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Unbiased Ensemble Square Root Filters

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Abstract

There is an established framework that describes a class of ensemble Kalman filter algorithms as square root filters (SRFs). These schemes carry out analyses by updating the ensemble mean and a square root of the ensemble covariance matrix. The matrix square root of the forecast covariance is post-

1 Introduction

Data assimilation seeks to solve the following problem: given an imperfect discrete model of the dynamics of a system and noisy observations of the system, find estimates of the state of the system. Sequential data assimilation techniques break this problem into a cycle of alternating forecast and analysis steps. In the forecast step the system dynamical model is used to evolve an earlier state estimate forward in time, giving a forecast state at the time of the latest observations. In the analysis step the observations are used to update the forecast state, giving an improved state estimate called the analysis. This analysis is used as the starting point for the next forecast.

Sequential data assimilation techniques include the optimal linear Kalman filter (KF) and its nonlinear generalisation, the extended Kalman filter (EKF) (Gelb, 1974; Jazwinski, 1970). As well as an estimate of the state of the system, these the ensemble size is small, but not so small that it is statistically unrepresentative, then the extra work needed to maintain an ensemble of state estimates is more than o set by the work saved through not maintaining a separate covariance matrix. The EnKF also does not use tangent linear operators, which eases implementation and may lead to a better handling of nonlinearity. The KF aspect of the EnKF appears in the analysis step, which is designed so that the implied updates of the ensemble mean and ensemble covariance matrix mimic those of the state vector and covariance matrix in the standard KF.

The EnKF was originally presented in Evensen (1994). An important subsequent development was the recognition by Burgers et al. (1998) (and independently by Houtekamer and Mitchell (1998)) of the need to use an ensemble of pseudo-random observation perturbations to obtain the right statistics from the analysis ensemble. Deterministic methods for forming an analysis ensemble with the right statistics have also been presented. The former approach to the EnKF is comprehensively reviewed in Evensen (2003), whilst previously-published variants of the latter approach are placed in a uniform framework in Tippett et al. (2003). These variants include the ensemble transform Kalman filter (ETKF) of Bishop et al. (2001), the ensemble adjustment Kalman filter (EAKF) of Anderson (2001), and the filter of Whitaker

fer (vsl 1. These

ewatseo03(o)-2.26a6442998(g73077(n)-339.324(a)-395(e)3.56659482(n)1.9i7.971424(e)-387.893(l)39.324(a)-3261693(h74 formulations of the analysis step of the EnKF whilst excluding those filters that do not have the desired analysis ensemble statistics.

This paper adopts a formal style of presentation with explicitly stated definitions and theorems. The purpose of the definitions is to clarify key concepts, especially the distinctions between the different types of filter. The theorems are stated explicitly to help distinguish them from the rest of the text. S space. The ensemble mean is the vector defined by

$$\bar{\mathbf{x}} = \frac{1}{m} \sum_{i}^{m} \mathbf{x}_i \tag{1}$$

The ensemble perturbation matrix is the $n \times m$ matrix defined by

$$\mathbf{X} = \frac{1}{\sqrt{m-1}} \left[\mathbf{x} - \bar{\mathbf{x}} \quad \mathbf{x}_2 - \bar{\mathbf{x}} \quad \quad \mathbf{x}_m - \bar{\mathbf{x}} \right] \tag{2}$$

The ensemble covariance matrix is the $n \times n$ matrix defined by

$$\mathbf{P} = \mathbf{X}\mathbf{X}^T = \frac{1}{m-1} \sum_{i}^{m} (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T \tag{3}$$

If the members of $\{\mathbf{x}_i\}$

$$\mathbf{P}^a = (\mathbf{X}^f - \mathbf{K}\mathbf{Y}^f)(\mathbf{X}^f)^T \tag{10}$$

$$\mathbf{K} = \mathbf{X}^f(\mathbf{Y}^f)^T\mathbf{D}^- \tag{11}$$

$$\mathbf{D} = \mathbf{Y}^f(\mathbf{Y}^f)^T + \mathbf{R} \tag{12}$$

An EnKF is *semi-deterministic* if its analysis step is deterministic.

