

A Brief Tutorial on the Ensemble Kalman Filter*

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Abstract

The ensemble Kalman filter (EnKF) is a recursive filter suitable for problems with a large number of variables, such as discretizations of partial differential equations in geophysical models. The EnKF originated as a version of the Kalman filter for large problems (essentially, the covariance matrix is replaced by the sample covariance), and it is now an important data assimilation component of ensemble forecasting. EnKF is related to the particle filter (in this context, a particle is the same thing as an ensemble member) but the EnKF makes the assumption that all probability distributions involved are Gaussian. This article briefly describes the derivation and practical implementation of the basic version of EnKF, and reviews several extensions.

1 Introduction

The Ensemble Kalman Filter (EnKF) is a Monte-Carlo implementation of the Bayesian update problem: Given a probability density function (pdf) of the state of the modeled system (the *prior*, called often the forecast in geosciences) and the data likelihood, the Bayes theorem is used to obtain pdf after the data likelihood has been taken into account (the *posterior*, often called the analysis). This is called a Bayesian update. The Bayesian update is combined with advancing the model in time, incorporating new data from time to time. The original Kalman Filter [18] assumes that all pdfs are Gaussian (the Gaussian assumption) and provides algebraic formulas for the change of the mean and covariance by the Bayesian update, as well as a formula for advancing the covariance matrix in time provided the system is linear. However, maintaining the covariance matrix is not feasible computationally for high-dimensional systems. For this reason, EnKFs were developed [9, 16]. EnKFs represent the distribution of the system state using a random sample, called an ensemble, and replace the covariance matrix by the sample covariance computed from the ensemble. One advantage of EnKFs is that advancing the pdf in time is achieved by simply advancing each member of the ensemble. For a survey of EnKF and related data assimilation techniques, see [12].

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2 A derivation of the EnKF

2.1 The Kalman Filter

Let us review first the Kalman filter. Let \mathbf{x} denote the n -dimensional state vector of a model, and assume that it has Gaussian probability distribution with mean μ and covariance Q , i.e., its pdf is

$$p(\mathbf{x}) \propto \exp\left(-\frac{1}{2}(\mathbf{x} - \mu)^T Q^{-1}(\mathbf{x} - \mu)\right).$$

Here and below, \propto means proportional; a pdf is always scaled so that its integral over the whole space is one. This probability distribution, called the *prior*, was evolved in time by running the model and now is to be updated to account for new data. It is natural to assume that the error distribution of the data is known; data have to come with an error estimate, otherwise they are meaningless. Here, the data \mathbf{d} is assumed to have Gaussian pdf with covariance R and mean $H\mathbf{x}$, where H is the so-called the observation matrix. The covariance matrix R describes the estimate of the error of the data; if the random errors in the entries of the data vector \mathbf{d} are independent, R is diagonal and its diagonal entries are the squares of the standard deviation (“error size”) of the error of the corresponding entries of the data vector \mathbf{d} . The value $H\mathbf{x}$ is what the value of the data would be for the state \mathbf{x} in the absence of data errors. Then the probability density $p(\mathbf{d}|\mathbf{x})$ of the the data \mathbf{d} conditional of the system state \mathbf{x} , called the data likelihood, is

$$p(\mathbf{d}|\mathbf{x}) \propto \exp\left(-\frac{1}{2}(\mathbf{d} - H\mathbf{x})^T R^{-1}(\mathbf{d} - H\mathbf{x})\right).$$

The pdf of the state and the data likelihood are combined to give the new probability density of the system state \mathbf{x} conditional on the value of the data \mathbf{d} (the *posterior*) by the Bayes theorem,

$$p(\mathbf{x}|\mathbf{d}) \propto p(\mathbf{d}|\mathbf{x}) p(\mathbf{x}).$$

The data \mathbf{d} is fixed once it is received, so denote the posterior state by $\hat{\mathbf{x}}$ instead of $\mathbf{x}|\mathbf{d}$ and the posterior pdf by $p(\hat{\mathbf{x}})$. It can be shown by algebraic manipulations [1] that the posterior pdf is also Gaussian,

$$p(\hat{\mathbf{x}}) \propto \exp\left(-\frac{1}{2}(\hat{\mathbf{x}} - \hat{\mu})^T \hat{Q}^{-1}(\hat{\mathbf{x}} - \hat{\mu})\right),$$

with the posterior mean $\hat{\mu}$ and covariance \hat{Q} given by the Kalman update formulas

$$\hat{\mu} = \mu + K(\mathbf{d} - H\mu), \quad \hat{Q} = (I - KH)Q,$$

where

$$K = QH^T (HQH^T + R)^{-1}$$

is the so-called Kalman gain matrix.

