

Ensemble square-root filters

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Abstract

Ensemble data assimilation methods can be formulated as *square-root filters*. A key step of ensemble data assimilation methods is the transformation of the forecast ensemble into an analysis ensemble with appropriate statistics. This transformation may be done stochastically by treating observations as random variables, or deterministically by requiring that the updated analysis perturbations satisfy the Kalman filter analysis error covariance equation. The nonuniqueness of the deterministic transformation used in square-root Kalman filters provides a framework to compare three recently proposed ensemble data assimilation methods.

1. Introduction

Data assimilation addresses the problem of producing useful analyses and forecasts given imperfect dynamical models and observations. The Kalman filter is the optimal data assimilation method for linear dynamics with additive, state-independent Gaussian model and observation error (Cohn, 1997). An attractive feature of the Kalman filter is its calculation of forecast and analysis error covariances, in addition to the forecast and analyses themselves. In this way, the Kalman filter produces estimates of forecast and analysis uncertainty, consistent with the dynamics and prescribed model and observation error statistics. However, the error covariance calculation component of the Kalman filter is difficult to implement in realistic systems because of *(i)* computational cost of error covariance calculations in systems with many degrees of freedom, *(ii)* nonlinearity of the dynamics and *(iii)* poorly characterized error sources.

Evensen (1994) proposed the ensemble Kalman filter (EnKF) to address the first two of these problems. In the EnKF, the forecast and analysis error covariances have ensemble representations. Ensemble size limits the number of degrees of freedom used to represent forecast and analysis errors, making Kalman filter error covariance calculations practical for modest ensemble sizes. The EnKF algorithm begins with an analysis ensemble whose mean is the current state-estimate or analysis and whose sample statistics reflect the analysis error. Then, the full nonlinear dynamics are applied to each analysis ensemble member to obtain a forecast ensemble. Sample statistics of the forecast ensemble represent forecast errors; in its simplest form, the EnKF only accounts for forecast error due to uncertain initial conditions and neglects forecast error due to model deficiencies. The forecast ensemble mean and covariance are then used to assimilate observations and compute an analysis and its error covariance. Finally, a new analysis ensemble with appropriate statistics is formed, and the cycle is repeated. The new analysis ensemble can be formed stochas-

tically (Houtekamer and Mitchell, 1998; Burgers et al., 1998) or deterministically (Bishop et al., 2001; Anderson, 2001; Whitaker and Hamill, 2001).

The purpose of this paper is to demonstrate that the EnKF and other ensemble data assimilation methods belong to the family of *square-root filters* (SRFs) and that deterministic analysis ensemble updates are implementations of Kalman square-root filters (Bierman, 1977; Maybeck, 1982). An immediate benefit of this identification is a unified context for understanding and comparing deterministic analysis ensemble update schemes (Bishop et al., 2001; Anderson, 2001; Whitaker and Hamill, 2001). SRFs, like ensemble representations of covariances, are not unique. We begin our discussion in Section 2 with a presentation of the square-root Kalman filter; issues related to implementation of ensemble SRFs are presented in Section 3; in Section 4 we summarize our results.

2. Square-root Kalman filter

Square-root Kalman filters algorithms, originally developed for space-navigation systems with limited computational word length, demonstrate superior numerical precision and stability compared to the standard Kalman filter algorithm (Bierman, 1977; Maybeck, 1982). SRFs by construction avoid loss of positive definiteness of the error covariance matrices. SRFs have been used in Earth Science data assimilation methods where error covariances are approximated by truncated eigenvector expansions (Verlaan and Heemink, 1997).