There is an alternative approach to extending an EnKF from linear to nonlinear observation operators, described in, for example, Evensen (2003, section 4.5). In this approach the state vector is augmented with a diagnostic variable that is the predicted observation vector:

$$\hat{\mathbf{x}} = \begin{pmatrix} \mathbf{x} \\ H(\mathbf{x}) \end{pmatrix} \tag{13}$$

and a linear observation operator is defined on augmented state space by

$$\hat{\mathbf{H}} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}$$

Definition 2 An *ensemble square root filter* is an ensemble filter in which the analysis ensemble is obtained by adding a column n-vector $\bar{\mathbf{x}}$ to the columns of a $n \times N$ matrix $\sqrt{N-1}\,\mathbf{X}$ where $\bar{\mathbf{x}}$ and $\mathbf{X}$ satisfy

$$
\begin{aligned}
\bar{\mathbf{x}} &= \overline{\mathbf{x}^f} + \mathbf{K}(\mathbf{y} - \overline{\mathbf{y}^f}) && (15)\\
\mathbf{X} &= \mathbf{X}^f\mathbf{T} && (16)\\
\mathbf{T}\mathbf{T}^T &= \mathbf{I} - (\mathbf{Y}^f)^T\mathbf{D}^{-}\,\mathbf{Y}^f && (17)
\end{aligned}
$$

Theorem 2 If T satisfies the matrix square root condition (17) and U is an $p \times p$ orthogonal matrix, then TU also satisfies (17).

Proof. Recall that an orthogonal matrix satisfies $U^T U = UU^T = I$. Thus $(TU)(TU)^T = TUU^T T^T = TT^T$ and so TU satisfies (17) if T does. □

Theorem 3 If X and X_2 are two $n \times p$ matrices such that $X X^T = X_2 X_2^T$, then there exists an orthogonal matrix U such that $X_2 = X U$.

Proof. This proof makes use of the singular value decomposition (SVD) of a matrix; see, for example, Golub and Van Loan (1996, section 2.5). Start by taking the SVD of X :

$$X = FGW^T \tag{19}$$

where G is an $n \times p$ diagonal matrix (in the sense that $g_{ij} = 0$ if $i \neq j$) and F and W are orthogonal matrices of sizes $n \times n$ and $p \times p$ respectively. Without loss of generality it may be assumed that G can be expressed in the form

$$G = \begin{bmatrix} G & 0 \\ 0 & 0 \end{bmatrix} \tag{20}$$

where G is a nonsingular diagonal matrix of size $r \times r$ for some r. The orthogonal matrix F can then be expressed in the form

$$F = \begin{bmatrix} F & F \end{bmatrix} \tag{21}$$

where F and F are column-orthogonal matrices of sizes $n \times r$ and $n \times (n - r)$ respectively (a column-orthogonal matrix is one in which the column vectors are orthonormal and thus the matrix satisfies $F^T F = I$). Similarly, W can be expressed in the form

$$W = \begin{bmatrix} W & W \end{bmatrix} \tag{22}$$

where W and W are column-orthogonal matrices of sizes $p \times r$ and $p \times (p - r)$ respectively. It may be verified by substitution in (19) that

$$X = F G W^T \tag{23}$$

Let ran(X) denote the range of X (the space of all n-vectors of the form X u where u is an arbitrary -vector). It follows from (23) that ran(X) □ ran(F G). Furthermore, since any r-vector v can be written in the form v = W^{T}u by setting u = W v, it follows that ran(X) = ran(F G).