2.2 The Ensemble Kalman Filter

The EnKF is a Monte Carlo approximation of the Kalman filter, which avoids evolving the covariance matrix of the pdf of the state vector \mathbf{x} . Instead, the distribution is represented by a collection of realizations, called an ensemble. So, let

$$X = [\mathbf{x}_1, \dots, \mathbf{x}_N] = [\mathbf{x}_i]$$

be an $n \times N$ matrix whose columns are a sample from the prior distribution. The matrix X is called the *prior ensemble*. Replicate the data \mathbf{d} into an $m \times N$ matrix

$$D = [\mathbf{d}_1, \dots, \mathbf{d}_N] = [\mathbf{d}_i]$$

so that each column \mathbf{d}_i consists of the data vector \mathbf{d} plus a random vector from the n -dimensional normal distribution $N(0, R)$. Then the columns of

$$\hat{X} = X + K(D - HX)$$

form a random sample from the posterior distribution. The EnKF is now obtained [17] simply by replacing the state covariance Q in Kalman gain matrix $K = QH^T (HQH^T + R)^{-1}$ by the sample covariance C computed from the ensemble members (called the *ensemble covariance*).

3 Theoretical analysis

It is commonly stated that the ensemble is a sample (that is, independent identically distributed random variables, i.i.d.) and its probability distribution is represented by the mean and covariance, thus assuming that the ensemble is normally distributed. Although the resulting analyses, e.g., [7], played an important role in the development of EnKF, both statements are false. The ensemble covariance is computed from all ensemble members together, which introduces dependence, and the EnKF formula is a nonlinear function of the ensemble, which destroys the normality of the ensemble distribution. For a mathematical proof of the convergence of the EnKF in the limit for large ensembles to the Kalman filter, see [23]. The core of the analysis is a proof that large ensembles in the EnKF are, in fact, nearly i.i.d. and nearly normal.

4 Implementation

4.1 Basic formulation

Here we follow [7, 10, 19]. Suppose the ensemble matrix X and the data matrix D are as above. The ensemble mean and the covariance are

$$E(X) = \frac{1}{N} \sum_{k=1}^N \mathbf{x}_k, \quad C = \frac{AA^T}{N-1},$$

where

$$A = X - E(X) = X - \frac{1}{N} (X \mathbf{e}_{N \times 1}) \mathbf{e}_{1 \times N},$$

and e denotes the matrix of all ones of the indicated size.

The posterior ensemble X^p is then given by

$$\hat{X} \approx X^p = X + CH^T (HCH^T + R)^{-1} (D - HX),$$

where the perturbed data matrix D is as above. It can be shown that *the posterior ensemble consists of linear combinations of members of the prior ensemble*.

Note that since R is a covariance matrix, it is always positive semidefinite and usually positive definite, so the inverse above exists and the formula can be implemented by the Choleski decomposition [19]. In [7, 10], R is replaced by the sample covariance $DD^T/(N-1)$ and the inverse is replaced by a pseudoinverse, computed using the Singular Values Decomposition (SVD).

Since these formulas are matrix operations with dominant Level 3 operations [14], they are suitable for efficient implementation using software packages such as LAPACK (on serial and shared memory computers) and ScaLAPACK (on distributed memory computers) [19]. Instead of computing the inverse of a matrix and multiplying by it, it is much better (several times cheaper and also more accurate) to compute the Choleski decomposition of the matrix and treat the multiplication by the inverse as solution of a linear system with many simultaneous right-hand sides [14].