The usual Kalman filter covariance evolution equations are

$$\mathbf{P}_k^f = \mathbf{M}_k \mathbf{P}_{k-1}^a \mathbf{M}_k^T + \mathbf{Q}_k, \quad (1)$$

$$\mathbf{P}_k^a = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_k^f, \quad (2)$$

where \mathbf{P}_k^f and \mathbf{P}_k^a are respectively the $n \times n$ forecast and analysis error covariance matrices at

time t_k , \mathbf{M}_k is the linear tangent dynamics, \mathbf{H}_k is the $p \times n$ observation operator, \mathbf{R}_k is the $p \times p$ observation error covariance, \mathbf{Q}_k is the $n \times n$ model error covariance matrix and $\mathbf{K}_k \equiv \mathbf{P}_k^f \mathbf{H}_k^T (\mathbf{H}_k \mathbf{P}_k^f \mathbf{H}_k^T + \mathbf{R}_k)^{-1}$ is the Kalman gain; n is the dimension of the system state; p is the number of observations. The error covariance evolution depends on the state estimates and observations through the linear tangent dynamics \mathbf{M}_k . Equation (1) describes the propagation of analysis errors by the dynamics with model error acting as a forcing. Equation (2) shows how an optimal data assimilation scheme uses observations to produce an analysis whose error is less than that of the forecast.

The forecast and analysis error covariance matrices are positive-definite and can be represented $\mathbf{P}_k^f = \mathbf{Z}_k^f \mathbf{Z}_k^{fT}$ and $\mathbf{P}_k^a = \mathbf{Z}_k^a \mathbf{Z}_k^{aT}$ where the matrices \mathbf{Z}_k^f and \mathbf{Z}_k^a are *matrix square-roots* of \mathbf{P}_k^f and \mathbf{P}_k^a respectively. Matrix square-roots are not unique; if an $n \times n$ covariance matrix \mathbf{P} has the representation $\mathbf{P} = \mathbf{Z}\mathbf{Z}^T$ where \mathbf{Z} is an $n \times m$ matrix, then it can also be represented as $\mathbf{P} = (\mathbf{Z}\mathbf{U})(\mathbf{Z}\mathbf{U})^T$ where \mathbf{U} is any $m \times m$ orthogonal transformation $\mathbf{U}\mathbf{U}^T = \mathbf{U}^T\mathbf{U} = \mathbf{I}$. The projection $\|\mathbf{x}^T \mathbf{Z}\|^2 = \mathbf{x}^T \mathbf{P} \mathbf{x}$ of an n -vector \mathbf{x} onto the matrix square-root \mathbf{Z} is uniquely determined, as is the subspace spanned by the columns of \mathbf{Z} . Covariance matrix square-roots are closely related to ensemble representations. Suppose the m -member analysis ensemble consists of the n -vectors $\{\mathbf{s} + \mathbf{s}_1, \mathbf{s} + \mathbf{s}_2, \dots, \mathbf{s} + \mathbf{s}_m\}$; \mathbf{s} is the ensemble mean and \mathbf{s}_i , $1 \leq i \leq m$, are the m mean-zero analysis perturbations. Assuming that the analysis ensemble adequately represents analysis error, the analysis error covariance is given by

$$\mathbf{P}_k^a = \frac{1}{m-1} \sum_{i=1}^m \mathbf{s}_i \mathbf{s}_i^T = \frac{1}{m-1} \mathbf{S} \mathbf{S}^T, \quad (3)$$

where the $n \times m$ matrix \mathbf{S} is given by $\mathbf{S} \equiv [\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_m]$. Therefore a matrix square-root of the analysis error covariance matrix \mathbf{P}_k^a is the matrix of scaled analysis perturbation ensemble members $\mathbf{Z}_k^a = (m-1)^{-1/2} \mathbf{S}$.

The square-root Kalman filter algorithm replaces error covariance evolution equations (1) and (2) with equations for the evolution of forecast and analysis error covariance square-roots \mathbf{Z}_k^f and \mathbf{Z}_k^a in such a manner that the full error covariance matrices are not formed. Neglecting the model error \mathbf{Q}_k , (1) can be replaced by

$$\mathbf{Z}_k^f = \mathbf{M}_k \mathbf{Z}_{k-1}^a . \quad (4)$$

In the ensemble context, (4) means to apply the linear tangent dynamics to each column of the \mathbf{Z}_{k-1}^a , that is, to each scaled analysis perturbation ensemble member. Practically, (4) is implemented by applying the full nonlinear dynamics to each analysis ensemble member.

