ON THE CONVERGENCE OF THE ENSEMBLE KALMAN FILTER

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Abstract. Convergence of the ensemble Kalman filter in the limit for large ensembles to the Kalman filter is proved. In each step of the filter, convergence of the ensemble sample covariance follows from a weak law of large numbers for exchangeable random variables, Slutsky's theorem gives weak convergence of ensemble members, and L^p bounds on the ensemble then give L^p convergence.

Keywords: Data assimilation, ensemble, asymptotics, convergence, filtering, exchangeable random variables

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1. Introduction

Data assimilation, a topic of importance in many disciplines, uses statistical estimation to update the state of a running model based on new data. One of the most succesful recent data assimilation methods is the ensemble Kalman filter (EnKF). EnKF is a Monte-Carlo approximation of the Kalman filter (KF), with the covariance in the KF replaced by the sample covariance computed from an ensemble of realizations. Because the EnKF does not need to maintain the state covariance matrix, it can be implemented efficiently for high-dimensional problems. Although the EnKF formulas rely on the assumption that the distribution of the state and the data likelihood are normal, the ensemble can robustly describe an arbitrary state probability distribution. Thus, in spite of errors such as smearing of the state distribution towards normality [9], the EnKF is often used for nonlinear systems. In many practical problems in geosciences, it is observed that reasonably small ensembles (typically 25 to 100) are sufficient [5]. Heuristic justifications of this fact exist and convergence can be further accelerated by localization, such as covariance tapering [7].

A large body of literature on the EnKF and variants exists, but rigorous probabilistic analysis is lacking. It is commonly assumed that the ensemble is a sample (that is, i.i.d.) and it is normally distributed. Although the resulting analyses played an important role in the development of EnKF, both assumptions are false. The ensemble covariance is computed from all ensemble members together, thus introducing dependence, and the EnKF formula is a nonlinear function of the ensemble, thus destroying the normality of the ensemble distribution.

For example, the analysis in [5] is based on the comparison of the covariance of the analysis ensemble and the covariance of the filtering distribution. [7] notes that if the ensemble sample covariance is a consistent estimator, then Slutsky's theorem yields the convergence in probability of the gain matrix. [8] studies the interplay of numerical and stochastic errors. All of these analyses assume that the ensemble covariance converges in some sense in the limit for large ensembles, yet a rigorous justification has not been available yet.

This paper provides a rigorous proof that the EnKF converges to the KF in the limit for large ensembles and for normal state probability distribution and normal data likelihood. The present analysis does not assume that the ensemble members are independent or normally distributed. The ensemble members are shown to be exchangeable random variables bounded in L^p, which provides properties that replace independence and normality. An argument using uniform integrability and Slutsky's theorem is then possible.

The result is valid for the EnKF version of Burgers, van Leeuven, and Evensen [5] in the case of constant state space dimension, a linear model, normal data likelihood and initial state distributions, and ensemble size going to infinity. This EnKF version involves randomization of data. Efficient variants of EnKF without randomization exist [2, 10], but they are not the subject of this paper.

Probabilistic analysis of the performance of the EnKF on nonlinear systems, for non-normal state probability distributions, as well as analysis of the speed of convergence of the EnKF to the KF and the dependence of the required ensemble size on the state dimension, are outside of the scope of this paper and left to future research. Some computational experiments and heuristic explanations can be found in [3].

2. Preliminaries

The Euclidean norm of column vectors in $\mathbb{R}^m$, $m \geq 1$, and the induced matrix norm are denoted by $\|\cdot\|$, and $^{\mathrm{T}}$ is the transpose. The stochastic L^p norm of a random element X is $\|X\|_p = (E(\|X\|^p))^{1/p}$. The j-th entry of a vector X is $[X]_j$ and the i,j entry of a matrix $Y \in \mathbb{R}^{m\times n}$ is $[Y]_{ij}$. Weak convergence (i.e., convergence in distribution) is denoted by $\Rightarrow$; weak convergence to a constant is the same as convergence in probability. *All convergence is for* $N \to \infty$. We denote by $X_N = [X_{Ni}]_{i=1}^N = [X_{N1}, \dots, X_{NN}]$, with various superscripts and for various $m \geq 1$, an ensemble of N random elements, called members, with values in $\mathbb{R}^m$. Thus, an ensemble is a random $m \times N$ matrix with the ensemble members as columns. Given two ensembles X_N and Y_N, the stacked ensemble $[X_N; Y_N]$ is defined as the block random matrix