4.2 Observation matrix-free implementation

It is usually inconvenient to construct and operate with the matrix H explicitly; instead, a function $h(x)$ of the form

$$h(\mathbf{x}) = H\mathbf{x}, \quad (1)$$

is more natural to compute. The function h is called the *observation function* or, in the inverse problems context, the *forward operator*. The value of $h(\mathbf{x})$ is what the value of the data would be for the state \mathbf{x} assuming the measurement is exact. Then [19, 22] the posterior ensemble can be rewritten as

$$X^p = X + \frac{1}{N-1} A (HA)^T P^{-1} (D - HX)$$

where

$$HA = HX - \frac{1}{N} ((HX) \mathbf{e}_{N \times 1}) \mathbf{e}_{1 \times N},$$

and

$$P = \frac{1}{N-1} HA (HA)^T + R,$$

with

$$\begin{aligned} [HA]_i &= H\mathbf{x}_i - H \frac{1}{N} \sum_{j=1}^N \mathbf{x}_j \\ &= h(\mathbf{x}_i) - \frac{1}{N} \sum_{j=1}^N h(\mathbf{x}_j). \end{aligned}$$

Consequently, the ensemble update can be computed by evaluating the observation function h on each ensemble member once and the matrix H does not need to be known explicitly. This formula also holds [19] for an observation function $h(\mathbf{x}) = H\mathbf{x} + \mathbf{f}$ with a fixed offset \mathbf{f} , which also does not need to be known explicitly. The above formula has been commonly used for a nonlinear observation function h , such as the position of a hurricane vortex [8]. In that case, the observation function is essentially approximated by a linear function from its values at the ensemble members.

4.3 Implementation for a large number of data points

For a large number m of data points, the multiplication by P^{-1} becomes a bottleneck. The following alternative formula [19, 22] is advantageous when the number of data points m is large (such as when assimilating gridded or pixel data) and the data error covariance matrix R is diagonal (which is the case when the data errors are uncorrelated), or cheap to decompose (such as banded due to limited covariance distance). Using the Sherman-Morrison-Woodbury formula [15]

$$(R + UV^T)^{-1} = R^{-1} - R^{-1}U(I + V^T R^{-1}U)^{-1}V^T R^{-1},$$

with

$$U = \frac{1}{N-1}HA, \quad V = HA,$$

gives

$$\begin{aligned} P^{-1} &= \left(R + \frac{1}{N-1}HA(HA)^T \right)^{-1} \\ &= R^{-1} \left[I - \frac{1}{N-1}(HA) \left(I + (HA)^T R^{-1} \frac{1}{N-1}(HA) \right)^{-1} (HA)^T R^{-1} \right], \end{aligned}$$

which requires only the solution of systems with the matrix R (assumed to be cheap) and of a system of size N with m right-hand sides. See [19] for operation counts.

5 Further extensions

The EnKF version described here involves randomization of data. For filters without randomization of data, see [2, 11, 25].

Since the ensemble covariance is rank-deficient (there are many more state variables, typically millions, than the ensemble members, typically less than a hundred), it has large terms for pairs of points that are spatially distant. Since in reality the values of physical fields at distant locations are not that much correlated, the covariance matrix is tapered off artificially based on the distance, which results in better approximation of the covariance for small ensembles [13], such as typically used in practice. Further development of this idea gives rise to localized EnKF algorithms [3, 24].

For problems with coherent features, such as firelines, squall lines, and rain fronts, there is a need to adjust the simulation state by distorting the state in space as well as by an additive correction to the state. The morphing EnKF [5, 20] employs intermediate states, obtained by techniques borrowed from image registration and morphing, instead of linear combinations of states.

EnKFs rely on the Gaussian assumption, though they are of course used in practice for nonlinear problems, where the Gaussian assumption is not satisfied. Related filters attempting to relax the Gaussian assumption in EnKF while preserving its advantages include filters that fit the state pdf with multiple Gaussian kernels [4], filters that approximate the state pdf by Gaussian mixtures [6], a variant of the particle filter with computation of particle weights by density estimation [20, 21], and a variant of the particle filter with thick tailed pdfs to alleviate particle filter degeneracy [26].

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