Next, analysis error covariance equation (2) is replaced with an equation for the analysis error covariance square-root \mathbf{Z}_k^a . This equation determines how to form an analysis ensemble with appropriate statistics. Initial implementations of the EnKF formed the new analysis ensemble by updating each forecast ensemble member using the same analysis equations, equivalent to applying the linear operator $(\mathbf{I} - \mathbf{K}_k \mathbf{H}_k)$ to the forecast perturbation ensemble \mathbf{Z}_k^f . This procedure gives an analysis ensemble whose statistics do not include uncertainty due to observation error and so underestimates analysis error. A *stochastic* solution to this problem proposed independently by Houtekamer and Mitchell (1998) and Burgers et al. (1998) was to compute analyses using each forecast ensemble member and, instead of using a single realization of the observations, to use an ensemble of simulated observations whose statistics reflect the observation error. This method is equivalent to the analysis perturbation ensemble update

$$\mathbf{Z}_k^a = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{Z}_k^f + \mathbf{K}_k \mathbf{w}_k , \quad (5)$$

where \mathbf{w}_k is a mean-zero, Gaussian random vector of length p with covariance $\langle \mathbf{w}_k \mathbf{w}_k^T \rangle = \mathbf{R}_k$. The perturbed observation analysis equation (5) gives an analysis perturbation ensemble with correct

expected statistics:

$$\begin{aligned}\langle \mathbf{Z}_k^a (\mathbf{Z}_k^a)^T \rangle &= (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_k^a (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k)^T + \mathbf{K}_k \mathbf{R}_k \mathbf{K}_k^T \\ &= \mathbf{P}_k^a.\end{aligned}\quad (6)$$

However, the perturbed observation approach introduces an additional source of sampling error that (i) reduces analysis error covariance accuracy and (ii) increases the probability of underestimating analysis error covariance (Whitaker and Hamill, 2001). A Monte Carlo method that avoids perturbed observations is described in Pham (2001).

Square-root Kalman filters provide a *deterministic* algorithm for transforming the forecast ensemble into an analysis ensemble with consistent statistics. The ‘‘Potter method’’ for the square-root Kalman filter analysis update (Bierman, 1977) is obtained by first rewriting (2) as

$$\begin{aligned}\mathbf{P}_k^a &= \mathbf{Z}_k^a \mathbf{Z}_k^{aT} = (\mathbf{I} - \mathbf{P}_k^f \mathbf{H}_k^T (\mathbf{H}_k \mathbf{P}_k^f \mathbf{H}_k^T + \mathbf{R}_k)^{-1} \mathbf{H}_k) \mathbf{P}_k^f \\ &= \mathbf{Z}_k^f \mathbf{Z}_k^{fT} - \mathbf{Z}_k^f \mathbf{Z}_k^{fT} \mathbf{H}_k^T (\mathbf{H}_k \mathbf{Z}_k^f \mathbf{Z}_k^{fT} \mathbf{H}_k^T + \mathbf{R}_k)^{-1} \mathbf{H}_k \mathbf{Z}_k^f \mathbf{Z}_k^{fT} \\ &= \mathbf{Z}_k^f (\mathbf{I} - \mathbf{Z}_k^{fT} \mathbf{H}_k^T (\mathbf{H}_k \mathbf{Z}_k^f \mathbf{Z}_k^{fT} \mathbf{H}_k^T + \mathbf{R}_k)^{-1} \mathbf{H}_k \mathbf{Z}_k^f) \mathbf{Z}_k^{fT}.\end{aligned}\quad (7)$$

