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Nonlinear Measurement Function in the Ensemble Kalman Filter

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ABSTRACT

The optimal Kalman gain was analyzed in a rigorous statistical framework. Emphasis was placed on a comprehensive understanding and interpretation of the current algorithm, especially when the measurement function is nonlinear. It is argued that when the measurement function is nonlinear, the current ensemble Kalman Filter algorithm seems to contain implicit assumptions: the forecast of the measurement function is unbiased or the nonlinear measurement function is linearized. While the forecast of the model state is assumed to be unbiased, the two assumptions are actually equivalent.

On the above basis, we present two modified Kalman gain algorithms. Compared to the current Kalman gain algorithm, the modified ones remove the above assumptions, thereby leading to smaller estimated errors. This outcome was confirmed experimentally, in which we used the simple Lorenz 3-component model as the test-bed. It was found that in such a simple nonlinear dynamical system, the modified Kalman gain can perform better than the current one. However, the application of the modified schemes to realistic models involving nonlinear measurement functions needs to be further investigated.

Key words: ensemble Kalman filter, measurement function, data assimilation.

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1. Introduction

Atmospheric and oceanic flows can be described by a system of stochastic partial differential equations (sPDE). Within this framework, not only can the dynamical system be stochastically forced, but the observations can also be considered stochastic processes rather than single numerical values. The most commonly used sPDE model is the state-space model, in which the dynamical model describes the evolution of the state variable over time, whereas the measurement model explains how the measurement relates to the state variable:

$$\begin{aligned} x_t &= M(x_{t-1}, \eta_{t-1}) \quad \text{(dynamic model)} \\ y_t &= h(x_t, \varepsilon_t) \quad \text{(measurement model)} \end{aligned} , \qquad (1)$$

where x_t denotes the state variable at time, t; t is the time index; η_t is the dynamical process noise; ε_t is the measurement noise; and y_t is the measurement. The functions M and h describe the evolution of the state variable over time and the relationship between the measurement and state, respectively.

In general, data assimilation is used to estimate the model states by combining the observational and model forecast data (e.g., Talagrand and Bouttier, 2007). Thus, a data assimilation system consists of three components: a dynamical model, a measurement (observation) model, and an assimilation scheme. Neither the dynamical model nor the measurement model is perfect. Errors in both model and observation play a critical role in the assimilation process. Therefore, they should be estimated and modeled accurately.

In general, assimilation methods can be classified into two categories: variational and sequential. Variational methods, such as the three-dimensional variational (3DVAR) method and four-dimensional variational (4DVAR) method (e.g., Le Dimet and Talagrand, 1986; Courtier et al., 1998), are batch methods; whereas sequential methods, such as the Kalman filter (KF) (proposed by Kalman, 1960), are part of estimation theory. Methods in both categories have had great success in atmosphere–ocean data assimilation. In November 1997, the European Centre for Medium-Range Weather Forecasts (ECMWF) introduced ~~the first~~ 4DVAR method to the operational global analysis system (e.g., Klinker et al., 2000). The ensemble Kalman filter (EnKF) was first introduced to the operational ensemble prediction system by the Canadian Meteorological Centre (CMC) in January 2005 (Houtekamer et al., 2005).

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An ideal case of data assimilation is when all the equations are linear and the noise is additive. Thus, Eq. (1) may become:

$$\begin{aligned} x_t &= \mathbf{M}x_{t-1} + \eta_{t-1} \\ y_t &= \mathbf{H}x_t + \varepsilon_t \end{aligned} , \tag{2}$$