Let P = X X^T. Then P = F G W^{T}W GF^T = F G^{2}F^T. Thus ran(P) □ ran(F G). Furthermore, since any r-vector v can be written in the form v = G F^{T}u by setting u = F G$^-$ v, it follows that

$$\text{ran(P) = ran(F G) = ran(X)} \tag{24}$$

By the hypothesis of the theorem P = X$_2$X$_2^T$ as well. Therefore

$$\text{ran}(X_2) = \text{ran(P)} = \text{ran(F G)} \tag{25}$$

It follows that every column of X$_2$ can be expressed as a linear combination of the columns of F G . Thus there exists an × r matrix W̃ such that

$$X_2 = \text{F G } \tilde{W}^T \tag{26}$$

Now

$$\text{F G}^2\text{F}^T = \text{P} = X_2 X_2^T = \text{F G } \tilde{W}^T \tilde{W} \text{ G F}^T \tag{27}$$

Pre-multiplying the first and last terms of this chain of equations by G$^-$ F^T and post-multiplying by F G$^-$ gives I = W̃^{T}W̃ . Thus W̃ is a column-orthogonal matrix and may be extended to a full × orthogonal matrix

$$\tilde{W} = \begin{bmatrix} \tilde{W} & \tilde{W} \end{bmatrix} \tag{28}$$

It may be verified by substitution that

$$X_2 = \text{FG}\tilde{W}^T \tag{29}$$

and thus

$$X_2 = \text{X W}\tilde{W}^T \tag{30}$$

Here W and W̃ are orthogonal matrices, and so therefore is WW̃^{T}. Thus the theorem is proven by setting U = WW̃^{T}. □

matrix $\mathbf{U}$ such that $\mathbf{X}^a = \tilde{\mathbf{X}}\mathbf{U}$. Let $\mathbf{T} = \mathbf{T}\ \mathbf{U}$. Then $\mathbf{X}^a = \mathbf{X}^f\mathbf{T}$ and $\mathbf{T}$ satisfies (17) by theorem 2. □

The results of this section make it possible to characterise the structure of the set of all ensemble SRF filters in terms of a well-known group of matrices; see appendix A for details.

4 Bias

A fact that appears to have been overlooked by Tippett et al. (2003) is that the ensemble SRF framework encompasses filters that are not EnKFs. To see this, suppose that an arbitrary ensemble SRF is a semi-deterministic EnKF. Then it follows from (9) and (15) that $\tilde{\mathbf{x}}$ equals the analysis ensemble mean $\overline{\mathbf{x}^a}$ and that $\tilde{\mathbf{X}}$ equals the analysis ensemble perturbation matrix $\mathbf{X}^a$. However, (2) implies that the sum of the columns of an ensemble perturbation matrix must be zero, and this does not necessarily follow from (16) and (17), which are the only constraints on $\tilde{\mathbf{X}}$. To see this, let $\mathbf{T}$ be a particular solution of (17). Then by theorem 2 a more general solution is $\mathbf{TU}$ where $\mathbf{U}$ is an arbitrary $m \times m$ orthogonal matrix. The corresponding general value of $\tilde{\mathbf{X}}$ is

$$\tilde{\mathbf{X}} = \mathbf{X}^f\mathbf{T}\mathbf{U} \tag{32}$$

Now let $\mathbf{1}$ be a column m-vector in which every element is 1; that is

$$\mathbf{1} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \tag{33}$$

The sum of the columns of $\tilde{\mathbf{X}}$ is

$$\tilde{\mathbf{X}}\mathbf{1} = \mathbf{X}^f\mathbf{T}\mathbf{U}\mathbf{1} \tag{34}$$

Thus $\tilde{\mathbf{X}}$ is a valid ensemble perturbation matrix if and only if $\mathbf{U1}$ lies in the null space of ensemble collapses to a point), there will be at least some choices of $\mathbf{U}$ that give $\tilde{\mathbf{X}}\mathbf{1} \neq \mathbf{0}$ and hence an $\tilde{\mathbf{X}}$ that is invalid as an ensemble perturbation matrix. In these cases the ensemble SRF cannot be a valid semi-deterministic EnKF.

To see the effect of treating an ensemble SRF that is not a valid semi-deterministic EnKF as though it were, let $\mathbf{x}'_i$ denote the ith column of $\sqrt{N-1}\,\tilde{\mathbf{X}}$, and let

deviations are close to one-tenth of the amplitude of the oscillations in the truth. The same covariance matrix is used in generating a random initial ensemble, centred on the true initial state.

