

On the Convergence of a Non-linear Ensemble Kalman Smoother

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Abstract

Ensemble methods, such as the ensemble Kalman filter (EnKF), the local ensemble transform Kalman filter (LETKF), and the ensemble Kalman smoother (EnKS) are widely used in sequential data assimilation, where state vectors are of huge dimension. Little is known, however, about the asymptotic behavior of ensemble methods. In this paper, we prove convergence in L^p of ensemble Kalman smoother to the Kalman smoother in the large-ensemble limit, as well as the convergence of EnKS-4DVAR, which is a Levenberg-Marquardt-like algorithm with EnKS as the linear solver, to the classical Levenberg-Marquardt algorithm in which the linearized problem is solved exactly.

1 Introduction

Data assimilation is the process of blending estimates of a given system state, in the form of observational information and a prior knowledge [18]. The Kalman filter/smoothing (KF/KS) [6, 8, 14] and the three and four-dimensional variational assimilation system (3DVAR/4DVAR) [7, 31] are among well-known algorithms used in data assimilation. Kalman filters estimate the state sequentially by seeking an analysis that minimizes the posterior variance, while the 3DVAR and 4DVAR methods produce posterior maximum likelihood solutions through minimization of an objective function. For high-dimensional problems, the ensemble Kalman filter/smoothing (EnKF/EnKS) [16, 8] and their variants have been proposed as Monte Carlo derivative-free alternatives to the KF and KS, with the intractable state covariance in the KF or in the KS replaced by the sample covariance computed from an ensemble of realizations.

The purpose of this paper is to provide theoretical results for the method originally proposed in [25], called EnKS-4DVAR. The EnKS-4DVAR method uses an ensemble Kalman smoother as a linear solver in the Gauss-Newton or Levenberg-Marquardt method to minimize the weak-constraint 4DVAR objective function. Further details on implementation and computational results can be found in [25].

The equivalence of the Kalman smoother and incremental variational data assimilation has been known for a long time; see, e.g., [2, 21]. Hybridization of variational and ensemble-based methods has been a topic of interest among researchers in recent years [11, 35, 34, 29, 4, 5]. The maximum

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ensemble likelihood filter (MELF) [35] uses repeated EnKF on the tangent problem to minimize the objective function over the span of the ensemble. The iterated ensemble Kalman filter (IEnKF) [29] solves the Euler equations for the minimum by Newton’s method, preconditioned by a square root ensemble Kalman filter, while [4] adds a regularization term, similar to the Levenberg-Marquardt method, and [5] extends the IEnK method to strong-constraint 4DVAR. The IEnKF uses a scaling of the ensemble, called the “bundle variant” to approximate the derivatives (tangent operators), achieving a similar effect as the use of finite differences here. The four-dimensional ensemble-based variational data assimilation (4DEnVar) of [23, 24, 22] minimizes the 4DVAR objective function over the span of the ensemble.

Usually, in the formulation of the ensemble based methods (EnKF/EnKS and their variants), each ensemble member is considered as a vector in \mathbf{R}^n , that is, each vector is regarded as a sample point of a random vector. In this paper, we investigate a different way to interpret such algorithms, similarly as in [26, 19], namely, each ensemble member is considered as a random vector and not merely as vector of \mathbf{R}^n . In fact, the elements of the EnKF/EnKS can be seen as random vectors instead of their realizations. Surprisingly, in this case little is known about the asymptotic behavior of the EnKF/EnKS and other related ensemble methods. This is in contrast to particle filters, for which the asymptotic behavior as the number of particles increases to infinity is well studied. An important question related to EnKF/EnKS and related ensemble methods is a law of large numbers-type theorem as the size of the ensemble grows to infinity. In [26, 19], it was proved that the ensemble mean and covariance of EnKF converge to those of the KF, as the number of ensemble members grows to infinity, but the convergence results are not dimension independent. The analysis in [26] relies on the fact that ensemble members are exchangeable and uses the uniform integrability theorem, which does not provide convergence rates; in [19], stochastic inequalities for the random matrices and vectors are used to obtain the classical rate $1/\sqrt{N}$, where N is the ensemble size, but it relies on entry-by-entry arguments. Convergence in L^p with the rate $1/\sqrt{N}$ independent of dimension (including infinite) was obtained recently for the square root ensemble Kalman filter [17]. These analyses apply to each time step separately rather than for the long-time behavior. The EnKF was proved to be well-posed and to stay within a bounded distance from the truth, for a class of dynamical systems, with the whole state observed, and when a sufficiently large covariance inflation is used [15].

In this paper, we extend the convergence result of [26] to EnKS, and apply the extension to EnKS-4DVAR. The randomness of the elements of EnKS implies that, in contrast to the EnKS-4DVAR algorithm presented in [25], the coefficients and the solution of the linearized subproblem at each iteration are random. We investigate also the asymptotic behavior of this algorithm. We show the convergence of the EnKS to the KS in L^p for all $p \in [1, \infty)$ in the large ensemble limit, in the sense that the ensemble mean and covariance constructed by EnKS method converge to the mean and covariance of the KS respectively in L^p . Finally, we show the convergence of the EnKS-4DVAR iterates to their corresponding iterates in the classical Levenberg-Marquardt algorithm. Since the EnKS-4DVAR algorithm uses finite differences for approximating derivatives, (i) we start by showing the convergence in probability of its iterates to the iterates generated by the algorithm with exact derivatives as the finite differences parameter goes to zero, (ii) then we prove the convergence in L^p of its iterates as the size of the ensemble grows to infinity.

The paper is organized as follows: in Section 2 we recall some definitions and preliminary results that will be useful throughout the paper. Section 3 introduces nonlinear data assimilation. Section 4 contains the statements of the KF and the EnKF, and recalls the convergence properties of the

EnKF as the ensemble size increases to infinity. Section 5 gives statements of the KS and the EnKS, and extends the convergence properties of the EnKF as the ensemble size goes to infinity, to the EnKS. Finally, Section 6 recalls the EnKS-4DVAR algorithm and presents the convergence properties.

2 Preliminaries

We recall definition of sequence of random vectors exchangeability, the notion of convergence in probability and in L^p of random elements. Then we present several lemmas, which will be useful for the following of the paper.

Definition 1 (Exchangeability of random vectors). *A set of N random vectors $[X^1, \dots, X^N]$ is exchangeable if their joint distribution is invariant to a permutation of the indices; that is, for any permutation π of the numbers $1, \dots, N$ and any Borel set B ,*

$$\mathbb{P}([X^{\pi(1)}, \dots, X^{\pi(N)}] \in B) = \mathbb{P}([X^1, \dots, X^N] \in B).$$

Clearly, an i.i.d sequence is exchangeable.

If X is a random element (either vector or matrix), we use $|X|$ to denote the usual Euclidean norm (for vectors) or spectral norm (for a matrix). For $1 \leq p < \infty$, denote

$$\|X\|_p = E(|X|^p)^{1/p}.$$

The space L^p (of vectors or matrices) consists of all random elements X (with values in the same space) such that the $E(|X|^p) < \infty$. Identifying random elements equal a.s., we have that $\|\cdot\|_p$ is a norm on the space L^p . Convergence in L^p is defined as the convergence in this norm. Note that if the element X is deterministic,

$$\|X\|_p = E(|X|^p)^{1/p} = (|X|^p)^{1/p} = |X|.$$

Definition 2 (Convergence in probability). *A sequence (X^k) of random vectors converges in probability towards the random vector X if for all $\epsilon > 0$,*

$$\lim_{k \rightarrow \infty} \mathbb{P}(|X^k - X| \geq \epsilon) = 0,$$

i.e.,

$$\forall \epsilon > 0 \forall \tilde{\epsilon} > 0 \exists k_0 \forall k \geq k_0 : \mathbb{P}[|X^k - X| \leq \epsilon] \geq 1 - \tilde{\epsilon}.$$

Convergence in probability will be denoted by

$$X^k \xrightarrow{P} X \text{ as } k \rightarrow \infty.$$

The concept of convergence in probability and the notation are extended in an obvious manner to the case when the random vectors are indexed by $\tau > 0$. Then

$$X^\tau \xrightarrow{P} X \text{ as } \tau \rightarrow 0$$

means

$$\forall \epsilon > 0 \forall \tilde{\epsilon} > 0 \exists \tau_0 > 0 \forall 0 < \tau < \tau_0 : \mathbb{P}[|X^\tau - X| \leq \epsilon] \geq 1 - \tilde{\epsilon}.$$

We state the following lemmas, which will be used in this paper.

Lemma 1. *If random elements Y^1, \dots, Y^N are exchangeable, and Z^1, \dots, Z^N are also exchangeable, and independent from Y^1, \dots, Y^N , then $Y^1 + Z^1, \dots, Y^N + Z^N$ are exchangeable.*

Lemma 2. *If random elements Y^1, \dots, Y^N are exchangeable, and*

$$Z^k = F\left(Y^1, \dots, Y^N, Y^k\right),$$

where F is measurable and permutation invariant in the first N arguments, then Z^1, \dots, Z^N are also exchangeable.

For the proof of the previous two lemmas, we refer to [26].

Lemma 3 (Uniform integrability). *If (X^k) is a bounded sequence in L^p and $X^k \xrightarrow{P} X$, then $\|X^k - X\|_q \rightarrow 0$ for all $1 \leq q < p$.*

Proof. The proof is an exercise on uniform integrability [3, page 338]: Let $1 \leq q < p$. The sequence $\left(E\left(|X^k - X|^{q(p/q)}\right)\right)$ is bounded and $p/q > 1$, thus the sequence $(|X^k - X|^q)$ is uniformly integrable. Since $|X^k - X| \xrightarrow{P} 0$, and thus $|X^k - X|^q \xrightarrow{P} 0$, it follows that $E(|X^k - X|^q) \rightarrow 0$. \square

Lemma 4 (Continuous mapping theorem). *Let X^k be a sequence of random elements with values on a metric space \mathcal{A} , such that $X^k \xrightarrow{P} X$. Let f be a continuous function from \mathcal{A} to another metric space \mathcal{B} . Then $f(X^k) \xrightarrow{P} f(X)$.*

We refer to [33, Theorem 2.3] for a proof.

3 The nonlinear data assimilation problem

Consider the following classical system of stochastic equations with additive Gaussian noise, which appears in different fields, such as weather forecasting and hydrology,

$$X_0 \sim N(x_b, B) \tag{1}$$

$$X_i = \mathcal{M}_i(X_{i-1}) + \mu_i + V_i, \quad V_i \sim N(0, Q_i), \quad i = 1, \dots, k \tag{2}$$

$$y_i = \mathcal{H}_i(X_i) + W_i, \quad W_i \sim N(0, R_i), \quad i = 1, \dots, k, \tag{3}$$

with independent perturbations V_i and W_i . The operators \mathcal{M}_i and \mathcal{H}_i are the model operators and the observation operators, respectively, and they are assumed to be continuously differentiable. When they are linear, we denote them by M_i and H_i , respectively. The index i denotes the time index and k denotes the number of time steps. While the outputs y_i are observed, the state X_i and the noise variables V_i and W_i are hidden. The quantities B , Q_i and R_i are the covariance matrices of X_0 , V_i and W_i respectively. The quantity μ_i is a deterministic vector. The objective is to estimate the hidden states X_1, \dots, X_k .