Next, the $m \times p$ matrix $\mathbf{V}_k \equiv (\mathbf{H}_k \mathbf{Z}_k^f)^T$ and the $p \times p$ innovation covariance matrix $\mathbf{D}_k \equiv \mathbf{V}_k^T \mathbf{V}_k + \mathbf{R}_k$ are defined. Then (2) can be written as

$$\mathbf{P}_k^a = \mathbf{Z}_k^a \mathbf{Z}_k^{aT} = \mathbf{Z}_k^f (\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T) \mathbf{Z}_k^{fT}, \quad (8)$$

so that the analysis perturbation ensemble is

$$\mathbf{Z}_k^a = \mathbf{Z}_k^f \mathbf{X}_k \mathbf{U}_k, \quad (9)$$

where $\mathbf{X}_k \mathbf{X}_k^T = (\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T)$ and \mathbf{U}_k is an arbitrary $m \times m$ orthogonal matrix. As formulated, the updated ensemble \mathbf{Z}_k^a is a linear combination of the columns of \mathbf{Z}_k^f and is obtained by inverting the $p \times p$ matrix \mathbf{D}_k and computing a matrix square-root of the $m \times m$ matrix $(\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T)$.

3. Ensemble SRFs

a. Forecast ensemble

Ensemble size is limited by the computational cost of applying the forecast model to each ensemble member. Small ensembles have few degrees of freedom available to represent errors and suffer from sampling error that further degrades covariance representation. Sampling error leads to loss of accuracy and underestimation of error covariances that can cause filter divergence. Techniques to deal with this problem are distance-dependent covariance filtering and covariance inflation (Whitaker and Hamill, 2001). Neglecting model error in (1) also causes the forecast error covariance to be underestimated, a problem that can be lessened by covariance inflation.

When the model error covariance \mathbf{Q}_k has large-scale structure, a reasonable representation is an ensemble or square-root decomposition $\mathbf{Q}_k = \mathbf{Z}_k^d \mathbf{Z}_k^{dT}$ where \mathbf{Z}_k^d is an $n \times q$ matrix. Then, a square-root of \mathbf{P}_k^f is the $n \times (m + q)$ matrix

$$\mathbf{Z}_k^f = [\mathbf{M}\mathbf{Z}_k^a \mathbf{Z}_k^d] . \quad (10)$$

With this model error representation, ensemble size grows by q with each forecast/analysis cycle. Ensemble size can be limited by computing the singular value decomposition of the ensemble and discarding components with small variance. When the model error covariance \mathbf{Q}_k is approximated as an operator, for instance a correlation model, Lanczos methods can be used to compute the leading eigenmodes of $\mathbf{M}_k \mathbf{P}_{k-1}^a (\mathbf{M}_k \mathbf{Z}_{k-1}^a)^T + \mathbf{Q}_k$ and form \mathbf{Z}_k^f (Cohn and Todling, 1996). Perturbing model physics, as done in *system simulation*, explicitly accounts for some aspects of model error (Houtekamer et al., 1996).

b. Analysis ensemble

Standard methods for computing the matrix square-root of $(\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T)$ and the updated analysis perturbation ensemble \mathbf{Z}_k^a are not always well-suited to typical Earth Science data assimilation applications where the state-dimension n and the number of observations p are large (Bierman, 1977; Maybeck, 1982). A direct approach is to solve first the linear system $\mathbf{D}_k \mathbf{Y}_k = \mathbf{H}_k \mathbf{Z}_k^f$ for the $p \times m$ matrix \mathbf{Y}_k , that is, to solve

$$(\mathbf{H}_k \mathbf{P}_k^f \mathbf{H}_k^T + \mathbf{R}_k) \mathbf{Y}_k = \mathbf{H}_k \mathbf{Z}_k^f, \quad (11)$$

as is done in the first step of the PSAS algorithm (Cohn et al., 1998). Then, the $m \times m$ matrix $\mathbf{I} - \mathbf{V}^T \mathbf{D}^{-1} \mathbf{V} = \mathbf{I} - (\mathbf{H}_k \mathbf{Z}_k^f)^T \mathbf{Y}_k$ is formed, its matrix square-root computed and applied to \mathbf{Z}_k^f .