where $\mathbf{M}$ and $\mathbf{H}$ are linear operators of the model and measurement, respectively. The optimal solution among sequential methods to Eq. (2) is provided by the KF under the assumption that the noise is Gaussian. The operators $\mathbf{M}$ and $\mathbf{H}$ must be linear in the KF as indicated in the update equation for forecast error covariance and in the Kalman gain. Thus, approximating techniques must be employed for nonlinear dynamics. A common approach is to linearize the nonlinear model, which is the key attribute of the Extended KF (EKF) (e.g., Jazwinski, 1970). Furthermore, the difficulty of the linearization of complex nonlinear models (e.g., general circulation models) forces one to use other possible alternatives to update the forecast error covariance, which was the motivation for other KF-based derivatives, such as the EnKF. The EnKF was initially introduced by Evensen (1994); it estimates the forecast error covariance using multiple integrations of the same models from subtly different initial conditions (ensemble), thereby avoiding the complicated—even intractable in some cases—linearization of nonlinear dynamical models. Because it is easy to implement and its algorithm is simple, the EnKF has attracted much attention and has been widely used in atmospheric and oceanic sciences in recent years (e.g., Evensen, 2003; Deng et al., 2012). In particular, the issues related to the implementation and potential concerns of the standard EnKF have become less significant with the advent of advanced and more efficient algorithms, such as the ensemble square-root filters (EnSRF), local ensemble transform Kalman filters (LETKF), maximum likelihood ensemble filter (MLEF), and localization and inflation schemes (e.g., Ito and Xiong, 2000; Anderson, 2001; Tippett et al., 2003; Hunt et al., 2007).

Despite the fact that EnKF-based filters have gained great success in many applications, there still exist some concerns. For example, the current Kalman gain algorithm of the EnKF actually originated from a natural extension of the KF or EKF, which is for linear cases. There has been no comprehensive discussion in the literature as to whether such a natural extension holds for the nonlinear estimate of Eq (1). Another example is the treatment of nonlinear measurement functions. In a classic EnKF with nonlinear measurement functions, the Kalman gain was written in a different way by decomposing the forecast error covariance matrix (see section 2.2 for details), thus allowing a direct evaluation of the nonlinear measurement function, as proposed by Houtekamer and Mitchell (2001; referred to as HM2001 hereafter). However, this algorithm was presented based on scientific intuition and there is a lack of rigorous mathematical proof (see section 2.2 for details). Thus, the current EnKF algorithm deserves further analysis in a statistically rigorous sense, to better understand and apply the EnKF. In fact, we can find in the following sections that a general Kalman gain algorithm can be derived for the nonlinear estimate, Eq. (1), which provides a better understanding of the EnKF, including some potential concerns about the EnKF, e.g., why the current EnKF algorithms often underestimate the prediction error covariance and need an inflation scheme (Furrer and Bengtsson, 2007; Anderson, 2007). In particular, we can find that the nonlinear measurement treatment in the classic EnKF contains an implicit assumption; that is, the forecast of the measurement function $h(\hat{x}_{t,\mathrm{b}})$ is unbiased or the mean of the forecast $(\overline{h(\hat{x}_{t,\mathrm{b}})})$ equals the forecast of the mean $(h(\overline{\hat{x}}_{t,\mathrm{b}}))$ where $\hat{x}_{t,\mathrm{b}}$ is model forecast, and the over-bar is the mean over the ensembles. This implicit assumption may impact the accuracy of the estimation.

This paper first examines the current EnKF algorithm based on a rigorous definition of model error and observation error, and a general form of the Kalman filter for Eq. (1). In particular, we explore the treatment of nonlinear measurement functions used in the EnKF in a rigorous statistical sense with detailed derivations. On this basis, two modified schemes of Kalman gain are proposed. Section 2 provides a brief review of the KF family methods, including the EKF and EnKF. A generalized KF algorithm for the nonlinear state-space model, Eq. (1), is also presented in section 2. In section 3, we analyze the Kalman gain algorithm used in the current EnKF and then develop two modified algorithms with a detailed statistical derivation. In section 4, the results from tests that were conducted on these Kalman gain algorithms using a low-dimensional 3-component Lorenz model are reported. Finally, ~~a~~ discussions and conclusions are presented in section 5.