Definition 3. *The distribution of X_k from (1)–(3) conditioned on y_1, \dots, y_{k-1} is called prior distribution. The filtering, or posterior, distribution is the distribution of X_k , conditioned on the observations of the data y_1, \dots, y_k . The smoothing distribution is the joint distribution of X_0, \dots, X_k , conditioned on the observations of data y_1, \dots, y_k .*

In geosciences, the prior is usually called forecast and the posterior is called analysis. In Table 1, we collect the notation for state vectors and their ensembles for reference.

Symbol	Random	Meaning	First used in Sec.
X_i	yes	the state at time i	3
$X_{i \ell}$	no	the mean of X_i given data $y_{1:\ell}$	4.1
$P_{i \ell}$	no	the covariance of X_i given data $y_{1:\ell}$	4.1
$X_{i \ell}^n$	yes	member n of an ensemble approximating X_i given $y_{1:\ell}$	4.2
$\bar{X}_{i \ell}^N$	yes	the sample mean of the ensemble $X_{i \ell}^1, \dots, X_{i \ell}^N$	4.2
$P_{i \ell}^N$	yes	the sample covariance of the ensemble $X_{i \ell}^1, \dots, X_{i \ell}^N$	4.2
$U_{i \ell}^n$	yes	member n of a reference ensemble approximating X_i given $y_{1:\ell}$	4.3
$X_{0:i}$	yes	composite state $[X_0, \dots, X_i]$ at times $0, \dots, i$	5.1
$X_{0:i \ell}$	no	the mean of $X_{0:i}$	5.1
$P_{0:i \ell}$	no	the covariance of $X_{0:i}$	5.1
$X_{0:i \ell}^n$	yes	member n of ensemble approximating X_i given $y_{1:\ell}$	5.2
$\bar{X}_{0:i \ell}^N$	yes	the sample mean of the ensemble $X_{0:i \ell}^1, \dots, X_{0:i \ell}^N$	5.2
$P_{0:i,0:i \ell}^N$	yes	the sample covariance of the ensemble $X_{0:i \ell}^1, \dots, X_{0:i \ell}^N$	5.2
$U_{0:i \ell}^n$	yes	member n of reference ensemble approximating X_i given $y_{1:\ell}$	5.3
x_b	no	the background state	6.1
x_i	no	the unknown state in 4DVAR minimization	6.1
$x_{0:k}$	no	the unknown composite state in the 4DVAR minimization	6.1
$x_i^j, x_{0:k}^j$	no	the iterate j in the 4DVAR minimization	6.2
$X_{0:i \ell}^{j,n}$	yes	member n of ensemble approximating $x_{0:i}^j$	6.3
$\bar{X}_{0:i \ell}^{j,N}$	yes	the sample mean of the ensemble $X_{0:i \ell}^{j,1}, \dots, X_{0:i \ell}^{j,N}$ using	6.3
$X_{0:k k}^{j,n,N_j}$	yes	member n from ensemble of size N_j	6.3
$X_{0:i \ell}^{j,n,\tau}$	yes	member n of the ensemble approximating $x_{0:i}^j$ with step τ	6.4
$\bar{X}_{0:i \ell}^{j,n,\tau}$	yes	the sample mean of the ensemble $X_{0:i \ell}^{j,1,\tau}, \dots, X_{0:i \ell}^{j,N,\tau}$	6.4
$\Delta_{i \ell}^{j,n}$	yes	4DVAR increment ensemble members $X_{i \ell}^{j,n} - x_i^{j-1,n}$	6.4

Table 1: Notation for state vectors.

4 Kalman filtering

4.1 Kalman filter

The Kalman filter [13] provides an efficient computational recursive means to estimate the state of the process X_k in the linear case, i.e., when \mathcal{M}_i and \mathcal{H}_i , $i = 1, \dots, k$, are linear. Denote the mean and the covariance of X_i given the data y_1, \dots, y_ℓ , by

$$X_{i|\ell} = E(X_i|y_1, \dots, y_\ell), \quad P_{i|\ell} = P(X_i|y_1, \dots, y_\ell),$$

respectively. In the linear case, the probability distribution of the process X_k given the data up to the time k is Gaussian, therefore it is characterized by its mean and covariance matrix, which can be computed as follows.

Algorithm 1 (Kalman filter). For $i = 0$, set $X_{0|0} = x_b$ and $P_{0|0} = B$. For $i = 1, \dots, k$,

$$X_{i|i-1} = M_i X_{i-1|i-1} + \mu_i, \quad (\text{advance the mean in time}) \quad (4)$$

$$P_{i|i-1} = M_i P_{i-1|i-1} M_i^T + Q_i, \quad (\text{advance the covariance in time})$$

$$K_i = P_{i|i-1} H_i^T (H_i P_{i|i-1} H_i^T + R_i)^{-1} \quad (\text{the Kalman gain})$$

$$X_{i|i} = X_{i|i-1} + K_i (y_i - H_i X_{i|i-1}), \quad (\text{update the mean from the observation } i) \quad (5)$$

$$P_{i|i} = (I - K_i H_i) P_{i|i-1} \quad (\text{update the covariance from the observation } i) \quad (6)$$

In atmospheric sciences, the update (5)–(6) is referred to as the analysis step.

Lemma 5. The distribution $N(X_{k|k}, P_{k|k})$ from the Kalman filter is the filtering distribution.

See, e.g., [1, 30] for the proof.

If the dimension of the hidden state X_k is large, the covariance matrices $P_{k|k-1}$ and $P_{k|k}$ are large dense matrices, hence storing such matrices in memory with the current hardware is almost impossible, and the matrix products in the computation of $P_{k|k-1}$ are also problematic. To solve these problems, the idea is to use ensemble methods.

4.2 Ensemble Kalman filter (EnKF)

The idea behind the ensemble Kalman filter is to use Monte Carlo samples and the corresponding empirical covariance matrix instead of the forecast covariance matrix $P_{k|k-1}$ [8]. Denote by n the ensemble member index, $n = 1, \dots, N$.

Algorithm 2 (EnKF). For $i = 0$, $X_{0|0}^n \sim N(x_b, B)$. For $i = 1, \dots, k$, given an analysis ensemble $X_{i-1|i-1}^1, \dots, X_{i-1|i-1}^N$ at time $i - 1$, the ensemble at time i is built as

$$X_{i|i-1}^n = M_i X_{i-1|i-1}^n + \mu_i + V_i^n, \quad V_i^n \sim N(0, Q_i), \quad (7)$$

$$X_{i|i}^n = X_{i|i-1}^n + P_{i|i-1}^N H_i^T (H_i P_{i|i-1}^N H_i^T + R_i)^{-1} (y_i - W_i^n - H_i X_{i|i-1}^n) \quad W_i^n \sim N(0, R_i), \quad (8)$$

where $P_{i|i-1}^N$ is the covariance estimate from the ensemble $\left[X_{i|i-1}^n \right]_{n=1}^N$,

$$P_{i|i-1}^N = \frac{1}{N-1} \sum_{n=1}^N (X_{i|i-1}^n - \bar{X}_{i|i-1}^N) (X_{i|i-1}^n - \bar{X}_{i|i-1}^N)^T, \quad \text{where } \bar{X}_{i|i-1}^N = \frac{1}{N} \sum_{n=1}^N X_{i|i-1}^n.$$

The empirical covariance matrix $P_{i|i-1}^N$ is never computed or stored, indeed to compute the matrix products $P_{i|i-1}^N H_i^T$ and $H_i P_{i|i-1}^N H_i^T$ only matrix-vector products are needed:

$$\begin{aligned} P_{i|i-1}^N H_i^T &= \frac{1}{N-1} \sum_{n=1}^N (X_{i|i-1}^n - \bar{X}_{i|i-1}^N) (X_{i|i-1}^n - \bar{X}_{i|i-1}^N)^T H_i^T \\ &= \frac{1}{N-1} \sum_{n=1}^N (X_{i|i-1}^n - \bar{X}_{i|i-1}^N) h_n^T, \end{aligned} \quad (9)$$

$$H_i P_{i|i-1}^N H_i^T = H_i \frac{1}{N-1} \sum_{n=1}^N (X_{i|i-1}^n - \bar{X}_{i|i-1}^N) (X_{i|i-1}^n - \bar{X}_{i|i-1}^N)^T H_i^T = \frac{1}{N-1} \sum_{n=1}^N h_n h_n^T, \quad (10)$$

where

$$h_n = H_i \left(X_{i|i-1}^n - \bar{X}_{i|i-1}^N \right). \quad (11)$$

Note that the i.i.d. random vectors (V_i^1, \dots, V_i^N) are simulated here with the same statistics as the additive Gaussian noise V_i in the original state in eq. (2). The i.i.d. random vectors (W_i^1, \dots, W_i^N) are simulated here with the same statistics as the additive Gaussian noise W_i in the original state in eq. (3). The initial ensemble $[X_{0|0}]_{n=1}^N$ is simulated as i.i.d. Gaussian random vectors with mean x_b and covariance B , i.e. with the same statistics as the initial state X_0 .

4.3 Convergence of the EnKF

For theoretical purposes, we define an auxiliary ensemble $U_{i|i} = [U_{i|i}^n]_{n=1}^N$, $i = 0, \dots, k$, called the *reference ensemble*, in the same way as the ensemble $X_{i|i} = [X_{i|i}^n]_{n=1}^N$, but this time for the updates of the ensemble $U_{i|i}$ we use the exact covariances instead of their empirical estimates. The realizations of the random perturbations V_i^n and W_i^n in both ensembles are the same. Thus, for $i = 0$, $U_{0|0}^n = X_{0|0}^n$ and for $i = 1, \dots, k$, we build $U_{i|i}$ up to time i conditioned on observations up to time i ,

$$U_{i|i-1}^n = M_i U_{i-1|i-1}^n + \mu_i + V_i^n, \quad V_i^n \sim N(0, Q_i), \quad n = 1, \dots, N, \quad (12)$$

$$U_{i|i}^n = U_{i|i-1}^n + P_{i|i-1} H_i^T (H_i P_{i|i-1} H_i^T + R_i)^{-1} \left(y_i - W_i^n - H_i U_{i|i-1}^n \right), \quad (13)$$

where $W_i^n \sim N(0, R_i)$ is a random perturbation, and $P_{i|i-1}$ is the covariance of $U_{i|i-1}^1$

$$P_{i|i-1} = E \left[\left(U_{i|i-1}^n - E(U_{i|i-1}^n) \right) \left(U_{i|i-1}^n - E(U_{i|i-1}^n) \right)^T \right].$$

Note that the only difference between the two ensembles $X_{k|k}$ and $U_{k|k}$ is that for the construction of $X_{k|k}$, we use the empirical prediction covariance $P_{k|k-1}^N$ of the ensemble, which depends on all ensemble members, instead of the exact covariance. Therefore, $X_{k|k}^n$, $n = 1, \dots, N$, are in general dependent. On the other hand:

Lemma 6. *The members of the ensemble $[U_{k|k}^n]_{n=1}^N$ are i.i.d and the distribution of each $U_{k|k}^n$ is the same as the filtering distribution.*

Proof. The proof is by induction and the same as in [26, Lemma 4], except we take the additional perturbation V_k^n into account. Since $[V_k^n]_{n=1}^N$ are Gaussian and independent of everything else by assumption, $[U_{k|k}^n]_{n=1}^N$ are independent and Gaussian. The forecast covariance $P_{k|k-1}$ is constant (non-random), and, consequently, the analysis step (13) is a linear transformation, which preserves the independence of the ensemble members and the Gaussianity of the distribution. It is known that the members of the reference ensemble have the same mean and covariance as given by the Kalman filter [6, eq. (15) and (16)]. The proof is completed by noting that a Gaussian distribution is determined by its mean and covariance. \square

Theorem 3. *For any $i = 0, \dots, k$, the random matrix*

$$\begin{bmatrix} X_{i|i}^1, \dots, X_{i|i}^N \\ U_{i|i}^1, \dots, U_{i|i}^N \end{bmatrix} \quad (14)$$

has exchangeable columns, and

$$X_{i|i}^1 \rightarrow U_{i|i}^1,$$

in all L^p , $1 \leq p < \infty$, as $N \rightarrow \infty$. Also,

$$\begin{aligned} \bar{X}_{i|i-1}^N &= \frac{1}{N} \sum_{n=1}^N X_{i|i}^n \rightarrow E \left(U_{i|i}^1 \right), \\ P_{i|i-1}^N &= \frac{1}{N-1} \sum_{n=1}^N \left(X_{i|i-1}^n - \bar{X}_{i|i-1}^N \right) \left(X_{i|i-1}^n - \bar{X}_{i|i-1}^N \right)^\top \\ &\rightarrow P_{i|i-1} = E \left[\left(U_{i|i-1}^1 - E \left(U_{i|i-1}^1 \right) \right) \left(U_{i|i-1}^1 - E \left(U_{i|i-1}^1 \right) \right)^\top \right], \end{aligned}$$

in all L^p , $1 \leq p < \infty$, as $N \rightarrow \infty$.

Proof. The theorem is again a simple extension of that of [26, Theorem 1], by adding the model error V_i^n in each step of the induction over i . \square

Note that since (14) has exchangeable columns and $X_{i|i}^1 \rightarrow U_{i|i}^1$ in L^p , we have the same convergence result for every fixed n , $X_{i|i}^n \rightarrow U_{i|i}^n$ in all L^p , as $N \rightarrow \infty$.

5 Kalman smoothing

5.1 Kalman smoother (KS)

A smoother estimates the composite hidden state

$$X_{0:i} = \begin{bmatrix} X_0 \\ \vdots \\ X_i \end{bmatrix}$$

given all observations y_1, \dots, y_i . Again, the Kalman smoother provides the exact result in the linear Gaussian case. Denote by $X_{0:i|\ell}$ the expectation of the composite state $X_{0:i}$ given the observations y_1, \dots, y_ℓ , and by $P_{0:i|\ell}$ the corresponding covariance. In the linear case, we write the stochastic system (2)–(3) in terms of the composite state $X_{0:i}$ as

$$X_{0:i} = \begin{bmatrix} I_m & 0 & \dots & 0 \\ 0 & I_m & \vdots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & \ddots & I_m \\ 0 & \dots & 0 & M_i \end{bmatrix} X_{0:i-1} + \begin{bmatrix} 0 \\ \vdots \\ \mu_i \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ V_i \end{bmatrix} \quad (15)$$

$$= \begin{bmatrix} I_{m(i-1)} \\ M_i \end{bmatrix} X_{0:i-1} + \begin{bmatrix} 0 \\ \vdots \\ \mu_i \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ V_i \end{bmatrix}, \quad V_i \sim N(0, Q_i),$$

$$y_i = [0, \dots, H_i] X_{0:i} + W_i = \tilde{H}_i X_{0:i} + W_i, \quad W_i \sim N(0, R_i), \quad (16)$$

where m is the dimension of the state X_i , I_d is the identity matrix in $\mathbf{R}^{d \times d}$, and

$$\tilde{H}_i = [0, \dots, H_i], \quad \tilde{M}_i = [0, \dots, M_i]. \quad (17)$$

Applying the Kalman filter analysis step (4)–(6) to the observation (16) of the composite state $X_{0:i}$, we obtain the Kalman smoother:

$$\begin{aligned} X_{0:i|i-1} &= \begin{bmatrix} I_{m(i-1)} \\ \tilde{M}_i \end{bmatrix} X_{0:i-1|i-1} + \begin{bmatrix} 0 \\ \vdots \\ \mu_i \end{bmatrix} = \begin{bmatrix} X_{0:i-1|i-1} \\ M_i X_{i-1,i-1} + \mu_i \end{bmatrix}, \\ P_{0:i|i-1} &= \begin{bmatrix} I_{m(i-1)} \\ \tilde{M}_i \end{bmatrix} P_{0:i-1|i-1} \begin{bmatrix} I_{m(i-1)} \\ \tilde{M}_i \end{bmatrix}^T + \begin{bmatrix} 0 & 0 \\ 0 & Q_i \end{bmatrix} \\ &= \begin{bmatrix} P_{0:i-1|i-1} & P_{0:i-1|i-1} \tilde{M}_i^T \\ \tilde{M}_i P_{0:i-1|i-1} & \tilde{M}_i P_{0:i-1|i-1} \tilde{M}_i^T + Q_i \end{bmatrix}, \\ K_i &= P_{0:i|i-1} \tilde{H}_i^T \left(R_i + \tilde{H}_i P_{0:i|i-1} \tilde{H}_i^T \right)^{-1} \\ &= P_{0:i|i-1} \tilde{H}_i^T \left(R_i + H_i P_{i,i|i-1} H_i^T \right)^{-1}, \\ X_{0:i|i} &= X_{0:i|i-1} + K_i \left(y_i - \tilde{H}_i X_{0:i|i-1} \right) = X_{0:i|i-1} + K_i \left(y_i - H_i X_{i|i-1} \right), \\ P_{0:i|i} &= \left(I_{mi} - K_i \tilde{H}_i \right) P_{0:i|i-1}. \end{aligned}$$

Lemma 7. *The distribution $N(X_{0:k|k}, P_{0:k,0:k|k})$ from the Kalman smoother is the smoothing distribution, and its mean $X_{0:k|k}$ is the solution of the least squares problem,*

$$X_{0:k|k} = \underset{x_{0:k}}{\operatorname{argmin}} \left(|x_0 - x_b|_{B^{-1}}^2 + \sum_{i=1}^k |x_i - M_i x_{i-1} - \mu_i|_{Q_i^{-1}}^2 + \sum_{i=1}^k |y_i - H_i x_i|_{R_i^{-1}}^2 \right). \quad (18)$$

Proof. The mean $X_{0:k|k}$ maximizes the joint posterior probability density of the composite state $X_{0:k}$ given $y_{1:k}$, which is proportional to

$$e^{-\frac{1}{2}|x_0 - x_b|_{B^{-1}}^2} e^{-\frac{1}{2} \sum_{i=1}^k |x_i - M_i x_{i-1} - \mu_i|_{Q_i^{-1}}^2} e^{-\frac{1}{2} \sum_{i=1}^k |y_i - H_i x_i|_{R_i^{-1}}^2}$$

from the Bayes theorem. □

Again, when m is large, the covariance matrices $P_{0:i|i-1}$ and $P_{0:i|i}$ are very large and the matrix products in the computation of $P_{0:i|i-1}$ is also problematic to implement, and we turn to ensemble methods.

5.2 Ensemble Kalman smoother (EnKS)

In the ensemble Kalman smoother [8], the covariances are replaced by approximations from the ensemble. Let

$$\left[\begin{bmatrix} X_{0|j}^1 \\ \vdots \\ X_{i|j}^1 \end{bmatrix}, \dots, \begin{bmatrix} X_{0|j}^N \\ \vdots \\ X_{i|j}^N \end{bmatrix} \right] = \left[X_{0:i|j}^1, \dots, X_{0:i|j}^N \right] = \left[X_{0:i|j}^n \right]_{n=1}^N$$

denote an ensemble of N model states over time up to i , conditioned on the observations up to time j .

Algorithm 4 (EnKS). For $i = 0$, the ensemble $\left[X_{0|0}^n\right]_{n=1}^N$ consists of i.i.d. Gaussian random variables

$$X_{0|0}^n \sim N(x_b, B). \quad (19)$$

For $i = 1, \dots, k$, advance the model to time i by

$$X_{i|i-1}^n = M_i X_{i-1|i-1}^n + \mu_i + V_i^n, \quad V_i^n \sim N(0, Q_i), \quad n = 1, \dots, N. \quad (20)$$

Incorporate the observation at time i ,

$$y_i = \tilde{H}_i X_i + W_i, \quad W_i \sim N(0, R_i)$$

into the ensemble of composite states $\left[X_{0:i|i-1}^1, \dots, X_{0:i|i-1}^N\right]$ in the same way as for the EnKF update,

$$X_{0:i|i}^n = X_{0:i|i-1}^n + P_{0:i|i-1}^N \tilde{H}_i^T \left(\tilde{H}_i P_{0:i|i-1}^N \tilde{H}_i^T + R_i \right)^{-1} \left(y_i - W_i^n - H_i X_{i|i-1}^n \right) \quad (21)$$

where $P_{0:i|i-1}^N$ is a covariance estimate from the ensemble $X_{0:i|i-1}$ and $W_i^n \sim N(0, R_i)$ are random perturbations. Similarly as in (9)–(11), only the following matrix-vector products are needed:

$$\begin{aligned} P_{0:i|i-1}^N \tilde{H}_i^T &= \frac{1}{N-1} \sum_{n=1}^N \left(X_{0:i|i-1}^n - \bar{X}_{0:i|i-1}^N \right) \left(X_{i|i-1}^n - \bar{X}_{i|i-1}^N \right)^T H_i^T \\ &= \frac{1}{N-1} \sum_{n=1}^N \left(X_{0:i|i-1}^n - \bar{X}_{0:i|i-1}^N \right) h_n^T, \end{aligned} \quad (22)$$

$$\tilde{H}_i^T P_{0:i|i-1} \tilde{H}_i^T = H_i \frac{1}{N-1} \sum_{n=1}^N \left(X_{i|i-1}^n - \bar{X}_{i|i-1}^N \right) \left(X_{i|i-1}^n - \bar{X}_{i|i-1}^N \right)^T H_i^T = \frac{1}{N-1} \sum_{n=1}^N h_n h_n^T, \quad (23)$$

where again

$$h_n = H_i \left(X_{i|i-1}^n - \bar{X}_{i|i-1}^N \right) \quad (24)$$

and

$$\bar{X}_{\ell|i-1}^N = \frac{1}{N} \sum_{n=1}^N X_{\ell|i-1}^n. \quad (25)$$

5.3 Convergence of the EnKS

Just as for the EnKF, we construct an ensemble $U_{0:k|k} = [U_{0:k|k}^n]_{n=1}^N$ in the same way as the ensemble $\left[X_{0:k|k}^n\right]_{n=1}^N$, but for the updates of the ensemble $U_{0:k|k}$ we use the exact covariances instead of their empirical estimates. So, for $i = 0$, $U_{0|0}^n = X_{0|0}^n$, and for $i = 1, \dots, k$, $n = 1, \dots, N$,

$$\begin{aligned} U_{i|i-1}^n &= M_i U_{i-1|i-1}^n + \mu_i + V_i^n, \quad V_i^n \sim N(0, Q_i), \\ U_{0:i|i}^n &= U_{0:i|i-1}^n + P_{0:i|i-1} \tilde{H}_i^T \left(\tilde{H}_i P_{0:i|i-1} \tilde{H}_i^T + R_i \right)^{-1} \left(y_i - W_i^n - H_i U_{i|i-1}^n \right), \\ W_i^n &\sim N(0, R_i), \end{aligned}$$

where $P_{0:i|i-1}$ is the covariance of $U_{0:i|i-1}^1$.