$$[X_N; Y_N] = \begin{bmatrix} X_N \\ Y_N \end{bmatrix} = \left[\begin{bmatrix} X_{N1} \\ Y_{N1} \end{bmatrix}, \dots, \begin{bmatrix} X_{NN} \\ Y_{NN} \end{bmatrix} \right] = [X_{Ni}; Y_{Ni}]_{i=1}^N.$$

If all the members of X_N are identically distributed, we write $E(X_{N1})$ and $\mathrm{Cov}(X_{N1})$ for their common mean vector and covariance matrix. The ensemble sample mean and ensemble sample covariance matrix are the random elements $\overline{X}_N = \frac{1}{N}\sum_{i=1}^{N} X_{Ni}$ and $C(X_N) = \overline{X_N X_N^{\mathrm{T}}} - \overline{X}_N \overline{X}_N^{\mathrm{T}}$.

We will work with ensembles such that the joint distribution of the ensemble X_N is invariant under a permutation of the ensemble members. Such ensemble is called *exchangeable*. That is, an ensemble X_N is exchangeable if and only if $\Pr(X_N \in B) = \Pr(X_N \Pi \in B)$ for every Borel set $B \subset \mathbb{R}^{m\times N}$ and every permutation matrix $\Pi \in \mathbb{R}^{N\times N}$. The covariance between any two members of an exchangeable ensemble is the same, $\mathrm{Cov}(X_{Ni}, X_{Nj}) = \mathrm{Cov}(X_{N1}, X_{N2})$, $i \neq j$.

Lemma 2.1. *Suppose X_N and D_N are exchangeable, the random elements X_N and D_N are independent, and $Y_{Ni} = F(X_N, X_{Ni}, D_{Ni})$, $i = 1,\dots,N$, where F is measurable and permutation invariant in the first argument, i.e. $F(X_N\Pi, X_{Ni}, D_{Ni}) = F(X_N, X_{Ni}, D_{Ni})$ for any permutation matrix Π. Then Y_N is exchangeable.*

Proof. Write $Y_N = \mathbf{F}(X_N, D_N)$, where

$$\mathbf{F}(X_N, D_N) = [F(X_N, X_{N1}, D_{N1}), \dots, F^{(k)}(X_N, X_{NN}, D_{NN})].$$

Let Π be a permutation matrix. Then $Y_N\Pi = \mathbf{F}(X_N\Pi, D_N\Pi)$. Because X_N is exchangeable, the distributions of X_N and $X_N\Pi$ are identical. Similarly, the distributions of D_N and $D_N\Pi$ are identical. Since X_N and D_N are independent, the joint distributions of (X_N, D_N) and $(X_N\Pi, D_N\Pi)$ are identical. Thus, for any Borel set $B \subset \mathbb{R}^{n\times N}$,

$$\begin{aligned}\Pr(Y_N\Pi \in B) &= E(1_B(Y_N\Pi)) = E(1_B(\mathbf{F}(X_N\Pi, D_N\Pi))) \\ &= E(1_B(\mathbf{F}(X_N, D_N))) = \Pr(Y_N \in B),\end{aligned}$$

thus Y_N is exchangeable. □

We now prove a weak law of large numbers for nearly i.i.d. exchangeable ensembles.