2. The standard KF, EKF, and EnKF and their generalized algorithm

2.1. *KF and EKF*

An ideal case in data assimilation is when the forecast and measurement models are both linear and the errors are Gaussian, as described by Eq. (2). The solution among sequential methods to this case is provided by the KF. Below, the primary equations of the KF are displayed, and attention is drawn to the characteristic properties of the algorithm, applying to the time step, t. The detailed derivation of these equations can be found in the literature (e.g., Simon, 2006).

$$\hat{x}_{t,\mathrm{a}} = \hat{x}_{t,\mathrm{b}} + K[y_t - \hat{y}_t] , \tag{3}$$

$$K = P_{t,\mathrm{b}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}P_{t,\mathrm{b}}\mathbf{H}^{\mathrm{T}} + R)^{-1} , \tag{4}$$

$$P_{t,\mathrm{a}} = (I - K\mathbf{H})P_{t,\mathrm{b}} , \tag{5}$$

$$P_{t,\mathrm{b}} = \mathbf{M}P_{t-1,a}\mathbf{M}^{\mathrm{T}} + Q , \tag{6}$$

$$\hat{x}_{t,\mathrm{b}} = \mathbf{M}\hat{x}_{t-1,\mathrm{a}} , \tag{7}$$

$$\hat{y}_t = \mathbf{H}\hat{x}_{t,\mathrm{b}} , \tag{8}$$

where $\hat{x}_{t,\mathrm{a}}$ and $\hat{x}_{t,\mathrm{b}}$ are model analysis and forecast, respectively, at time step t. $\boldsymbol{I}$ is unity matrix. The model errors η_t and observed errors ε_t have zero mean and variance values $\mathrm{var}(\eta_t) =< \eta_t, \eta_t^{\mathrm{T}} >= Q$, $\mathrm{var}(\varepsilon_t) =< \varepsilon_t, \varepsilon_t^{\mathrm{T}} >= R$. The variables $P_{t,\mathrm{a}}$ and $P_{t,\mathrm{b}}$ represent the analysis and forecast error covariance, respectively.

In Eq. (3), y_t is the true value of measurement by Eq. (1) or Eq. (2). Often, it is approximated by observation $y_{t,\mathrm{o}}$. If the random nature of the true measurement is considered, y_t should be the observation $y_{t,\mathrm{o}}$ perturbed by noise, resulting in an analysis ensemble. Thus, the $\hat{x}_{t,\mathrm{a}}$ in Eq. (3) should be understood as the mean of the analysis when $y_{t,\mathrm{o}}$ is used directly instead of y_t, if we assume the observation $y_{t,\mathrm{o}}$ is unbiased. This strategy should be followed in the KF-family of filters discussed in this paper. This also explains why the perturbed observation (i.e., $y_{t,\mathrm{o}}+\varepsilon_t$, where ε_t is noise) is often used in applying Eq. (3) in the EnKF.

The above equations consider the evolution of the forecast (background) error covariance with time and are controlled by the dynamical model operator $\mathbf{M}$. Equations (3)–(8) constitute the framework of the Kalman filter for Eq. (2). If the forecast error covariance P_t^b is prescribed as a constant in time, the estimate is called the optimal interpolation (OI).

In deriving Eqs. (4)–(6), both the dynamical model $\mathbf{M}$ and the measurement model $\mathbf{H}$ should be assumed to be linear and the errors to be Gaussian. Therefore, the standard KF only works for linear models and Gaussian distribution. If the dynamical model and/or the measurement model are not linear, the KF cannot be directly applied. Instead, linearization must be performed prior to applying the KF. The analytically linearized version of the KF is called the extended KF (EKF), which solves the state-space estimate problem of Eq. (1). The disparities and similarities between the EKF and the KF include the following: (1) both the Kalman gain K and the update equation of forecast error covariance have the same form, with the use of the linear and linearized state model; (2) the forecast model and the measurement model are different, with linear Eq. (2) for the KF and nonlinear Eq. (1) for the EKF; (3) Eqs. (7) and (8) are different, with linear model $\mathbf{M}$ and linear measurement function $\mathbf{H}$ used for the KF, and nonlinear model M and nonlinear measurement function H used for the EKF.

2.2. *EnKF*

A challenge in the EKF is to update the prediction error covariance using Eq. (6), which requires linearization of the nonlinear model M. The linearization of a nonlinear model is often technically difficult and even intractable in some cases, e.g., in non-continuous functions. Another drawback of the EKF is the neglect of the contributions from higher-order statistical moments in calculating the error covariance.