Since the Kalman smoother is nothing else than the Kalman filter for the composite state $X_{0:k}$, the same induction step as in Theorem 3 applies for each i , and we have the following.

Lemma 8. *The random elements $U_{0:k|k}^1, \dots, U_{0:k|k}^N$ are i.i.d and the distribution of each $U_{0:k|k}^n$ is the same as the smoothing distribution. In particular, $E(U_{0:k|k}) = X_{0:k|k}$, with $X_{0:k|k}$ is the least squares solution (18).*

Theorem 5. *For each time step $i = 0, \dots, k$, the random matrix*

$$\begin{bmatrix} X_{0:i|i}^1, \dots, X_{0:i|i}^N \\ U_{0:i|i}^1, \dots, U_{0:i|i}^N \end{bmatrix}.$$

has exchangeable columns, and $X_{0:i|i}^1 \rightarrow U_{0:i|i}^1$, $\bar{X}_{0:i|i}^N \rightarrow E(U_{0:i|i}^1)$, and $P_{0:i|i}^N \rightarrow P_{0:i|i}$ in L^p as $N \rightarrow \infty$, for all $1 \leq p < \infty$.

6 Variational data assimilation and 4DVAR

6.1 4DVAR as an optimization problem

We estimate the compound state $X_{0:k}$ of the stochastic system (1)–(3), conditioned on the observations y_1, \dots, y_k , by the maximum posterior probability density,

$$\mathbb{P}(x_{0:k}|y_{1:k}) \propto e^{-\frac{1}{2} \left(|x_0 - x_b|_{B^{-1}}^2 + \sum_{i=1}^k |x_i - \mathcal{M}_i(x_{i-1}) - \mu_i|_{Q_i^{-1}}^2 + \sum_{i=1}^k |y_i - \mathcal{H}_i(x_i)|_{R_i^{-1}}^2 \right)} \rightarrow \max_{x_{0:k}},$$

which is the same as solving the nonlinear least squares problem for the composite state $x_{0:k}$,

$$|x_0 - x_b|_{B^{-1}}^2 + \sum_{i=1}^k |x_i - \mathcal{M}_i(x_{i-1}) - \mu_i|_{Q_i^{-1}}^2 + \sum_{i=1}^k |y_i - \mathcal{H}_i(x_i)|_{R_i^{-1}}^2 \rightarrow \min_{x_{0:k}}. \quad (26)$$

Numerical solution of the nonlinear least squares problem (26) is the essence of weak-constraint 4-dimensional variational data assimilation (4DVAR) [9, 31].

6.2 The Levenberg-Marquardt method and incremental 4DVAR

Consider an approximate solution $x_{0:k}^{j-1}$ of the nonlinear least squares problem (26). We seek a better approximation $x_{0:k}^j$. Linearizing the model and the observation operators at $x_{0:k}^{j-1}$ by their tangent operators and adding a penalty term to control the size of the increment $x_{0:k}^j - x_{0:k}^{j-1}$, yields the linear least squares problem for $x_{0:k}^j$ in the Levenberg-Marquardt (LM) method [20, 27] for the solution of the nonlinear least squares (26).

Algorithm 6 (LM method). *Given $x_{0:k}^0$ and $\gamma \geq 0$, compute the iterations $x_{0:k}^j$ for $j = 1, 2, \dots$, as the solutions of the least squares problem linearized at $x_{0:k}^{j-1}$,*

$$\begin{aligned} x_{0:k}^j = \operatorname{argmin}_{x_{0:k}} & |x_0 - x_b|_{B^{-1}}^2 + \sum_{i=1}^k \left| x_i - \mathcal{M}_i(x_{i-1}^{j-1}) - \mathcal{M}'_i(x_{i-1}^{j-1})(x_{i-1} - x_{i-1}^{j-1}) - \mu_i \right|_{Q_i^{-1}}^2 \\ & + \sum_{i=1}^k \left| y_i - \mathcal{H}_i(x_i^{j-1}) - \mathcal{H}'_i(x_i^{j-1})(x_i - x_i^{j-1}) \right|_{R_i^{-1}}^2 + \sum_{i=1}^k \gamma |x_i - x_i^{j-1}|^2. \end{aligned} \quad (27)$$

For $\gamma = 0$, (27) becomes the Gauss-Newton method, which can converge at a rate close to quadratic, but convergence is not guaranteed even locally. Under suitable technical assumptions, the LM method is guaranteed to converge globally if the regularization parameter γ is large enough [28, 10], and a suitable sequence of penalty parameters $\gamma_j \geq 0$ changing from step to step can be found adaptively. The LM method is a precursor of the trust-region method in the sense that it seeks to determine when the faster Gauss-Newton method ($\gamma = 0$) is applicable and when it is not and should be blended with a slower but safer gradient descent method ($\gamma > 0$). In this paper, we consider only the case of a constant penalty parameter $\gamma > 0$.

The Gauss-Newton method for the solution of nonlinear least squares is known in atmospheric sciences as incremental 4DVAR [7]. The use of Levenberg-Marquardt iterations was proposed by [32].

6.3 LM-EnKS with tangent operators

From (18), it follows that the linear least squares problem (27) can be interpreted as finding the maximum posterior probability density for a linear stochastic system with all Gaussian probability distributions. The penalty terms $\gamma|x_i - x_i^{j-1}|^2$ are implemented as additional independent observations [12] of the form

$$x_i^{j-1} = x_i + E_i, \quad E_i \sim N\left(0, \frac{1}{\gamma}I_m\right), \quad i = 1, \dots, k.$$

Lemma 9. *The LM iterate $x_{0:k}^j$, defined by (27), equals to the mean*

$$x_{0:k}^j = E\left(X_{0:k|k}^j\right),$$

of the smoothing distribution of the stochastic system

$$X_0^j \sim N(x_b, B), \tag{28}$$

$$X_i^j = \mathcal{M}'_i(x_{i-1}^{j-1})\left(X_{i-1}^j - x_{i-1}^{j-1}\right) + \mathcal{M}_i(x_{i-1}^{j-1}) + \mu_i + V_i^j, \quad V_i^j \sim N(0, Q_i) \quad i = 1, \dots, k, \tag{29}$$

$$\tilde{y}_i = \tilde{\mathcal{H}}_i(x_i^{j-1}) + \tilde{\mathcal{H}}'_i(x_i^{j-1})\left(X_i^j - x_i^{j-1}\right) + \tilde{W}_i^j, \quad \tilde{W}_i^j \sim N(0, \tilde{R}_i), \quad i = 1, \dots, k, \tag{30}$$

where

$$\tilde{y}_i = \begin{bmatrix} y_i \\ x_i^{j-1} \end{bmatrix}, \quad \tilde{\mathcal{H}}_i = \begin{bmatrix} \mathcal{H}_i \\ I_m \end{bmatrix}, \quad \tilde{R}_i = \begin{bmatrix} R_i & 0 \\ 0 & \frac{1}{\gamma}I_m \end{bmatrix}, \tag{31}$$

or, equivalently

$$X_0^j \sim N(x_b, B), \tag{32}$$

$$X_i^j = M_i^j X_{i-1}^j + \tilde{\mu}_i^j + V_i^j, \quad V_i^j \sim N(0, Q_i) \quad i = 1, \dots, k, \tag{33}$$

$$\tilde{y}_i^j = \tilde{H}_i^j X_i^j + \tilde{W}_i^j, \quad \tilde{W}_i^j \sim N(0, \tilde{R}_i), \quad i = 1, \dots, k, \tag{34}$$

where

$$M_i^j = \mathcal{M}'_i(x_{i-1}^{j-1}), \quad \tilde{\mu}_i^j = \mathcal{M}_i(x_{i-1}^{j-1}) + \mu_i - \mathcal{M}'_i(x_{i-1}^{j-1})x_{i-1}^{j-1},$$

$$\tilde{H}_i^j = \tilde{\mathcal{H}}'_i(x_i^{j-1}), \quad \tilde{y}_i^j = \tilde{y}_i + \tilde{\mathcal{H}}'_i(x_i^{j-1})x_i^{j-1} - \tilde{\mathcal{H}}_i(x_i^{j-1}).$$

Proof. The system (28)–(30) has the same form as the original problem (1)–(3) and all distributions are Gaussian, hence Lemma 7 applies. \square

Corollary 7. *The LM iterate x^j is the mean found from the Kalman smoother (15)–(17), applied to the linear stochastic system (28)–(30).*

However, since the dimension of the state is generally large, we apply the EnKS (19)–(25) to solve (28)–(30) approximately. In each LM iteration $j = 1, 2, \dots$, the linearized least squares solution x^j is approximated by the sample mean $\bar{X}_{0:k|k}^{j, N_j}$ from the EnKS and the least squares are linearized at the previous iterate $\bar{X}_{0:k|k}^{j-1, N_{j-1}}$ rather than at x^{j-1} . However, for $j = 0$ this notation is formal for the sake of consistency only. There is no ensemble for $j = 0$.

Algorithm 8. *Given an initial approximation $x_{0:k}^0$, and $\gamma \geq 0$. Initialize*

$$\tilde{x}^j = \bar{X}_{0:k|k}^{j, N_j} = x_{0:k}^0 \quad \text{for } j = 0.$$

LM loop: For $j = 1, 2, \dots$. Choose an ensemble size N_j .