Fig. 1 shows the difference between the filter and the truth for and r. There are considerable intervals of time during which the true state of the system (represented by zero on the vertical axis) is outside the band defined by the ensemble mean ± ensemble standard deviation. This suggests that the ensemble statistics may be inconsistent with the actual error. This is confirmed by computing the fraction of analyses having an ensemble mean within one ensemble standard deviation of the perturbation matrix and thus has columns that sum to zero. Therefore $\tilde{\mathbf{X}}\mathbf{1} = \mathbf{0}$ and the ensemble SRF is unbiased.

Suppose conversely that a filter is an unbiased ensemble SRF. Unbiasedness implies that $\tilde{\mathbf{x}}$ is the mean of the analysis ensemble and $\tilde{\mathbf{X}}$ is the analysis ensemble perturbation matrix. Equation (15) implies that $\overline{\mathbf{x}^a}$ satisfies (9) in the definition of a semi-deterministic EnKF, whilst theorem 1 implies that $\mathbf{P}^a$ satisfies (10) in the same definition. Therefore the filter in a semi-deterministic EnKF. □

6 Conditions for an unbiased ensemble SRF

Definitions 2 and 3 in conjunction with theorem 8 reduce the problem of constructing a semi-deterministic EnKF to finding a solution $\mathbf{T}$ of the matrix square root condition (17) and checking that the matrix $\tilde{\mathbf{X}}$ defined by (16) satisfies $\tilde{\mathbf{X}}\mathbf{1} = \mathbf{0}$. It would be useful to replace this condition on $\tilde{\mathbf{X}}$ with one on $\mathbf{T}$, so that the problem of finding a semi-deterministic EnKF is reduced to one of finding $\mathbf{T}$ satisfying certain conditions. Such conditions for $\mathbf{T}$ are provided in this section. It is assumed throughout that $\mathbf{T}$ satisfies the matrix square root condition (17). The first theorem gives an additional sufficient condition for the resulting ensemble SRF to be unbiased.

Theorem 9 If $\mathbf{1}$ is an eigenvector of $\mathbf{T}$, then the ensemble SRF is unbiased.

Proof. By hypothesis $\mathbf{T}\mathbf{1} = \ \mathbf{1}$ for some scalar . Therefore $\tilde{\mathbf{X}}\mathbf{1} = \mathbf{X}^f\mathbf{T}\mathbf{1} = \ \mathbf{X}^f\mathbf{1} = \mathbf{0}$. Therefore the filter is unbiased. □

An important special case is that of a symmetric $\mathbf{T}$. This is the subject of the following theorem and its corollary.

Theorem 10 If $\mathbf{T}$ is symmetric, then $\mathbf{1}$ is an eigenvector of $\mathbf{T}$.

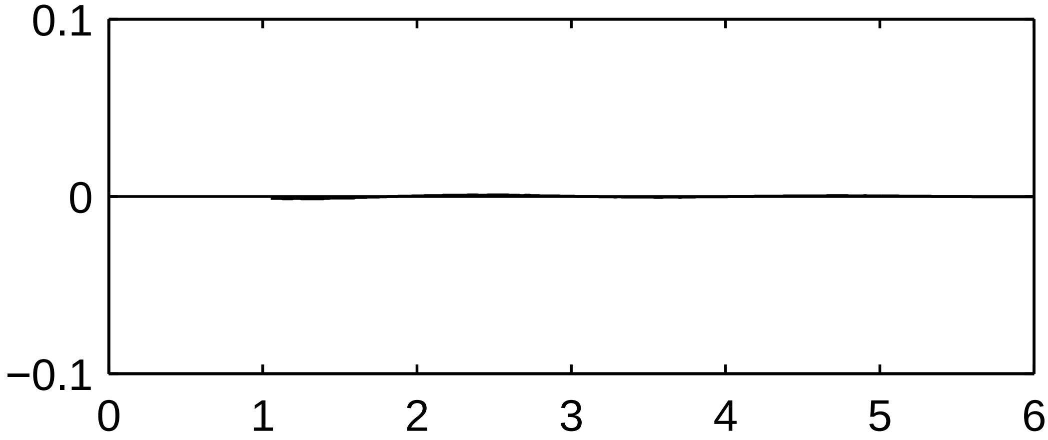
Proof. Since $\mathbf{Y}^f$ is an ensemble perturbation matrix, it satisfies $\mathbf{Y}^f\mathbf{1} = \mathbf{0}$. Therefore it follows from (17) that $\mathbf{T}^2\mathbf{1} = \mathbf{1}$ for symmetric $\mathbf{T}$. Thus $\mathbf{1}$ is an eigenvector of $\mathbf{T}^2$. But the eigenvectors of the square of a symmetric matrix are the same as those of the original matrix. Therefore $\mathbf{1}$ is an eigenvector of $\mathbf{T}$. □