When observation errors are uncorrelated, observations can be efficiently assimilated one at a time or *serially* (Houtekamer and Mitchell, 2001). In the case of a single observation, $p = 1$, \mathbf{V}_k is a column-vector and the innovation \mathbf{D}_k is a scalar. In this case, a matrix square-root of $(\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T)$ can be computed in closed form by taking the *ansatz*

$$\mathbf{I} - \mathbf{D}_k^{-1} \mathbf{V}_k \mathbf{V}_k^T = (\mathbf{I} - \beta_k \mathbf{V}_k \mathbf{V}_k^T) (\mathbf{I} - \beta_k \mathbf{V}_k \mathbf{V}_k^T)^T, \quad (12)$$

and solving for the scalar β_k , which gives $\beta_k = (\mathbf{D}_k \pm \sqrt{\mathbf{R}_k \mathbf{D}_k})^{-1}$. This result is a special case of the general result that

$$\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T = (\mathbf{I} - \mathbf{V}_k \mathbf{B}_k \mathbf{V}_k^T) (\mathbf{I} - \mathbf{V}_k \mathbf{B}_k \mathbf{V}_k^T)^T, \quad (13)$$

where the $p \times p$ matrix \mathbf{B}_k is given by $\mathbf{B}_k \equiv (\mathbf{D}_k \pm \mathbf{R}_k^{1/2} \mathbf{D}_k^{1/2})^{-1}$ (Andrews, 1968). The analysis ensemble update for $p = 1$ is

$$\mathbf{Z}_k^a = \mathbf{Z}_k^f (\mathbf{I} - \beta_k \mathbf{V}_k \mathbf{V}_k^T). \quad (14)$$

At observation locations, the analysis error ensemble is related to the forecast error ensemble by $\mathbf{H}_k \mathbf{Z}_k^a = (1 - \beta_k \mathbf{V}_k^T \mathbf{V}_k) \mathbf{H}_k \mathbf{Z}_k^f$. The scalar factor $(1 - \beta_k \mathbf{V}_k^T \mathbf{V}_k)$ has absolute value less than or equal to one and is positive when the plus sign is chosen in the definition of β_k .

In Whitaker and Hamill (2001) the analysis perturbation ensemble is found from

$$\mathbf{Z}_k^a = (\mathbf{I} - \tilde{\mathbf{K}}_k \mathbf{H}_k) \mathbf{Z}_k^f, \quad (15)$$

where the matrix $\tilde{\mathbf{K}}_k$ is a solution of the nonlinear equation

$$(\mathbf{I} - \tilde{\mathbf{K}}_k \mathbf{H}_k) \mathbf{P}_k^f (\mathbf{I} - \tilde{\mathbf{K}}_k \mathbf{H}_k)^T = \mathbf{P}_k^a. \quad (16)$$

In the case of a single observation, a solution of (16) is

$$\tilde{\mathbf{K}}_k = \left(1 + \sqrt{\frac{\mathbf{R}_k}{\mathbf{D}_k}} \right)^{-1} \mathbf{K}_k = \beta_k \mathbf{Z}_k^f \mathbf{V}_k, \quad (17)$$

where the plus sign is chosen in the definition of β_k . The corresponding analysis perturbation ensemble update

$$\mathbf{Z}_k^a = (\mathbf{I} - \tilde{\mathbf{K}}_k \mathbf{H}_k) \mathbf{Z}_k^f = (\mathbf{I} - \beta_k \mathbf{Z}_k^f \mathbf{V}_k \mathbf{H}_k) \mathbf{Z}_k^f = \mathbf{Z}_k^f (\mathbf{I} - \beta_k \mathbf{V}_k \mathbf{V}_k^T), \quad (18)$$

is identical to (14). Observations with correlated errors, e.g., radiosonde height observations from the same sounding, can be handled by applying the whitening transformation $\mathbf{R}_k^{-1/2}$ to the observations to form a new observation set with uncorrelated errors.