EnKS loop: For $i = 0$, the ensemble $\left[X_{0|0}^{j, n}\right]_{n=1}^{N_j}$ consists of i.i.d. Gaussian random variables

$$X_{0|0}^{j, n} \sim N(\tilde{x}_0^0, B).$$

For $i = 1, \dots, k$, advance the model in time (the forecast step) by

$$\begin{aligned} X_{i|i-1}^{j, n} &= \mathcal{M}'_i \left(\bar{X}_{i-1|k}^{j-1, N_{j-1}} \right) \left(X_{i-1|i-1}^{j, n} - \bar{X}_{i-1|k}^{j-1, N_{j-1}} \right) + \mathcal{M}_i \left(\bar{X}_{i-1|k}^{j-1, N_{j-1}} \right) + \mu_i + V_i^{j, n}, \\ V_i^{j, n} &\sim N(0, Q_i), \quad n = 1, \dots, N_j. \end{aligned} \quad (35)$$

Incorporate the observations at time i into the ensemble of composite states $\left[X_{0:i|i-1}^{j, n}\right]_{n=1}^{N_j}$ in the same way as in the EnKF analysis step,

$$\begin{aligned} X_{0:i|i}^{j, n} &= X_{0:i|i-1}^{j, n} + P_{0:i|i-1}^{j, N_j} \tilde{H}_i^{jT} \left(\tilde{H}_i^j P_{0:i|i-1}^{j, N_j} \tilde{H}_i^{jT} + \tilde{R}_i \right)^{-1} \\ &\quad \cdot \left(\tilde{y}_i - \tilde{W}_i^{j, n} - \tilde{\mathcal{H}}_i \left(\bar{X}_{i|k}^{j-1, N_{j-1}} \right) - \tilde{\mathcal{H}}'_i \left(\bar{X}_{i|k}^{j-1, N_{j-1}} \right) \left(X_{i|i-1}^{j, n} - \bar{X}_{i|k}^{j-1, N_{j-1}} \right) \right), \\ \tilde{W}_i^{j, n} &\sim N(0, \tilde{R}_i) \end{aligned} \quad (36)$$

where $P_{0:i|i-1}^{j, N_j}$ is the sample covariance from the ensemble $\left[X_{0:i|i-1}^{j, n}\right]_{n=1}^{N_j}$. Similarly as in (9)–(11),

only the following matrix-vector products are needed:

$$\begin{aligned}
P_{0:i|i-1}^{j,N_j} \tilde{H}_i^{j\text{T}} &= \frac{1}{N_j - 1} \sum_{n=1}^{N_j} \left(X_{0:i|i-1}^{j,n} - \bar{X}_{0:i|i-1}^{j,N_j} \right) \left(X_{i|i-1}^{j,n} - \bar{X}_{i|i-1}^{j,N_j} \right)^{\text{T}} \tilde{H}_i^{j\text{T}} \\
&= \frac{1}{N_j - 1} \sum_{n=1}^{N_j} \left(X_{0:i|i-1}^{j,n} - \bar{X}_{0:i|i-1}^{j,N_j} \right) h_i^{j,n\text{T}}, \\
\tilde{H}_i^j P_{0:i|i-1}^{j,N_j} \tilde{H}_i^{j\text{T}} &= \frac{1}{N_j - 1} \sum_{n=1}^{N_j} \tilde{H}_i^j \left(X_{i|i-1}^{j,n} - \bar{X}_{i|i-1}^{j,N_j} \right) \left(X_{i|i-1}^{j,n} - \bar{X}_{i|i-1}^{j,N_j} \right)^{\text{T}} \tilde{H}_i^{j\text{T}} \\
&= \frac{1}{N_j - 1} \sum_{n=1}^{N_j} h_i^{j,n} h_i^{j,n\text{T}},
\end{aligned}$$

where

$$h_i^{j,n} = \tilde{H}_i^j \left(X_{i|i-1}^{j,n} - \bar{X}_{i|i-1}^{j,N_j} \right) = \tilde{\mathcal{H}}_i' \left(\bar{X}_{i|k}^{j-1,N_{j-1}} \right) \left(X_{i|i-1}^{j,n} - \bar{X}_{i|i-1}^{j,N_j} \right) \quad (37)$$

and

$$\bar{X}_{i|i-1}^{j,N_j} = \frac{1}{N_j} \sum_{n=1}^{N_j} X_{i|i-1}^{j,n}, \quad \bar{X}_{0:i|i-1}^{j,N_j} = \frac{1}{N_j} \sum_{n=1}^{N_j} X_{0:i|i-1}^{j,n}.$$

The next iterate is $\tilde{x}^j = \bar{X}_{0:k|k}^{j,N_j}$.

In the rest of this section, we study the asymptotic behavior of Algorithm 8 when the ensemble sizes $N_1, \dots, N_j \rightarrow \infty$. We start with an a-priori L^p bound on the ensemble members, independent of the ensemble size.

Assumption 9. *The model and observation operators, \mathcal{M}_i , and \mathcal{H}_i are continuously differentiable, with at most polynomial growth at infinity, and their Jacobians have at most polynomial growth at infinity, i.e. there exists $\kappa > 0$ and $s \geq 0$, such that $|\mathcal{M}_i(x)| \leq \kappa(1 + |x|^s)$, $|\mathcal{M}'_i(x)| \leq \kappa(1 + |x|^s)$, $|\mathcal{H}_i(x)| \leq \kappa(1 + |x|^s)$, and $|\mathcal{H}'_i(x)| \leq \kappa(1 + |x|^s)$ for all i and all x .*

Since we are interested in the convergence with the ensemble size, we need a notation to distinguish between $X_{0:k|k}^{j,n}$ coming from ensembles of different sizes N_j . Thus, when we need to make such distinction, we denote by $X_{0:k|k}^{j,n,N_j}$ the n -th ensemble member from the ensemble $\left[X_{0:k|k}^{j,1}, \dots, X_{0:k|k}^{j,N_j} \right]$ of size N_j in Algorithm 8, and similarly for other subscripts and superscripts.

Lemma 10. *For any $1 \leq p < \infty$, any $i = 0, \dots, k$ and any $j = 1, 2, \dots$, there exists a constant $C(i, j, p)$ such that in Algorithm 8,*

$$\left\| X_{0:i|i}^{j,n,N_j} \right\|_p \leq C(i, j, p) \quad (38)$$

for all $n = 1, \dots, N_j$ and all N_j .

Proof. Let $p \in [1, \infty)$. We will prove (38) by induction on the iteration number j . For $j = 1$, \tilde{x}^{j-1} is constant, otherwise, for $j \geq 2$, $\|\tilde{x}^{j-1}\|_p$ is bounded independently of the ensemble sizes by induction assumption because

$$\tilde{x}^{j-1} = \bar{X}_{0:k|k}^{j-1,N_{j-1}} = \frac{1}{N_{j-1}} \sum_{n=1}^{N_{j-1}} X_{0:k|k}^{j-1,n,N_{j-1}}.$$

For a fixed j , we now proceed by induction on the time step i . For $i = 0$, $X_{0|0}^{j,n} \sim N(x_0^0, B)$, thus $\|X_{0|0}^{j,n}\|_p$ does not depend on n or N_j . For $i = 1, \dots, k$, from (35), we have

$$\|X_{i|i-1}^{j,n}\|_p \leq \|\mathcal{M}'_i(\tilde{x}_{i-1}^{j-1})\|_{2p} \left(\|X_{i-1|i-1}^{j,n}\|_{2p} + \|\tilde{x}_{i-1}^{j-1}\|_{2p} \right) + \|\mathcal{M}_i(\tilde{x}_{i-1}^{j-1})\|_p + |\mu_i| + \|V_i^{j,n}\|_p.$$

From Assumption 9 and the fact that $V_i^{j,n}$ is normally distributed, there exist a constant C_p such that

$$\begin{aligned} \|X_{i|i-1}^{j,n}\|_p &\leq \kappa C_p \left(1 + \|\tilde{x}_{i-1}^{j-1}\|_{2ps}^s \right) \left(\|X_{i-1|i-1}^{j,n}\|_{2p} + \|\tilde{x}_{i-1}^{j-1}\|_{2p} \right) \\ &\quad + \kappa C_p \left(1 + \|\tilde{x}_{i-1}^{j-1}\|_{ps}^s \right) + |\mu_i| + C_p. \end{aligned}$$

Bounding \tilde{x}_{i-1}^{j-1} by the induction assumption on j and $X_{i-1|i-1}^{j,n}$ by the induction assumption on i , we have that $\|X_{0:i|i-1}^{j,n,N_j}\|_p$ is bounded independently of n and N_j . From equation (36), and the fact that $\tilde{H}_i^j = \tilde{\mathcal{H}}'_i(\tilde{x}_i^{j-1}) = [0, \dots, \mathcal{H}'_i(\tilde{x}_i^{j-1})]$ we conclude that

$$\begin{aligned} \|X_{0:i|i}^{j,n}\|_p &\leq \|X_{0:i|i-1}^{j,n}\|_p + \left\| P_{0:i|i-1}^{j,N_j} \tilde{\mathcal{H}}'^{\Gamma}(\tilde{x}_i^{j-1}) \left(\tilde{\mathcal{H}}'_i(\tilde{x}_i^{j-1}) P_{0:i|i-1}^{j,N_j} \tilde{\mathcal{H}}'^{\Gamma}(\tilde{x}_i^{j-1}) + \tilde{R}_i \right)^{-1} \right\|_{2p} \\ &\quad \cdot \left\| \tilde{y}_i - \tilde{W}_i^{j,n} - \mathcal{H}_i(\tilde{x}_i^{j-1}) - \tilde{\mathcal{H}}'_i(\tilde{x}_i^{j-1}) \left(X_{i|i-1}^{j,n} - \tilde{x}_i^{j-1} \right) \right\|_{2p}, \\ &\leq \|X_{0:i|i-1}^{j,n}\|_p + \|P_{0:i|i-1}^{j,N_j}\|_{8p} \|\tilde{\mathcal{H}}'^{\Gamma}(\tilde{x}_i^{j-1})\|_{8p} \\ &\quad \cdot \left\| \left(\tilde{\mathcal{H}}'_i(\tilde{x}_i^{j-1}) P_{0:i|i-1}^{j,N_j} \tilde{\mathcal{H}}'^{\Gamma}(\tilde{x}_i^{j-1}) + \tilde{R}_i \right)^{-1} \right\|_{4p} \\ &\quad \cdot \left(|\tilde{y}_i| + \|\tilde{W}_i^{j,n}\|_{2p} + \|\mathcal{H}_i(\tilde{x}_i^{j-1})\|_{2p} + \|\tilde{\mathcal{H}}'_i(\tilde{x}_i^{j-1})\|_{4p} \left(\|X_{i|i-1}^{j,n}\|_{4p} + \|\tilde{x}_i^{j-1}\|_{4p} \right) \right). \end{aligned}$$

Since \tilde{R}_i is positive definite and $P_{0:i|i-1}^{j,N_j}$ is positive semi definite, we have

$$\left\| \left(\tilde{\mathcal{H}}'_i(\tilde{x}_i^{j-1}) P_{0:i|i-1}^{j,N_j} \tilde{\mathcal{H}}'^{\Gamma}(\tilde{x}_i^{j-1}) + \tilde{R}_i \right)^{-1} \right\|_{4p} \leq |\tilde{R}_i^{-1}|. \quad (39)$$