Corollary 11 If T is symmetric, then the ensemble SRF is unbiased.

Although not as general as theorem 9, corollary 11 provides a particularly simple

Proof.

Since $\mathbf{C}^T$


0.1
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−0.1
0
1
2
3
4
5
6

augmented state space of the type discussed at the end of section 2 must be used to apply it to a nonlinear observation operator. Tippett et al. (2003, section 3a) outline how the EAKF may be expressed in post-multiplier form (16), but the demonstration glosses over a few details[2]. Therefore an alternative proof is presented here. This proof is based on the SVD of $\mathbf{X}^f$ instead of on the eigenvalue decomposition of $\mathbf{P}^f$ as in Tippett et al. (2003).

The first step is to construct the reduced SVD of $\mathbf{X}^f$ as in the proof of theorem 3:

$$\mathbf{X}^f = \mathbf{F}\ \mathbf{G}\ \mathbf{W}^T \tag{46}$$

where $\mathbf{G}$ is an $r \times r$ diagonal matrix of the nonzero singular values of $\mathbf{X}^f$ and $\mathbf{F}$

related to $\mathbf{G}$, $\mathbf{F}$, and $\mathbf{W}$ by (20), (21), and (22). The eigenvalue decomposition (47) extends to

$$(\mathbf{HFG})^T\mathbf{R}^{-}\,\mathbf{HFG} = \tilde{\mathbf{C}}\tilde{\mathbf{F}}\tilde{\mathbf{C}}^T \tag{51}$$

where $\tilde{\mathbf{C}}$ is orthogonal, $\tilde{\mathbf{F}}$ is diagonal, and both are $m \times m$. This is achieved by setting

$$\tilde{\mathbf{C}} = \begin{bmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \breve{\mathbf{C}} \end{bmatrix} \tag{52}$$

$$\tilde{\mathbf{F}} = \begin{bmatrix} \mathbf{F} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \tag{53}$$

where $\breve{\mathbf{C}}$ is an $(m - r) \times (m - r)$ orthogonal matrix. It may be verified by substitution that (51) is satisfied. Similarly it follows by substitution that $\mathbf{X}^a$ defined by (49) also satisfies

$$\mathbf{X}^a = \mathbf{FG}\tilde{\mathbf{C}}(\mathbf{I} + \tilde{\mathbf{F}})^{-\frac{1}{2}}\mathbf{W}^T = \mathbf{X}^f\mathbf{T} \tag{54}$$

where

$$\mathbf{T} = \mathbf{W}\tilde{\mathbf{C}}(\mathbf{I} + \tilde{\mathbf{F}})^{-1}$$

require a linear observation operator, but it will be shown below that this restriction can be eliminated. The filter is given by

$$\mathbf{X}^a = (\mathbf{I} - \tilde{\mathbf{K}}\mathbf{H})\mathbf{X}^f \tag{57}$$

where $\tilde{\mathbf{K}}$ is a solution of

$$(\mathbf{I} - \tilde{\mathbf{K}}\mathbf{H})\mathbf{P}^f(\mathbf{I} - \tilde{\mathbf{K}}\mathbf{H})^T = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}^f \tag{58}$$