In the EnKF, the prediction error covariance $P_{t,\mathrm{b}}$ used in Eq. (4) is estimated using an ensemble of model forecasts. The equation below was used for the EnKF to replace Eq. (6), while the other equations are kept the same, i.e.,

$$P_{t,\mathrm{b}} = \frac{1}{L-1}\sum_{i=1}^{L}(\hat{x}_{t,i,\mathrm{b}}-\overline{\hat{x}_{t,\mathrm{b}}})(\hat{x}_{t,i,\mathrm{b}}-\overline{\hat{x}_{t,\mathrm{b}}})^{\mathrm{T}}\ , \qquad (9)$$

where $\hat{x}_{t,i,\mathrm{b}}$ represents the forecast of the i-th member at step t and L is the ensemble size. The use of Eq. (9) avoids the task of processing Eq. (6), which requires the linearized operator $\mathbf{M}$ for the nonlinear model, M. In the Kalman gain [Eq. (4)], the measurement function $\mathbf{H}$ is still linear or linearized, which might cause concerns when the nonlinear measurement function is difficult to linearize. To avoid the linearization of a nonlinear measurement function, HM2001 re-wrote the Kalman gain [Eq. (4)] as follows:

$$K = P_{\mathrm{b}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}P_{\mathrm{b}}\mathbf{H}^{\mathrm{T}}+R)^{-1}\ , \qquad (10)$$

$$P_{\mathrm{b}}h^{\mathrm{T}} \equiv \frac{1}{L-1}\sum_{i=1}^{L}(\hat{x}_{i,\mathrm{b}}-\overline{\hat{x}_{\mathrm{b}}})(h(\hat{x}_{i,\mathrm{b}})-\overline{h(\hat{x}_{\mathrm{b}})})^{\mathrm{T}}\ , \qquad (11)$$

$$\mathbf{H}P_{\mathrm{b}}\mathbf{H}^{\mathrm{T}} \equiv \frac{1}{L-1}\sum_{i=1}^{L}(h(\hat{x}_{i,\mathrm{b}})-\overline{h(\hat{x}_{\mathrm{b}})})(h(\hat{x}_{i,\mathrm{b}})-\overline{h(\hat{x}_{\mathrm{b}})})^{\mathrm{T}}\ ; \qquad (12)$$

where $\overline{h(\hat{x}_{i,\mathrm{b}})}=\sum_{i=1}^{L}h(\hat{x}_{t,\mathrm{b}})/(\mathrm{L}-1)$ and i is the ensemble index.

The time step, t, is omitted in Eqs. (11) and (12) for simplicity. Equations (11) and (12) allow for a direct evaluation of the nonlinear measurement function H in calculating the Kalman gain. However, Eqs. (11) and (12) have not been proven mathematically. Tang and Ambadan (2009) argued that Eqs. (11) and (12) approximately hold only if the following is true:

$$\overline{h(\hat{x}_{i,\mathrm{b}})} = h(\overline{\hat{x}_{\mathrm{b}}})\ ; \qquad (13)$$

$$\hat{x}_{i,\mathrm{b}}-\overline{\hat{x}_{\mathrm{b}}}=\varepsilon_i,\ \mathrm{Norm}(\varepsilon_i)\ \text{is small for}\ i=1,2\ldots \qquad (14)$$

Under the conditions of Eqs. (13) and (14), Tang and Ambadan (2009) argued that Eqs. (11) and (12) actually linearize the nonlinear measurement functions h to $\mathbf{H}$. Therefore, the direct application of the nonlinear measurement function in Eqs. (11) and (12) imposes an implicit linearization process using ensemble members. In the next sections, we will find that Eqs. (11) and (12) actually held without requiring the conditions of Eqs. (13) and (14), if the measurement forecast $\hat{y}_t$ was unbiased. A further interpretation is the equivalence of Eqs. (13) and (14) with the unbiased forecast $\hat{y}_t$.