From [26, lemma 31] we have

$$\|P_{0:i|i-1}^{j,N_j}\|_{8p} \leq 2 \|X_{0:i|i-1}^{j,1}\|_{16p}^2. \quad (40)$$

From the inequalities (39) and (40), Assumption 9, and the fact that $\tilde{W}_i^{j,n}$ is normally distributed, there exists a constant \tilde{C}_p such that

$$\begin{aligned} \|X_{0:i|i}^{j,n}\|_p &\leq \|X_{0:i|i-1}^{j,n}\|_p + 2 \|X_{0:i|i-1}^{j,1}\|_{16p}^2 \kappa \tilde{C}_p \left(1 + \|\tilde{x}_i^{j-1}\|_{8ps}^s \right) \\ &\quad \left| \tilde{R}_i^{-1} \right| |\tilde{y}_i| + \tilde{C}_p + \kappa \tilde{C}_p \left(1 + \|\tilde{x}_i^{j-1}\|_{2ps}^s \right) \\ &\quad + \kappa \tilde{C}_p \left(1 + \|\tilde{x}_i^{j-1}\|_{4ps}^s \right) \left(\|X_{i|i-1}^{j,1}\|_{4p} + \|\tilde{x}_i^{j-1}\|_{4p} \right) \end{aligned}$$

Bounding \tilde{x}_i^{j-1} by the induction assumption on j and $X_{i-1|i-1}^{j,n}$ by the induction assumption on i , we obtain that $\left\| X_{0:i|i}^{j,n,N_j} \right\|_p$ is bounded independently of n and N_j . \square

At each iteration j of Algorithm 8, we define for theoretical purposes a reference ensemble $\left[U_{0:k|k}^1, \dots, U_{0:k|k}^{N_j} \right]$, similarly as in Section 5.3, and with the derivatives taken at the mean, rather than sample mean as in Algorithm 8: For $j = 0$, all $U_{i|i}^{j,n} = X_{i|i}^{j,n} = x^0$ are constants. For $j = 1, 2, \dots$, $U_{0|0}^{j,n} = X_{0|0}^{j,n}$ for $i = 0$, and for $i = 1, \dots, k$,

$$U_{i|i-1}^{j,n} = \mathcal{M}'_i \left(E \left(U_{i-1|i-1}^{j-1,1} \right) \right) \left(U_{i-1|i-1}^{j,n} - x_{i-1}^{j-1} \right) + \mathcal{M}'_i \left(E \left(U_{i-1}^{j-1,1} \right) \right) + \mu_i + V_i^{j,n}, \quad (41)$$

$$U_{0:i|i}^{j,n} = U_{0:i|i-1}^{j,n} + Q_{0:i}^j \tilde{\mathcal{H}}'_i \left(E \left(U_{i|k}^{j-1,1} \right) \right)^\top \left(\mathcal{H}'_i \left(E \left(U_{i|k}^{j-1,1} \right) \right) Q_i^j \mathcal{H}'_i \left(E \left(U_{i|k}^{j-1,1} \right) \right)^\top + \tilde{R}_i \right)^{-1} \\ \left(\hat{y}_i + \tilde{\mathcal{H}}'_i \left(E \left(U_{i|k}^{j-1,1} \right) \right) \left(E \left(U_{i|k}^{j-1,1} \right) - U_{i|i-1}^{j,1} \right) - \mathcal{H}_i \left(E \left(U_{i|i}^{j-1,1} \right) \right) - \tilde{W}_i^{j,1} \right) \quad (42)$$

where $Q_{0:i}^j = \text{Cov} \left(U_{0:i|i-1}^{j-1,1} \right)$ and $\hat{y}_i = \left[E \left(U_{i|k}^{j-1,1} \right) \right]$. We now show that the mean of the reference ensemble members is the solution of the linearized least squares (27), and thus the next LM iterate:

Lemma 11. $E(U_{0:k|k}^{j,1}) = x^j$, where x^j is the j -th iterate generated by the algorithm (6).

Proof. The proof proceeds by induction on the iteration number j . For $j = 0$ we have $U^{0,n} = x^0$ for all n by definition, thus $E(U^{0,1}) = x^0$. Let $j \geq 1$. From the induction assumption, the stochastic system (41)–(42) is linearized about the previous LM iterate x^{j-1} . By Lemma 8, $\left[U_{0:k}^{j,n} \right]_{n=1}^{N_j}$ are i.i.d. with the smoothing distribution, whose mean is the solution of the linearized least squares (27). \square

Lemma 12. For all iterations j and all times $i = 0, \dots, k$, the columns of the random matrix

$$\left[X_{0:i|i}^j; U_{0:i|i}^j \right] = \left[\begin{array}{c} X_{0:i|i}^{j,1}, \dots, X_{0:i|i}^{j,N_j} \\ U_{0:i|i}^{j,1}, \dots, U_{0:i|i}^{j,N} \end{array} \right] \quad (43)$$

are exchangeable.

Proof. We recall that for all $j \geq 1$, $\tilde{x}^j = \bar{X}_{0:k|k}^{j,N_j}$. In this proof we omit the subscripts of N_j and N_{j-1} . We use induction on the LM iteration number j . For $j = 0$ we have that for all $i = 0, \dots, k$, $X_{0:i|i}^{0,n} = x_{0:i}^0 = U_{0:i|i}^{0,n}$, and $U_{0:i|i}^{0,n}$ are i.i.d., therefore $\left[X_{0:i|i}^0; U_{0:i|i}^0 \right]$ are exchangeable. For $j \geq 1$, we use the induction on the time index i . For $i = 0$, $\left[U_{0|0}^{j,n} \right]_{n=1}^N$ are i.i.d., and $X_{0|0}^{j,n} = U_{0|0}^{j,n}$, therefore

$[X_{0|0}^j; U_{0|0}^j]$ are exchangeable. For $i = 1, \dots, k$, consider first the forecast step,

$$\begin{aligned} \begin{bmatrix} X_{i|i-1}^{j,n} \\ U_{i|i-1}^{j,n} \end{bmatrix} &= \begin{bmatrix} \mathcal{M}'_i(\bar{X}_{i-1|k}^{j-1,N}) & 0 \\ 0 & \mathcal{M}'_i(E(U_{i-1|k}^{j-1,1})) \end{bmatrix} \begin{bmatrix} X_{i-1|i-1}^{j,n} \\ U_{i-1|i-1}^{j,n} \end{bmatrix} \\ &+ \begin{bmatrix} \mathcal{M}_i(\bar{X}_{i-1|k}^{j-1,N}) - \mathcal{M}'_i(\bar{X}_{i-1|k}^{j-1,N}) \bar{X}_{i-1|k}^{j-1,N} + \mu_i \\ \mathcal{M}_i(E(U_{i-1|k}^{j-1,1})) - \mathcal{M}'_i(E(U_{i-1|k}^{j-1,1})) E(U_{i-1|k}^{j-1,1}) + \mu_i \end{bmatrix} + \begin{bmatrix} V_i^{j,n} \\ V_i^{j,n} \end{bmatrix} \\ &= F^i \left(\bar{X}_{i-1|k}^{j-1,N}, \begin{bmatrix} X_{i-1|i-1}^{j,n} \\ U_{i-1|i-1}^{j,n} \end{bmatrix}, \begin{bmatrix} V_i^{j,n} \\ V_i^{j,n} \end{bmatrix} \right), \end{aligned}$$

where F^i is a measurable function. The ensemble sample mean $\bar{X}_{i-1|k}^{j-1,N}$ is invariant to a permutation of ensemble members, and $V_i^j = [V_i^{j,1}, \dots, V_i^{j,N}]$ is exchangeable because its members are i.i.d. From the induction assumption on i we have that $[X_{i-1|i-1}^j; U_{i-1|i-1}^j]$ is exchangeable, and it is also independent from $\begin{bmatrix} V_i^j \\ V_i^j \end{bmatrix}$, therefore, using Lemma 2, $\begin{bmatrix} X_{i|i-1}^j \\ U_{i|i-1}^j \end{bmatrix}$ is exchangeable. The analysis step also preserves exchangeability:

$$\begin{aligned} \begin{bmatrix} X_{0:i|i}^{j,n} \\ U_{0:i|i}^{j,n} \end{bmatrix} &= \begin{bmatrix} X_{0:i|i-1}^{j,n} \\ U_{0:i|i-1}^{j,n} \end{bmatrix} + \begin{bmatrix} K_i^N & 0 \\ 0 & K_i \end{bmatrix} \\ &\left(\begin{bmatrix} \tilde{y}_i - \mathcal{H}'_i(\bar{X}_{i|k}^{j-1,N}) \bar{X}_{i|i}^{j-1,N} - \mathcal{H}_i(\bar{X}_{i|k}^{j-1,N}) - \tilde{W}_i^{j,n} \\ \hat{y}_i - \mathcal{H}'_i(E(U_{i|k}^{j-1,1})) E(U_{i|k}^{j-1,1}) - \mathcal{H}_i(E(U_{i|k}^{j-1,1})) - \tilde{W}_i^{j,n} \end{bmatrix} \right. \\ &\left. - \begin{bmatrix} \mathcal{H}'_i(\bar{X}_{i|k}^{j-1,N}) & 0 \\ 0 & \mathcal{H}'_i(E(U_{i|k}^{j-1,1})) \end{bmatrix} \begin{bmatrix} X_{i|i-1}^{j,n} \\ U_{i|i-1}^{j,n} \end{bmatrix} \right) \\ &= F^i \left(\bar{X}_{i|k}^{j-1,N}, P_{0:i|i-1}^{j,N}, \begin{bmatrix} X_{i|i-1}^{j,n} \\ U_{i|i-1}^{j,n} \end{bmatrix}, \begin{bmatrix} \tilde{W}_i^{j,n} \\ \tilde{W}_i^{j,n} \end{bmatrix} \right) \end{aligned}$$

because the Kalman gain matrices are functions of the ensemble members through $\bar{X}_{i|k}^{j-1,N}$ and $P_{0:i|i-1}^{j,N}$ only,

$$\begin{aligned} K_i^N &= \begin{bmatrix} P_{0|i-1}^{j,N} \mathcal{H}'_i(\bar{X}_{i|k}^{j-1,N})^\top \\ \vdots \\ P_{i|i-1}^{j,N} \mathcal{H}'_i(\bar{X}_{i|k}^{j-1,N})^\top \end{bmatrix} \left(\mathcal{H}'_i(\bar{X}_{i|k}^{j-1,N}) P_{i|i-1}^{j,N} \mathcal{H}'_i(\bar{X}_{i|k}^{j-1,N})^\top + \tilde{R}_i \right)^{-1}, \\ K_i &= \begin{bmatrix} Q_0^j \mathcal{H}'_i(E(U_{i|k}^{j-1,1}))^\top \\ \vdots \\ Q_i^j \mathcal{H}'_i(E(U_{i|k}^{j-1,1}))^\top \end{bmatrix} \left(\mathcal{H}'_i(E(U_{i|k}^{j-1,1})) Q_i^j \mathcal{H}'_i(E(U_{i|k}^{j-1,1}))^\top + \tilde{R}_i \right)^{-1} \end{aligned}$$

and the ensemble sample mean $\bar{X}_{i|k}^{j-1,N}$, and the ensemble sample covariance $P_{0:i|i-1}^{j,N}$ are invariant to a permutation of ensemble members, $\tilde{W}_i^j = [\tilde{W}_i^{j,1}, \dots, \tilde{W}_i^{j,N}]$ is exchangeable because, its members are i.i.d. and they are independent from $[X_{i|i-1}^{j,n}; U_{i|i-1}^{j,n}]$ is exchangeable. Therefore, using again Lemma 2, $[X_{0:i|i}^{j,n}; U_{0:i|i}^{j,n}]$ are exchangeable. \square

Theorem 10. For all j , and $n = 1, \dots, N_j$, $X_{0:k|k}^{j,n,N_j} \rightarrow U_{0:k|k}^{j,n}$ and $\bar{X}_{0:k|k}^{j,N_j} \rightarrow E(U_{0:k|k}^{j,1})$ as $\min\{N_1, \dots, N_j\} \rightarrow \infty$, in all L^p , $1 \leq p < \infty$.