$\mathbf{K}$ being the standard Kalman gain defined by (6). This equation ensures that the ensemble covariance matrix updates as in (5). A solution of (58) is given in Whitaker and Hamill (2002), based on Andrews (1968). This solution is

$$\begin{aligned}
\tilde{\mathbf{K}} &= \mathbf{P}^f\mathbf{H}^T\left(\left(\sqrt{\mathbf{H}\mathbf{P}^f\mathbf{H}^T + \mathbf{R}}\right)^T\right)^{-1}\left(\sqrt{\mathbf{H}\mathbf{P}^f\mathbf{H}^T + \mathbf{R}} + \sqrt{\mathbf{R}}\right)^{-1} \\
&= \mathbf{X}^f(\mathbf{Y}^f)^T\left(\sqrt{\mathbf{D}}^T\right)^{-1}\left(\sqrt{\mathbf{D}} + \sqrt{\mathbf{R}}\right)^{-1}
\end{aligned} \tag{59}$$

where, given a symmetric positive definite $p \times p$ matrix $\mathbf{V}$, the square root $\sqrt{\mathbf{V}}$ stands for a $p \times p$ matrix such that $\sqrt{\mathbf{V}}\sqrt{\mathbf{V}}^T = \mathbf{V}$. The general solution (59) is not considered in Tippett et al. (2003), which instead concentrates on the case of scalar observations where $p = 1$. However, it is not difficult to show that the more general form fits into the ensemble SRF framework. To do this, expand (57) and substitute (59) to obtain

$$\begin{aligned}
\mathbf{X}^a &= \mathbf{X}^f - \tilde{\mathbf{K}}\mathbf{Y}^f \\
&= \mathbf{X}^f - \mathbf{X}^f(\mathbf{Y}^f)^T\left(\sqrt{\mathbf{D}}^T\right)^{-1}\left(\sqrt{\mathbf{D}} + \sqrt{\mathbf{R}}\right)^{-1}\mathbf{Y}^f \\
&= \mathbf{X}^f\mathbf{T}
\end{aligned} \tag{60}$$

where

$$\mathbf{T} = \mathbf{I} - (\mathbf{Y}^f)^T\left(\sqrt{\mathbf{D}}^T\right)^{-1}\left(\sqrt{\mathbf{D}} + \sqrt{\mathbf{R}}\right)^{-1}\mathbf{Y}^f \tag{61}$$

Note that the linear operator $\mathbf{H}$ does not explicitly appear in this post-multiplier form of the filter, which may therefore be applied when the observation operator is nonlinear. It may be shown that $\mathbf{T}$ satisfies (17) as follows (which adapts a proof of Andrews (1968)):

$$\mathbf{T}\mathbf{T}^T = \left[\mathbf{I} - (\mathbf{Y}^f)^T\left(\sqrt{\mathbf{D}}^T\right)^{-1}\left(\sqrt{\mathbf{D}} + \sqrt{\mathbf{R}}\right)^{-1}\mathbf{Y}^f\right]$$

$$
\times \left(\mathbf{I} - (\mathbf{Y}^f)^T \left(\sqrt{\mathbf{D}}^T \right)^{-1} \left(\sqrt{\mathbf{D}} + \sqrt{\mathbf{R}} \right)^{-1} \mathbf{Y}^f \right)^T
$$

$$
= \left(\mathbf{I} - (\mathbf{Y}^f)^T \left(\sqrt{\mathbf{D}}^T \right)^{-1} \left(\sqrt{\mathbf{D}} + \sqrt{\mathbf{R}} \right)^{-1}
$$

$$
\times \left(\sqrt{\mathbf{D}} \left(\sqrt{\mathbf{D}} + \sqrt{\mathbf{R}} \right)^T + \left(\sqrt{\mathbf{D}} + \sqrt{\mathbf{R}} \right) \sqrt{\mathbf{D}}^T - \mathbf{Y}^f (\mathbf{T}
$$