Lemma 2.2. *If for all N, X_N, U_N are ensembles of $\mathbb{R}^1$ valued random variables, $[X_N; U_N]$ is exchangeable, $\mathrm{Cov}(U_{Ni}, U_{Nj}) = 0$ for all $i \neq j$, $U_{N1} \in L^2$ is the same for all N, and $X_{N1} \to U_{N1}$ in L^2, then $\overline{X}_N \Rightarrow E(U_{N1})$.*

Proof. Since X_N is exchangeable, $\mathrm{Cov}(X_{Ni}, X_{Nj}) = \mathrm{Cov}(X_{N1}, X_{N2})$ for all $i, j = 1,\dots,N$, $i \neq j$. Since $X_N - U_N$ is exchangeable, also $X_{N2} - U_{N2} \to 0$ in L^2. Then, using the identity $\mathrm{Cov}(X,Y) = E(XY) - E(X)E(Y)$ and Cauchy inequality for the L^2 inner product $E(XY)$, we have

$$\begin{aligned}&|\mathrm{Cov}(X_{N1}, X_{N2}) - \mathrm{Cov}(U_{N1}, U_{N2})| \\ &\qquad \leq 2\|X_{N1}\|_2 \|X_{N2} - U_{N2}\|_2 + 2\|U_{N2}\|_2 \|X_{N1} - U_{N1}\|_2,\end{aligned}$$

so $\mathrm{Cov}(X_{N1}, X_{N2}) \Rightarrow 0$. By the same argument, $\mathrm{Var}(X_{N1}) \Rightarrow \mathrm{Var}(U_{N1}) < +\infty$. Now $E(\overline{X}_N) = E(X_{N1}) \Rightarrow E(U_{N1})$ from $X_{N1} - U_{N1} \to 0$ in L^2, and

$$\begin{aligned}\mathrm{Var}(\overline{X}_N) &= \frac{1}{N^2} \sum_{i=1}^{N} \mathrm{Var}(X_{Ni}) + \sum_{i,j=1, j\neq j}^{N} \mathrm{Cov}(X_{Ni}, X_{Nj}) \\ &= \frac{1}{N} \mathrm{Var}(X_{N1}) + (1 - \frac{1}{N}) \mathrm{Cov}(X_{N1}, X_{N2}) \to 0,\end{aligned}$$

and the conclusion follows from Chebyshev inequality. □

The convergence of the ensemble sample covariance follows.

Lemma 2.3. *If for all N, X_N, U_N are ensembles of $\mathbb{R}^n$ valued random elements, $[X_N; U_N]$ is exchangeable, U_N are i.i.d., $U_{N1} \in L^4$ is the same for all N, and $X_{N1} \to U_{N1}$ in L^4, then $\overline{X}_N \Rightarrow E(U_{N1})$ and $C(X_N) \Rightarrow \mathrm{Cov}(U_{N1})$.*

Proof. From Lemma 2.2, it follows that $[\overline{X}_N]_j \Rightarrow [E(U_{N1})]_j$ for each entry $j = 1, \ldots, n$, so $\overline{X}_N \Rightarrow E(U_{N1})$. Let $Y_{Ni} = X_{Ni} X_{Ni}^{\mathrm{T}}$, so that $C(X_N) = \overline{Y}_N - \overline{X}_N \overline{X}_N^{\mathrm{T}}$. Each entry of $[Y_{Ni}]_{j\ell} = [X_{Ni}]_j [X_{Ni}]_\ell$ satisfies the assumptions of Lemma 2.2, so $[Y_{Ni}]_{j\ell} \Rightarrow E([U_{N1} U_{N1}^{\mathrm{T}}]_{j\ell})$. Convergence of the entries $[\overline{X}_N \overline{X}_N^{\mathrm{T}}]_{j\ell} = [\overline{X}_N]_j [\overline{X}_N]_\ell$ to $E([U_{N1}]_{j\ell}) E([U_{N1}^{\mathrm{T}}]_{j\ell})$ follows from the already proved convergence of $\overline{X}_N$ and Slutsky's theorem [6, p. 254]. Applying Slutsky's theorem again, we get $C(X_N) \Rightarrow \mathrm{Cov}(U_{N1})$. □