Proof. We will prove that for all $j \geq 0$ and all $1 \leq i \leq k$, $X_{0:i|i}^{j,1,N_j} \rightarrow U_{0:i|i}^{j,1}$ as $\min\{N_1, \dots, N_j\} \rightarrow \infty$, in all L^p , $1 \leq p < \infty$, and the convergence of the mean follows. Since $[X_{0:i|i}^{j,n}; U_{0:i|i}^{j,n}]_{n=1}^{N_j}$ are exchangeable, we only need to consider the convergence of $X_{0:i|i}^{j,1,N_j} \rightarrow U_{0:i|i}^{j,1}$. We use induction on the LM iteration number j . For $j = 0$, we have $X_{0:i|i}^{0,1,N_0} = x_{0:i}^0 = U_{0:i|i}^{0,1}$. For $j \geq 1$, we use induction on time index i . For $i = 0$, $X_{0|0}^{j,1,N_j} = U_{0|0}^{j,1}$. For $i = 1, \dots, k$, from induction assumption on j and i , we have $\bar{X}_{i-1|k}^{j-1,N_j} \rightarrow E(U_{i-1|k}^{j-1,1})$ and $X_{i-1|k}^{j,1,N_j} \rightarrow U_{i-1|k}^{j,1}$ in all L^p , $1 \leq p < \infty$, as $\min\{N_1, \dots, N_j\} \rightarrow \infty$. Convergence in L^p implies convergence in probability, and by the continuous mapping theorem,

$$\begin{aligned} X_{i|i-1}^{j,1,N_j} &= \mathcal{M}'_i \left(\bar{X}_{i-1|k}^{j-1,N_{j-1}} \right) X_{i-1|i-1}^{j,1,N_j} + \mathcal{M}_i \left(\bar{X}_{i-1|k}^{j-1,N_{j-1}} \right) \\ &\quad - \mathcal{M}'_i \left(\bar{X}_{i-1|k}^{j-1,N_{j-1}} \right) \bar{X}_{i-1|k}^{j-1,N_{j-1}} + \mu_i + V_i^{j,1} \\ &\stackrel{\text{P}}{\rightarrow} \mathcal{M}'_i \left(E \left(U_{i-1|k}^{j-1,1} \right) \right) U_{i-1|i-1}^{j,1} + \mathcal{M}_i \left(E \left(U_{i-1|k}^{j-1,1} \right) \right) \\ &\quad - \mathcal{M}'_i \left(E \left(U_{i-1|k}^{j-1,1} \right) \right) E \left(U_{i-1|k}^{j-1,1} \right) + \mu_i + V_i^{j,1} \\ &= U_{i|i-1}^{j,1} \end{aligned}$$

as $\min\{N_1, \dots, N_j\} \rightarrow \infty$. From Lemma 10, the sequence $\left\{ X_{0:i|i-1}^{j,1,N_j} \right\}_{N_j=1}^{\infty}$ is bounded in all L^p , $1 \leq p < \infty$, therefore by using the uniform integrability theorem we leverage the convergence in probability to convergence in all L^p , hence $X_{0:i|i-1}^{j,1,N_j} \rightarrow U_{0:i|i-1}^{j,1}$ and $\bar{X}_{0:i|i-1}^{j,N_j} \rightarrow E(U_{0:i|i-1}^{j,1})$ in all L^p . From [26] we have $P_{0:i|i-1}^{j,N_j} \stackrel{\text{P}}{\rightarrow} Q_{0:i}^j$, then, from the continuous mapping theorem, $K_i^{N_j} \stackrel{\text{P}}{\rightarrow} K_i$. From the fact that convergence in L^p implies convergence in probability, and using the continuous mapping theorem again, we conclude that

$$\begin{aligned} X_{0:i|i}^{j,1,N_j} &= X_{0:i|i-1}^{j,1,N_j} + K_i^{N_j} \left(\tilde{y}_i + \tilde{\mathcal{H}}'_i \left(\bar{X}_{i|k}^{j-1,N_{j-1}} \right) \bar{X}_{i|k}^{j-1,N_{j-1}} - \tilde{\mathcal{H}}_i \left(\bar{X}_{i|k}^{j-1,N_{j-1}} \right) \right) \\ &\quad - \tilde{W}_i^{j,1} - \tilde{\mathcal{H}}'_i \left(\bar{X}_{i|k}^{j-1,N_{j-1}} \right) X_{i|i-1}^{j,1,N_j} \\ &\stackrel{\text{P}}{\rightarrow} U_{0:i|i-1}^{j,1} + K_i \left(\hat{y}_i + \tilde{\mathcal{H}}'_i \left(E \left(U_{i|k}^{j-1,1} \right) \right) E \left(U_{i|k}^{j-1,1} \right) - \tilde{\mathcal{H}}_i \left(E \left(U_{i|k}^{j-1,1} \right) \right) \right) \\ &\quad - \tilde{W}_i^{j,1} - \tilde{\mathcal{H}}'_i \left(E \left(U_{i|k}^{j-1,1} \right) \right) U_{i|i-1}^{j,1} \\ &= U_{0:i|i}^{j,1}, \end{aligned}$$

as $\min\{N_1, \dots, N_j\} \rightarrow \infty$. Then we leverage the last convergence to the convergence in L^p using Lemma 10 and the uniform integrability again. \square

6.4 EnKS-4DVAR

To avoid computing with the tangent matrices $\mathcal{M}'_i(x_{i-1}^{j-1})$ and $\mathcal{H}'_i(x_i^{j-1})$, we take advantage of the fact that they occur in the EnKS only in matrix-vector products, and approximate the matrix-vector multiplications in Algorithm 8 by finite differences with a small step size $\tau > 0$, centered at the previous iterate. Thus, we use the approximations of the form

$$f'(x)y \approx \frac{f(x + \tau y) - f(y)}{\tau} \quad (44)$$

in (35), (36), and (37). Denote by an additional superscript τ the quantities computed in the resulting algorithm. This is the EnKS-4DVAR method originally proposed in [25].

Algorithm 11 (EnKS-4DVAR). *Given an initial approximation $x_{0:k}^0$, $\gamma > 0$, and $\tau > 0$. Initialize*

$$\bar{X}_{0:k|k}^{j,N_j,\tau} = x_{0:k}^0 \quad \text{for } j = 0.$$

LM loop: For $j = 1, 2, \dots$. Choose N_j the same as in Algorithm 8.

EnKS loop: For $i = 0$, the ensemble $\left[X_{0|0}^{j,n,\tau}\right]_{n=1}^{N_j}$ consists of i.i.d. Gaussian random variables

$$X_{0|0}^{j,n,\tau} \sim N(\tilde{x}_0^0, B).$$

For $i = 1, \dots, k$, advance the model in time (the forecast step) by

$$X_{i|i-1}^{j,n,\tau} = \frac{\mathcal{M}_i\left(\bar{X}_{i-1|k}^{j-1,N_{j-1},\tau} + \tau\left(X_{i-1|i-1}^{j,n,\tau} - \bar{X}_{i-1|k}^{j-1,N_{j-1},\tau}\right)\right) - \mathcal{M}_i\left(\bar{X}_{i-1|k}^{j-1,N_{j-1},\tau}\right)}{\tau}, \quad (45)$$

$$+ \mathcal{M}_i\left(\bar{X}_{i-1|k}^{j-1,N_{j-1},\tau}\right) + \mu_i + V_i^{j,n} \quad V_i^{j,n} \sim N(0, Q_i), \quad n = 1, \dots, N_j.$$

Incorporate the observations at time i into the ensemble of composite states $\left[X_{0:i|i-1}^{j,n,\tau}\right]_{n=1}^{N_j}$ by the analysis step

$$X_{0:i|i}^{j,n,\tau} = X_{0:i|i-1}^{j,n,\tau} + P_{0:i|i-1}^{j,N_j,\tau} \tilde{H}_i^{j,\tau T} \left(\tilde{H}_i^{j,\tau} P_{0:i|i-1}^{j,N_j,\tau} \tilde{H}_i^{j,\tau T} + \tilde{R}_i \right)^{-1} \quad (46)$$

$$\cdot \left(\tilde{y}_i - \tilde{W}_i^{j,n} - \tilde{\mathcal{H}}_i\left(\bar{X}_{i|k}^{j-1,N_{j-1},\tau}\right) \right.$$

$$\left. - \frac{\tilde{\mathcal{H}}_i\left(\bar{X}_{i|k}^{j-1,N_{j-1},\tau} + \tau\left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|k}^{j-1,N_{j-1},\tau}\right)\right) - \tilde{\mathcal{H}}_i\left(\bar{X}_{i|k}^{j-1,N_{j-1},\tau}\right)}{\tau} \right),$$

$$\tilde{W}_i^{j,n} \sim N\left(0, \tilde{R}_i\right)$$

where $P_{0:i|i-1}^{j,N_j,\tau}$ is the sample covariance from the ensemble $\left[X_{0:i|i-1}^{j,n,\tau}\right]_{n=1}^{N_j}$. Similarly as in (9)–(11),

only the following matrix-vector products are needed:

$$P_{0:i|i-1}^{j,N_j,\tau} \tilde{H}_i^{j,\tau\text{T}} = \frac{1}{N_j - 1} \sum_{n=1}^{N_j} \left(X_{0:i|i-1}^{j,n,\tau} - \bar{X}_{0:i|i-1}^{j,N_j,\tau} \right) \left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|i-1}^{j,N_j,\tau} \right)^{\text{T}} \tilde{H}_i^{j,\tau\text{T}}, \quad (47)$$

$$\begin{aligned} &= \frac{1}{N_j - 1} \sum_{n=1}^{N_j} \left(X_{0:i|i-1}^{j,n,\tau} - \bar{X}_{0:i|i-1}^{j,N_j,\tau} \right) h_i^{j,n,\tau\text{T}} \\ \tilde{H}_i^j P_{0:i|i-1}^{j,N_j,\tau} \tilde{H}_i^{j,\tau\text{T}} &= \frac{1}{N_j - 1} \sum_{n=1}^{N_j} \tilde{H}_i^{j,\tau} \left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|i-1}^{j,N_j,\tau} \right) \left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|i-1}^{j,N_j,\tau} \right)^{\text{T}} \tilde{H}_i^{j,\tau\text{T}} \\ &= \frac{1}{N_j - 1} \sum_{n=1}^{N_j} h_i^{j,n,\tau} h_i^{j,n,\tau\text{T}}, \end{aligned} \quad (48)$$

where

$$h_i^{j,n,\tau} = \tilde{H}_i^{j,\tau} \left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|i-1}^{j,N_j,\tau} \right) = \frac{\tilde{\mathcal{H}}_i \left(\tau \left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|i-1}^{j,N_j,\tau} \right) + \bar{X}_{i|k}^{j-1,N_{j-1},\tau} \right) - \tilde{\mathcal{H}}_i \left(\bar{X}_{i|k}^{j-1,N_{j-1},\tau} \right)}{\tau} \quad (49)$$

and

$$\bar{X}_{i|i-1}^{j,N_j,\tau} = \frac{1}{N_j} \sum_{n=1}^{N_j} X_{i|i-1}^{j,n,\tau}, \quad \bar{X}_{0:i|i}^{j,N_j,\tau} = \frac{1}{N_j} \sum_{n=1}^{N_j} X_{0:i|i}^{j,n,\tau}.$$

The next LM iterate is $\tilde{x}^{j,\tau} = \bar{X}_{0:k|k}^{j,N_j,\tau}$.

