quad (9)$$

Here h_i is the length of interpolation interval with respect to $\mathcal{M}_{i+1,i}$.

The similarity between the sDDF and the EnUKF is that both the filters need to generate symmetric sigma points. However, in the EnUKF, these symmetric points are generated for the purpose of statistical approximations. In contrast, in the sDDF these symmetric system states are used for the purpose of interpolation. Another major difference between the EnUKF and the sDDF lies in that, in the EnUKF one needs to conduct an SVD to generate sigma points, which is avoided in the sDDF, due to the simplifications made in its derivation [12]. Therefore the sDDF is computationally more efficient than the EnUKF if the ensemble size is no larger than the dimension of the dynamical system.

NUMERICAL RESULTS

We use the 40-dimensional Lorenz and Emanuel model [14] (LE98 model hereafter) for illustration, whose governing equations are given by

$$\frac{dx_i}{dt} = (x_{i+1} - x_{i-2})x_{i-1} - x_i + 8, i = 1, \dots, 40. \quad (10)$$

The fourth-order Runge-Kutta method is used to numerically integrate the system 200 steps forward, with a constant integration step of 0.05. We generate the synthetic observations through the following system

$$\mathbf{y}_i = \mathbf{x}_i + \mathbf{v}_i, \quad (11)$$

where \mathbf{v}_i follows the Gaussian distribution $N(\mathbf{v}_i : \mathbf{0}, \mathbf{I}_{40})$, with \mathbf{I}_{40} being the 40-dimensional identity matrix. The observations are made for every integration step.

We first compare the performance of the sDDF, the EnUKF and the ETKF with various ensemble sizes. In the context of ensemble filtering, it is customary to conduct covariance inflation and localization to improve the performance of the filters [15]. Here we follow [16] and [13] to conduct covariance inflation and localization, respectively, which introduces two parameters, the inflation factor δ and the length scale l_c of covariance localization, to the filters. To examine the effects of δ and l_c on the filter performance, in the experiment we also vary their values in certain ranges. The concrete settings of the experiment are as follows: In both the sDDF and the EnUKF, the ensemble size p is in the form of $p = 2n + 1$. In the EnUKF the $(2n + 1)$ -member ensembles are generated by the first n pairs of leading eigenvalues and eigenvectors of a sample covariance. Thus n shall be no larger than 40, the dimension of the LE98 model. For this reason, in the EnUKF we let $n = 5, 10, 20, 40$ (corresponding to ensemble sizes of 11, 21, 41, 81). However, in the sDDF n can be any positive integer number. To include the scenario with relatively large ensemble sizes, in the sDDF we let $n = 5, 10, 20, 40, 80, 160, 320$ (corresponding to ensemble sizes of 11, 21, 41, 81, 321, 641). For comparison, we let the ensemble sizes of the ETKF equal those of the sDDF. The values of δ and l_c depend on the

choice of the ensemble size, which are given in Table 1. To reduce statistical fluctuations, we repeat all the experiments for 20 times.

We use the root mean squared error (RMSE) to measure the filter performance. Due to the space limitation, we are not able to present the full details of our experiment results. Instead, we only report in Table 1 the minimum RMSEs \hat{e}_{min} that the three filters can achieve within the tested ranges of δ and l_c . From Table 1, we have the following observation: The ETKF outperforms both the EnUKF and the sDDF in the small sample scenario (say, with the ensemble size $p = 11$), in that the ETKF has the lowest \hat{e}_{min} . As the ensemble size p keeps increasing to around the dimension of the LE98 model (say $p = 41$), the gap between the three filters is narrowed. Increasing p further thereafter makes the sDDF and the EnUKF outperform the ETKF instead.

Our explanation of the experiment results is the following. For a relatively small ensemble size p (say $p = 11$), there exist substantial rank deficiencies in the (sample) analysis covariances of the sDDF and the EnUKF in comparison to that of the ETKF. This is because, in the small sample scenario, given an ensemble size $p = 2n + 1$, the rank of the analysis covariance of the ETKF in general is $2n$, while the ranks of the analysis covariances of the sDDF and the EnUKF are only n , due to the symmetry in sigma points. Therefore, although the presence of symmetry may help the sDDF and the EnUKF to reduce the effect of sampling errors, the effect of rank deficiency dominates the filters' performance and make the sDDF and the EnUKF under-perform the ETKF. On the other hand, when the ensemble size becomes comparable to the dimension of the dynamical system or even higher, there are no substantial rank deficiencies in the analysis covariances in the sDDF and the EnUKF, and the presence of the symmetry in the analysis ensembles helps the sDDF and the EnUKF to outperform the ETKF instead. Finally, we note that in the experiments, the EnUKF outperforms the sDDF in most cases, since some simplifications are made in the derivation of the sDDF for computational efficiency [12].

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