The analysis ensemble statistics produced by a biased ensemble SRF are undesirable for a number of reasons beyond the simple fact that a biased mean tends to put the filter's best state estimate in the wrong place. Such a bias would not be too great a problem if it were accompanied by an increase in the size of the error estimate provided by the filter's covariance matrix. Users of the output would then be aware of the increased error, although they would remain unaware that part of the error is systematic rather than random. However, as is shown in section 4, there a best state estimate is maintained separately from the ensemble, which still provides the measurement of estimation error. The forecast and analysis perturbation matrices are taken relative to the forecast and analysis best state estimates rather than the ensemble means. It is not necessary for the columns of these matrices to sum to zero and hence there is no need to impose an unbiasedness condition in the analysis step: the ensemble perturbation matrices may be updated using $\mathbf{X}^a = \mathbf{X}^f\mathbf{T}$ where $\mathbf{T}$ is any solution of the matrix square root condition (17). An example of such a filter is the maximum likelihood ensemble filter (MLEF) of Zupanski (2005), in which the analysis step updates the best state estimate using 3D-Var (with a cost function that uses the forecast ensemble covariance matrix instead of a static background error covariance matrix) and updates the ensemble perturbations using the ETKF. Although that paper references the original ETKF of Bishop et al. (2001), it is in fact the revised ETKF of Wang et al. (2004) that is used [3].

Finally, it must be stated the the type of bias discussed in this paper is not the only type of bias that may be encountered with an EnKF. Inconsistent ensemble statistics have been observed in formulations of the EnKF other than the original ETKF. Houtekamer and Mitchell (1998) present results showing problems with a stochastic EnKF and Anderson (2001) discusses the issue in the context of the EAKF. The causes of the inconsistencies in these cases must be different to that of the ETKF bias established in section 8.1. The authors attribute them to the use of small ensembles and to other approximations made in the course of deriving the filters. Various solutions to the problem have been proposed in the literature. Houtekamer and Mitchell (1998) use a pair of ensembles with the covariance calculated from each ensemble being used to assimilate observations into the other. The justification for such an approach is discussed further in van Leeuwen (1999) and Houtekamer and Mitchell (1999). Anderson (2001) uses a tunable scalar covariance inflation factor. The more fundamental problems of model and observation biases are not addressed here. Such biases may be estimated using data assimilation with an augmented state vector (e.g., Nichols (2003)). The incorporation of these

[3] By Zupanski (2005, (10) and (12)) the post-multiplier matrix is $\mathbf{V}(\mathbf{I}+\mathbf{\Lambda})^{-1/2}\mathbf{V}^{\mathrm{T}}$ in the notation of that paper, which corresponds to (45) in this paper

techniques into the ensemble SRF framework is left for future work.

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A Structure of the set of ensemble SRFs

This appendix uses the results of section 3 to describe the se

cancelled from both sides of this equation to give U = U . Therefore U is unique.
□

Theorems 2 and 18 imply the following description of the set of all solutions T of (17) in terms of the group $O($) of all × orthogonal matrices.

Corollary 19 Let T be a solution of (17). Then U ↔ T U defines a one-to-one correspondence between $O($) and the solutions T of (17).

Thus the set of all ensemble SRFs is in one-to-one correspondence with $O($).

B The Two-Dimensional Swinging Spring

The two-dimensional swinging spring (Lynch, 2003) consists of a heavy bob of mass suspended from a fixed point in a uniform gravitational field of acceleration g by a light spring of unstretched length and elasticity k. The bob is constrained to move in a vertical plane. The system coordinates are polar coordinates r, (r measured from the point of suspension, measured from the downward vertical) and the corresponding generalised momenta p_r, p_θ. The equations of motion are

$$\dot{} = \frac{p_\theta}{\ r^2} \qquad (64)$$

$$\dot{p}_\theta = \ gr \sin$$

Theorem 20 Suppose that $\mathbf{X}^f$ is nondegenerate and that $\mathbf{T}$ is the post-multiplier matrix of an unbiased ensemble SRF. Then $\mathbf{U} \leftrightarrow \mathbf{T}\mathbf{U}$ defines a one-to-one correspondence between the subgroup of all matrices $\mathbf{U}$ in $O(N)$ that have $\mathbf{1}$ as an eigenvector and the set of post-multiplier matrices of unbiased ensemble SRFs.