3. Formulation of the EnKF

Consider an initial state given as the random variable $U^{(0)}$. In step k, the state $U^{(k-1)}$ is advanced in time by applying the model $M^{(k)}$ to obtain $U^{(k),f} = M^{(k)}(U^{(k-1)})$, called the prior or the forecast, with probability density function (pdf) $p_{U^{(k),f}}$. The data in step k are given as measurements $d^{(k)}$ with a known error distribution, and expressed as the data likelihood $p(d^{(k)}|u)$. The new state $U^{(k)}$ conditional on the data, called the posterior or the analysis, then has the density $p_{U^{(k)}}$ given by the Bayes theorem, $p_{U^{(k)}}(u) \propto p(d^{(k)}|u) p_{U^{(k),f}}(u)$, where $\propto$ means proportional. This is the discrete time filtering problem. The distribution of $U^{(k)}$ is called the filtering distribution.

Assume that $U^{(0)} \sim N(u^{(0)}, Q^{(0)})$, the model is linear, $M^{(k)} : u \mapsto A^{(k)} u + b^{(k)}$, and the data likelihood is normal conditional on given state $u^{(k),f}$,

$$p\left(d^{(k)}|u^{(k),f}\right) \propto e^{-\frac{1}{2}\left(H^{(k)}u^{(k),f} - d^{(k)}\right)^{\mathrm{T}} R^{(k)^{-1}} \left(H^{(k)}u^{(k),f} - d^{(k)}\right)}$$

where $\propto$ means proportional, $H^{(k)}$ is the given observation matrix and $R^{(k)}$ is the given data error covariance. The data error is assumed to be independent of the model state. Then the filtering distribution is normal, $U^{(k)} \sim N(u^{(k)}, Q^{(k)})$, and it satisfies the KF recursions [1]

$$u^{(k),f} = E(U^{(k),f}) = A^{(k)} u^{(k)} + b^{(k)}, \quad Q^{(k),f} = \mathrm{Cov}\, U^{(k),f} = A^{(k)^{\mathrm{T}}} Q^{(k)} A^{(k)}, \tag{3.1}$$

$$u^{(k)} = u^{(k),f} + K^{(k)}(d^{(k)} - H^{(k)} u^{(k),f}), \quad Q^{(k)} = (I - K^{(k)} H^{(k)}) Q^{(k),f}, \tag{3.2}$$

where the Kalman gain matrix $K^{(k)}$ is given by

$$K^{(k)} = Q^{(k),f} H^{(k)\mathrm{T}} (H^{(k)} Q^{(k),f} H^{(k)\mathrm{T}} + R^{(k)})^{-1}. \tag{3.3}$$

The EnKF is obtained by replacing the exact covariance $Q^{(k)}$ by the ensemble sample covariance and adding noise to the data in order to avoid a shrinking of the ensemble spread and to obtain the correct filtering covariance [5], cf. Lemma 3.1 below.

Let $U_i^{(0)} \sim N(u^{(0)}, Q^{(0)})$ and $D_i^{(k)} \sim N(d^{(k)}, R^{(k)})$ be independent for all $k, i \geq 1$. Given N, choose the initial ensemble and the perturbed data as the first N terms of the respective sequence, $U_{Ni}^{(0)} = U_i^{(0)}$, $i = 1, \ldots, N$, $D_{Ni}^{(k)} = D_i^{(k)}$, $i = 1, \ldots, N$, $k = 1, 2, \ldots$ The ensembles produced by EnKF are $X_N^{(0)} = U_N^{(0)}$ and

$$X_{Ni}^{(k),f} = M^{(k)}(X_{Ni}^{(k-1)}), \quad i = 1, \ldots, N. \tag{3.4}$$

$$X_N^{(k)} = X_N^{(k),f} + K_N^{(k)}(D_N^{(k)} - H^{(k)} X_N^{(k),f}), \tag{3.5}$$

where $K_N^{(k)}$ is the ensemble sample gain matrix,

$$K_N^{(k)} = Q_N^{(k),f} H^{(k)T} (H^{(k)} Q_N^{(k),f} H^{(k)T} + R^{(k)})^{-1}, \quad Q_N^{(k),f} = C(X_N^{(k),f}). \tag{3.6}$$