Another approach to computing the updated analysis ensemble is to use the Sherman-Morrison-Woodbury identity (Golub and Van Loan, 1996) to show that

$$\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T = \left(\mathbf{I} + \mathbf{Z}_k^{fT} \mathbf{H}_k^T \mathbf{R}_k^{-1} \mathbf{H}_k \mathbf{Z}_k^f \right)^{-1}. \quad (19)$$

The $m \times m$ matrix on the right hand side of (19) is practical to compute when the operator $\mathbf{R}_k^{-1/2}$ is available to apply to $\mathbf{H}_k \mathbf{Z}_k^f$. This approach avoids inverting the $p \times p$ matrix \mathbf{D}_k and is used in the

ensemble transform filter Kalman filter (ET KF) where the analysis update is (Bishop et al., 2001)

$$\mathbf{Z}_k^a = \mathbf{Z}_k^f \mathbf{C}_k (\mathbf{\Gamma}_k + \mathbf{I})^{-1/2}; \quad (20)$$

$\mathbf{C}_k \mathbf{\Gamma}_k \mathbf{C}_k^T$ is the eigenvalue decomposition of $\mathbf{Z}_k^{fT} \mathbf{H}_k^T \mathbf{R}_k^{-1} \mathbf{H}_k \mathbf{Z}_k^f$. Note that the matrix \mathbf{C}_k of orthonormal eigenvectors is not uniquely determined.¹ Comparison with (19) shows that $\mathbf{C}_k (\mathbf{\Gamma}_k + \mathbf{I})^{-1} \mathbf{C}_k^T$ is the eigenvalue decomposition of $\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T$ and thus that $\mathbf{C}_k (\mathbf{\Gamma}_k + \mathbf{I})^{-1/2}$ is a square-root of $(\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T)$.

In the *ensemble adjustment Kalman filter* (EAKF) the form of the analysis ensemble update is (Anderson, 2001)

$$\mathbf{Z}_k^a = \mathbf{A}_k \mathbf{Z}_k^f; \quad (21)$$

the ensemble adjustment matrix \mathbf{A}_k is defined by

$$\mathbf{A}_k \equiv \mathbf{F}_k \mathbf{G}_k \tilde{\mathbf{C}}_k (\mathbf{I} + \tilde{\mathbf{\Gamma}}_k)^{-1/2} \mathbf{G}_k^{-1} \mathbf{F}_k^T, \quad (22)$$

where $\mathbf{P}_k^f = \mathbf{F}_k \mathbf{G}_k^2 \mathbf{F}_k^T$ is the eigenvalue decomposition of \mathbf{P}_k^f and the orthogonal matrix $\tilde{\mathbf{C}}_k$ is chosen so that $\tilde{\mathbf{C}}_k^T \mathbf{G}_k \mathbf{F}_k^T \mathbf{H}_k^T \mathbf{R}_k^{-1} \mathbf{H}_k \mathbf{F}_k \mathbf{G}_k \tilde{\mathbf{C}}_k = \tilde{\mathbf{\Gamma}}_k$ is diagonal.² The cost of computing the eigenvalue decomposition of \mathbf{P}_k^f depends on both the state-dimension n and the ensemble size m . Choosing the orthogonal matrix $\tilde{\mathbf{C}}_k$ to be $\tilde{\mathbf{C}}_k = \mathbf{G}_k^{-1} \mathbf{F}_k^T \mathbf{Z}_k^f \mathbf{C}_k$ gives that $\tilde{\mathbf{\Gamma}}_k = \mathbf{\Gamma}_k$ and that the ensemble adjustment matrix is

$$\mathbf{A}_k = \mathbf{Z}_k^f \mathbf{C}_k (\mathbf{I} + \mathbf{\Gamma}_k)^{-1/2} \mathbf{G}_k^{-1} \mathbf{F}_k^T. \quad (23)$$