Proof. This follows from corollary 19 and theorems 13 and 14. □

The subgroup in theorem 20 is given more concrete form by the following theorem.

Theorem 21 There is a one-to-one correspondence between the subgroup of all matrices in $O(N)$ that have $\mathbf{1}$ as an eigenvector and the group $O(1) \times O(N-1)$.

Proof. Let $\mathbf{W}$ be an orthogonal matrix in which the first column is a scalar multiple of $\mathbf{1}$. Then $\mathbf{U} \leftrightarrow \mathbf{W}^T\mathbf{U}\mathbf{W}$ is a one-to-one correspondence between $O(N)$ and itself. Under this correspondence, matrices $\mathbf{U}$ that have $\mathbf{1}$ as an eigenvector correspond to matrices that have the coordinate vector

$$\mathbf{e} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{68}$$

as an eigenvector. The latter matrices are those of the form

$$\begin{pmatrix} \mathbf{U} & \mathbf{0} \\ \mathbf{0} & \mathbf{U}_2 \end{pmatrix} \tag{69}$$

where $\mathbf{U}$ is an element of $O(1)$ (that is to say $\mathbf{U} = \pm 1$) and $\mathbf{U}_2$ is an element of $O(N-1)$. This establishes the required correspondence. □

Thus, in the case of nondegenerate $\mathbf{X}^f$, the set of all unbiased ensemble SRFs is in one-to-one correspondence with $O(1) \times O(N-1)$.

References

J. L. Anderson. An ensemble adjustment Kalman filter for data assimilation. Mon. Wea. Rev., 129:2884–2903, 2001.

A. Andrews. A square root formulation of the Kalman covariance equations. AIAA J., 6:1165–1166, 1968.

C. H. Bishop, B. J. Etherton, and S. J. Majumdar. Adaptive sampling with the ensemble transform Kalman filter. Part I: Theoretical aspects. Mon. Wea. Rev., 129:420–436, 2001.

G. Burgers, P. J. van Leeuwen, and G. Evensen. Analysis scheme in the ensemble Kalman filter. Mon. Wea. Rev., 126:1719–1724, 1998.

G. Evensen. Sequential data assimilation with a nonlinear quasi-geostrophic model using Monte Carlo methods to forecast error statistics. J. Geophys. Res., 99(C5): 10143–10162, 1994.

G. Evensen. The Ensemble Kalman Filter: Theoretical formulation and practical implementation. Ocean Dynamics, 53:343–367, 2003.

A. Gelb, editor. Applied Optimal Estimation. The M.I.T. Press, 1974. 374 pp.

G. H. Golub and C. F. Van Loan. Matrix Computations. The Johns Hopkins University Press, 3rd edition, 1996. 694 pp.

P. R. Halmos. Finite-Dimensional Vector Spaces. Springer-Verlag, 1974. 200 pp.

P. L. Houtekamer and H. L. Mitchell. Data assimilation using an ensemble Kalman filter technique. Mon. Wea. Rev., 126:796–811, 1998.

P. L. Houtekamer and H. L. Mitchell. Reply. Mon. Wea. Rev., 127:1378–1379, 1999.

A. H. Jazwinski. Stochastic Processes and Filtering Theory. Academic Press, 1970. 376 pp.

P. Lynch. Introduction to initialization. In R. Swinbank, V. Shutyaev, and W. A. Lahoz, editors, Data Assimilation for the Earth System, pages 97–111. Kluwer Academic Publishers, 2003.

N. K. Nichols. Treating model error in 3-d and 4-d data assimilation. In R. Swinbank, V. Shutyaev, and W. A. Lahoz, editors, Data Assimilation for the Earth System, pages 127–135. Kluwer Academic Publishers, 2003.