Our analysis of the EnKF is based on the observation that the ensembles $X_N^{(k)}$ are a perturbation of auxiliary ensembles $U_N^{(k)}$. The ensembles $U_N^{(k)}$ are obtained from the same initial ensemble by applying the KF formulas to each ensemble member separately and using the same corresponding member of perturbed data,

$$U_{Ni}^{(k),f} = M^{(k)}(U_{Ni}^{(k-1)}), \quad i = 1, \ldots, N, \tag{3.7}$$

$$U_N^{(k)} = U_N^{(k),f} + K^{(k)}(D_N^{(k)} - H^{(k)} U_N^{(k),f}). \tag{3.8}$$

The auxiliary ensembles $U_N^{(k)}$ are introduced for theoretical puposes only and they do not play any role in the EnKF algorithm. The next lemma shows that $U_N^{(k)}$ is a sample from the filtering distribution.

Lemma 3.1. *For all $k = 1, 2, \ldots$, $U_N^{(k)}$ is i.i.d. and $U_{N1}^{(k)} \sim N(u^{(k)}, Q^{(k)})$.*

Proof. The statement is true for $k = 0$ by definition of $U_N^{(0)}$. Assume that it is true for $k - 1$ in place of k. The ensemble $U_N^{(k)}$ is i.i.d. and normally distributed because it is an image under a linear map of the normally distributed i.i.d. ensemble with members $[U_{Ni}^{(k-1)}, D_{Ni}^{(k)}]$, $i = 1, \ldots, N$. Further, $D_N^{(k)}$ and $U_{Ni}^{(k),f}$ are independent, so from [5, eq. (15) and (16)], $U_{N1}^{(k)}$ has the correct mean and covariance, which determines the normal distribution of $U_{N1}^{(k)}$ uniquely. □

4. Convergence analysis

Lemma 4.1. *There exist constants $c(k, p)$ for all k and all $p < \infty$ such that $\|X_{N1}^{(k)}\|_p \leq c(k, p)$ and $\|K_N^{(k)}\|_p \leq c(k, p)$ for all N.*

Proof. For $k = 0$, each $X_{Ni}^{(k)}$ is normal. Assume $\|X_{N1}^{(k-1)}\|_p \le c(k-1,p)$ for all N. Then

$$\|X_{N1}^{(k),f}\|_p = \|A^{(k)} X_{N1}^{(k-1)} + b^{(k)}\|_p \le \|A^{(k)}\| \|X_{N1}^{(k-1)}\|_p + \|b^{(k)}\| \le \mathrm{const}(k,p).$$

By Jensen's inequality, for any X_N,

$$\|\frac{1}{N}\sum_{i=1}^{N} X_{N_i}\|_p \le \frac{1}{N}\sum_{i=1}^{N} \|X_{N_i}\|_p.$$

This gives $\|\overline{X}_N^{(k),f}\|_p \le \mathrm{const}(k,p)$ and

$$\begin{aligned}\|Q_N^{(k),f}\|_p &\le \frac{1}{N}\|X_{N1}^{(k),f} X_{N1}^{(k),f\mathrm{T}}\|_p + \frac{1}{N^2}\|X_{N1}^{(k),f}\|_p^2 \\ &\le \frac{1}{N}\|X_{N1}^{(k),f}\|_{2p}^2 + \frac{1}{N^2}\|X_{N1}^{(k),f}\|_p^2 \le \mathrm{const}(k,p),\end{aligned}$$

since from Cauchy inequality,

$$\|WZ\|_p \le E\left(\|W\|^p \|Z\|^p\right)^{\frac{1}{p}} \le E(\|W\|^{2p})^{\frac{1}{2p}} E(\|Z\|^{2p})^{\frac{1}{2p}} = \|W\|_{2p} \|Z\|_{2p}, \tag{4.1}$$