The EAKF analysis update (21) becomes

$$\mathbf{Z}_k^a = \mathbf{Z}_k^f \mathbf{C}_k (\mathbf{I} + \mathbf{\Gamma}_k)^{-1/2} \mathbf{G}_k^{-1} \mathbf{F}_k^T \mathbf{Z}_k^f, \quad (24)$$

¹For instance, the columns of \mathbf{C}_k that span the $(m-p)$ -dimensional null-space of $\mathbf{Z}_k^{fT} \mathbf{H}_k^T \mathbf{R}_k^{-1} \mathbf{H}_k \mathbf{Z}_k^f$ are determined only up to orthogonal transformations if the number of observations p is less than the ensemble size m .

²The appearance of \mathbf{G}_k^{-1} in the definition of the ensemble adjustment matrix \mathbf{A} seems to require the forecast error covariance \mathbf{P}_k^f to be invertible. However, the formulation is still correct when \mathbf{G}_k is $m' \times m'$ and \mathbf{F}_k is $n \times m'$ where m' is the number of nonzero eigenvalues of \mathbf{P}_k^f .

The EAKF analysis ensemble given by (24) is the same as applying the transformation $\mathbf{G}_k^{-1} \mathbf{F}_k^T \mathbf{Z}_k^f$ to the ET KF analysis ensemble. The matrix $\mathbf{G}_k^{-1} \mathbf{F}_k^T \mathbf{Z}_k^f$ is orthogonal and is, in fact, the matrix of right singular vectors of \mathbf{Z}_k^f . Therefore, $\mathbf{C}_k(1 + \mathbf{\Gamma}_k)^{-1/2} \mathbf{G}_k^{-1} \mathbf{F}_k^T \mathbf{Z}_k^f$ is a matrix square-root of $(\mathbf{I} - \mathbf{V}_k \mathbf{D}_k^{-1} \mathbf{V}_k^T)$.

4. Summary and Discussion

Ensemble forecast/assimilation methods use low-rank ensemble representations of forecast and analysis error covariance matrices. Since these ensemble are scaled square-roots of the error covariance matrices, ensemble data assimilation methods can be viewed as square-root filters (SRFs) (Bierman, 1977). Analysis ensembles can be constructed stochastically or deterministically. Deterministic construction of analysis ensembles eliminates one source of sampling error and in some examples leads to deterministic SRFs being more accurate than stochastic SRFs (Whitaker and Hamill, 2001). SRFs are not unique. This lack of uniqueness is illustrated in three different recently proposed ensemble data assimilation methods that use the Kalman square-root filter method to update the analysis ensemble (Bishop et al., 2001; Anderson, 2001; Whitaker and Hamill, 2001). Identifying the methods as SRFs allows a clearer discussion and comparison of their different analysis ensemble updates.

Small ensemble-size and model deficiencies lead to inaccurate ensemble representations of error covariances. Distance-dependent covariance filtering and covariance inflation have been proposed as solutions (Whitaker and Hamill, 2001). Hybrid methods using ensemble and correlation models to represent forecast error are another way of treating the problem of inaccurate ensemble representations (Hamill and Snyder, 2000). However, as currently implemented, hybrid methods require perturbed observations. Here we have presented deterministic methods of including model

error into a square-root or ensemble data assimilation system when the model error has large-scale representation.

In Estimation Theory, nonuniqueness of SRFs has been exploited to design filters with desirable computational and numerical properties. An open question is whether there are ensemble properties that would make a particular SRF implementation better than another, or if the only issue is computational cost. For instance, it may be possible to choose an analysis update scheme that preserves higher-order, non-Gaussian statistics of the forecast ensemble. This question can only be answered by detailed comparisons of different methods in a realistic setting where other details of the assimilation system such as modeling of systematic errors or data quality control may prove to be as important.

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