We now summarize the differences between the previous three algorithms. Algorithm 6 solves the linearized problem in each iteration exactly, while Algorithm 8 approximates the solution of the linearized problem by EnKS, and Algorithm 11 approximates also the linearized problem itself by finite differences.

We show that when the finite difference parameter $\tau \rightarrow 0$, the iterations of Algorithm 11 converge to their corresponding iterations of Algorithm 8 in probability. The following lemma is the cornerstone of the analysis of the finite differences here.

Lemma 13. *Let (X_τ) and (Y_τ) be random vectors such that $X_\tau \xrightarrow{\text{P}} X$ and $Y_\tau \xrightarrow{\text{P}} Y$ as $\tau \rightarrow 0$, $\tau > 0$, and f be twice continuously differentiable with the matrix of second order derivatives f'' bounded. Then,*

$$\frac{f(X_\tau + \tau Y_\tau) - f(X_\tau)}{\tau} \xrightarrow{\text{P}} f'(X)Y \text{ as } \tau \rightarrow 0, \tau > 0.$$

Proof. From Taylor expansion, for any x , y , and t ,

$$\left| \frac{f(x + ty) - f(x)}{t} - f'(x)y \right| \leq Mt|y|^2, \quad (50)$$

where $M = \frac{1}{2} \sup_{\xi} |f''(\xi)|$ in the matrix norm induced by the vector norm $|\cdot|$. Let $\varepsilon > 0$, $\tilde{\varepsilon} > 0$. Since $Y_\tau \xrightarrow{\text{P}} Y$, $\{Y_\tau\}$ is uniformly tight, that is, there exists K such that $\mathbb{P}[|Y_\tau| \leq K] \geq 1 - \tilde{\varepsilon}$ for all $\tau > 0$. Choose $\tau_1 = \frac{\varepsilon}{MK^2} > 0$. Using (50), it follows that for all $0 < \tau < \tau_1$,

$$\mathbb{P} \left[\left| \frac{f(X_\tau + \tau Y_\tau) - f(X_\tau)}{\tau} - f'(X_\tau)Y_\tau \right| \leq \varepsilon \right] \geq 1 - \tilde{\varepsilon}. \quad (51)$$

Since the mapping $(x, y) \mapsto f'(x)y$ is continuous and $(X_\tau, Y_\tau) \rightarrow (X, Y)$ in probability, it follows from the continuous mapping theorem that $f'(X_\tau)Y_\tau \rightarrow f'(X)Y$ in probability, hence there exists τ_2 such that for all $\tau < \tau_2$,

$$\mathbb{P} \left[\left| f'(X_\tau)Y_\tau - f'(X)Y \right| \leq \varepsilon \right] \geq 1 - \tilde{\varepsilon}. \quad (52)$$

Finally, using the triangle inequality, (51) and (52) imply

$$\mathbb{P} \left[\left| \frac{f(X_\tau + \tau Y_\tau) - f(X_\tau)}{\tau} - f'(X)Y \right| \leq 2\varepsilon \right] \geq 1 - 2\tilde{\varepsilon},$$

for all $0 < \tau < \min \{\tau_1, \tau_2\}$. \square

Theorem 12. *At each iteration j and time step i of Algorithm 11, $X_{0:i|i}^{j,n,\tau} \xrightarrow{\text{P}} X_{0:i|i}^{j,n}$ as $\tau \rightarrow 0$, where $X_{0:i|i}^{j,n}$ is the n -th member of the ensemble generated at j -th iteration in Algorithm 8 with the same random perturbations as in Algorithm 11.*

Proof. In this proof we omit the subscripts of N_j and N_{j-1} . The proof is by induction on the number of iterations j . For $j = 1$ we have $\bar{X}_{0:i|i}^{j-1,N,\tau} = \bar{X}_{0:i|i}^{j-1,N}$. For $j \geq 2$, we use induction on time step i . For $i = 0$ we have $X_{0|0}^{j,n,\tau} = x_b + V_b^n = X_{0|0}^{j,n}$. For $i = 1, \dots, k$, we have from the induction assumption on i , $X_{i-1|i-1}^{j,n,\tau} \xrightarrow{\text{P}} X_{i-1|i-1}^{j,n}$ as $\tau \rightarrow 0$. Then using Lemma 13, we have in (45) as $\tau \rightarrow 0$,

$$X_{i|i-1}^{j,n,\tau} = \frac{\mathcal{M}_i \left(\bar{X}_{i-1|k}^{j-1,N,\tau} + \tau \left(X_{i-1|i-1}^{j,n,\tau} - \bar{X}_{i-1|k}^{j-1,N,\tau} \right) \right) - \mathcal{M}_i \left(\bar{X}_{i-1|k}^{j-1,N,\tau} \right)}{\tau} \quad (53)$$

$$\begin{aligned} &+ \mathcal{M}_i \left(\bar{X}_{i-1|k}^{j-1,N,\tau} \right) + \mu_i \\ &\xrightarrow{\text{P}} \mathcal{M}'_i \left(\bar{X}_{i-1|k}^{j-1,N} \right) \left(X_{i-1|i-1}^{j,n} - \bar{X}_{i-1|k}^{j-1,N} \right) + \mathcal{M}_i \left(\bar{X}_{i-1|k}^{j-1,N} \right) + \mu_i + V_i^n = X_{i|i-1}^{j,n}. \end{aligned} \quad (54)$$

Similarly, using the induction assumption on j and Lemma 13, we have in (46) and in (49), respectively,

$$\begin{aligned} &\frac{\mathcal{H}_i \left(\bar{X}_{i|k}^{j-1,N,\tau} + \tau \left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|k}^{j-1,N,\tau} \right) \right) - \mathcal{H}_i \left(\bar{X}_{i|k}^{j-1,N,\tau} \right)}{\tau} \\ &\xrightarrow{\text{P}} \mathcal{H}'_i \left(\bar{X}_{i|i}^{j-1,N} \right) \left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|k}^{j-1,N,\tau} \right), \\ &\frac{\mathcal{H}_i \left(\bar{X}_{i|k}^{j-1,N,\tau} + \tau \left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|i-1}^{j-1,N,\tau} \right) \right) - \mathcal{H}_i \left(\bar{X}_{i|k}^{j-1,N,\tau} \right)}{\tau} \\ &\xrightarrow{\text{P}} \mathcal{H}'_i \left(\bar{X}_{i|k}^{j-1,N} \right) \left(X_{i|i-1}^{j,n,\tau} - \bar{X}_{i|i-1}^{j-1,N,\tau} \right). \end{aligned}$$

as $\tau \rightarrow 0$. In (11) gives

$$h_i^{j,n,\tau} \xrightarrow{\text{P}} h_i^{j,n} \text{ as } \tau \rightarrow 0. \quad (55)$$

Using (55) and the continuous mapping theorem in (48) and (47) gives

$$\begin{aligned} &P_{0:i|i-1}^{j,N,\tau} \tilde{H}_i^{j,\tau\text{T}} \xrightarrow{\text{P}} P_{0:i|i-1}^{j,N} \tilde{H}_i^{j\text{T}} \text{ as } \tau \rightarrow 0, \\ &\tilde{H}_i^{j,\tau} P_{0:i|i-1}^{j,N,\tau} \tilde{H}_i^{j,\tau\text{T}} \xrightarrow{\text{P}} \tilde{H}_i^j P_{0:i|i-1}^{j,N} \tilde{H}_i^{j\text{T}} \text{ as } \tau \rightarrow 0. \end{aligned}$$

Using also (53) in (46) and the continuous mapping theorem once more gives $X_{0:i|i}^{j,n,\tau} \xrightarrow{P} X_{0:i|i}^{j,n}$ as $\tau \rightarrow 0$. \square

Corollary 13. *For each j , $\lim_{\min\{N_1, \dots, N_j\} \rightarrow \infty} \lim_{\tau \rightarrow 0} \bar{X}_{0:k|k}^{j,N,\tau} = x^j$ in probability, where x^j is the j -th iterate of Algorithm 6.*

Proof. The proof follows immediately from Theorem 12, Theorem 10, and Lemma 11. \square

7 Conclusion

In this paper we have shown that: when the observation and the model operators are linear for any time step, the empirical mean and covariance of EnKS converge to the KS mean and covariance in the limit for large ensemble size in L^p for any $p \in [1, \infty)$. In the nonlinear case, i.e., in the case where the observation and the model operators are not necessary linear, we have shown the convergence of LM-EnKS iterations (Algorithm 11) in the limit for large ensemble size. The convergence is in the sense that (i) each iterate generated by Algorithm 11 converges in probability to its corresponding iterate of Algorithm 8 as the finite differences parameter goes to zero, (ii) and that each iterate generated by Algorithm 8 converges, in L^p for any $p \in [1, \infty)$, to its corresponding iterate of Algorithm 6 (the Levenberg-Marquardt algorithm) in the large-ensemble limit.

These proofs of convergence, and more generally the asymptotic behavior of the ensemble-based algorithms deserve further investigation. Here in the nonlinear case, we have given only the limit in probability of each iterate of Algorithm 11 as the finite differences parameter goes to zero and the ensemble sizes go to infinity. One may, for instance, try to prove stronger convergence results, especially to leverage the convergences in probability to convergences in L^p , and show the convergence rate of these algorithms following the spirit of [19]. The approach followed in this paper could be also extended to the case in which other variants of ensemble method, such as the square root ensemble Kalman filter [17], are used to approximately solve the linearized subproblem.

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