for any compatible random matrices W and Z. Since $H^{(k)} Q_N^{(k),f} H^{(k)\mathrm{T}}$ is symmetric positive semidefinite and $R^{(k)}$ is symmetric positive definite, it holds that

$$\|(H^{(k)} Q_N^{(k),f} H^{(k)\mathrm{T}} + R^{(k)})^{-1}\| \le \|(R^{(k)})^{-1}\| \le \mathrm{const}(k),$$

which, together with the bound on $\|Q_N^{(k),f}\|_p$, gives

$$\|K_N^{(k)}\|_p \le \|Q_N^{(k)}\|_p \,\mathrm{const}(k) \le \mathrm{const}(k,p).$$

Finally, we obtain the desired bound

$$\begin{aligned}\|X_{N1}^{(k)}\|_p &\le \|X_{N1}^{(k),f}\|_p + \|K_N^{(k)} D_{N1}^{(k)}\|_p + \|K_N^{(k)} H^{(k)} X_{N1}^{(k),f}\|_p \\ &\le \mathrm{const}(k,p)(\|X_{N1}^{(k),f}\|_p + \|K_N^{(k)}\|_p + \|K_N^{(k)}\|_{2p}\|X_{N1}^{(k),f}\|_{2p}) \le c(k,p),\end{aligned}$$

using again (4.1). □

Theorem 4.1. *For all k, $[X_N; U_N]$ is exchangeable and $X_{N1}^{(k)} \to U_{N1}^{(k)}$ in L^p for all $p < +\infty$, where U_N is i.i.d. with the filtering distribution.*

Proof. The ensembles $U_N^{(k)}$ are obtained by linear mapping of the i.i.d. initial ensemble $U_N^{(0)}$, so they are i.i.d. Since $X_{Ni}^{(0)} = U_{Ni}^{(0)}$, $[X_N^{(0)}; U_N^{(0)}]$ is exchangeable, and $X_{N1} = U_{N1}$. Suppose the statement holds for $k-1$ in place of k. The ensemble members are given by a recursion of the form

$$[X_{Ni}^{(k)}; U_{Ni}^{(k)}] = F^{(k)}(C(X_N^{(k-1)}), [X_{Ni}^{(k-1)}; U_{Ni}^{(k-1)}], D_{Ni}^{(k)}).$$

The ensemble sample covariance matrix C is permutation invariant, so $[X_N^{(k)}; U_N^{(k)}]$ is exchangeable by Lemma 2.1. Subtracting (3.5) and (3.8) gives

$$X_N^{(k),f} - U_N^{(k),f} = A^{(k)}(X_N^{(k-1)} - U_N^{(k-1)}),$$

and $X_N^{(k),f}$ and $U_N^{(k),f}$ satisfy the assumption of Lemma 2.3. Thus, $C(X_N^{(k),f}) \Rightarrow \mathrm{Cov}\, U_{N1}^{(k),f}$, $K_N^{(k)} \Rightarrow K^{(k)}$ by the mapping theorem [4, p. 334], and $X_{N1}^{(k)} \Rightarrow U_{N1}^{(k)}$

by Slutsky's theorem. Let $p < +\infty$. Since the sequence $\{X_{N1}^{(k)}\}_{N=1}^{\infty}$ is bounded in L^p by Lemma 4.1 and $X_{N1}^{(k)} \Rightarrow U_{N1}^{(k)}$, it follows that $X_{N1}^{(k)} \to U_{N1}^{(k)}$ in L^p by uniform integrability [4, p. 338]. $\square$

Using Lemma 2.3 and uniform integrability again, it follows that the ensemble mean and covariance converge to the filtering mean and covariance.

Corollary 4.1. *$\overline{X}_N^{(k)} \to u^{(k)}$ and $C(X_N^{(k)}) \to Q^{(k)}$ in L^p for all $p < +\infty$, where $u^{(k)}$ and $Q^{(k)}$ are the mean and the covariance of the filtering distribution.*

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