2.3. *General form of ensemble-based filters for Gaussian models*

As discussed in the preceding subsections, the linear or linearized measurement functions are still required in the optimal Kalman gain K in the KF, EKF and EnKF. In this subsection, we proceed with a general form of the Kalman gain, which does not contain the linear measurement operator. This general form was first introduced by Julier et al. (1995) when they developed the unscented Kalman filter and has been widely applied in the literature (e.g., Simon, 2006).

Following the general state-space model, Eq. (1), the state update equation can be written as:

$$\begin{aligned}\hat{x}_{t,\mathrm{a}} &= \hat{x}_{t,\mathrm{b}}+K_t(y_t-\hat{y}_t)\\ \hat{x}_{t,\mathrm{b}} &= M(\hat{x}_{t-1,\mathrm{a}})\\ \hat{y}_t &= h(\hat{x}_{t,\mathrm{b}})\end{aligned}$$

The analysis error is denoted by $\tilde{x}_{t,\mathrm{a}}=x_t-\hat{x}_{t,\mathrm{a}}$, the forecast error by $\tilde{x}_{t,\mathrm{b}}=x_t-\hat{x}_{t,\mathrm{b}}$, and the observation error by $\tilde{y}_t=y_t-\hat{y}_t$, where x_t and y_t are the true values at the time step t in the model state and measurement. For convenience, we omit the subscript t in the derivation below.

Considering an unbiased estimate, we have:

$$\begin{aligned}\tilde{x}_\mathrm{a} &= \tilde{x}_\mathrm{b} - K\tilde{y} ,\\ P_\mathrm{a} &= E[\tilde{x}_\mathrm{a}\tilde{x}_\mathrm{a}^\mathrm{T}] = E(\tilde{x}_\mathrm{b} - K\tilde{y})(\tilde{x}_\mathrm{b} - K\tilde{y})^\mathrm{T}\\ &= E(\tilde{x}_\mathrm{b}\tilde{x}_\mathrm{b}^\mathrm{T} - \tilde{x}_\mathrm{b}\tilde{y}^\mathrm{T}K^\mathrm{T} - K\tilde{y}\tilde{x}_\mathrm{b}^\mathrm{T} + K\tilde{y}\tilde{y}^\mathrm{T}K^\mathrm{T}) ,\\ P_\mathrm{a} &= P_{\tilde{x}_\mathrm{b}\tilde{x}_\mathrm{b}} - P_{\tilde{x}_\mathrm{b}\tilde{y}}K^\mathrm{T} - KP_{\tilde{y}\tilde{x}_\mathrm{b}} + KP_{\tilde{y}\tilde{y}}K^\mathrm{T} ,\end{aligned}$$

Where E[·] is the expectation. Under the Gaussian distribution assumption, the optimal estimate as the trace of the minimum P_a is:

$$\begin{aligned}\frac{\partial[\mathrm{tr}(P_\mathrm{a})]}{\partial K} &= 0 ,\\ -P_{\tilde{x}_\mathrm{b}\tilde{y}} - P_{\tilde{y}\tilde{x}_\mathrm{b}} + 2KP_{\tilde{y}\tilde{y}} &= 0 ,\\ K &= P_{\tilde{x}_\mathrm{b}\tilde{y}}P_{\tilde{y}\tilde{y}}^{-1} ,\\ P_\mathrm{a} &= P_{\tilde{x}_\mathrm{b}\tilde{x}_\mathrm{b}} - KP_{\tilde{x}_\mathrm{b}\tilde{y}} ,\end{aligned}$$

A summary of the main equations discussed above is listed below:

$$\hat{x}_{t,\mathrm{a}} = \hat{x}_{t,\mathrm{b}} + K[y_t - \hat{y}_t] , \tag{15}$$

$$K_t = P_{\tilde{x}_\mathrm{b}\tilde{y}}P_{\tilde{y}\tilde{y}}^{-1} , \tag{16}$$

$$P_\mathrm{a} = P_{\tilde{x}_\mathrm{b}\tilde{x}_\mathrm{b}} - KP_{\tilde{x}_\mathrm{b}\tilde{y}} , \tag{17}$$

$$\hat{x}_{t,\mathrm{b}} = M(\hat{x}_{t-1,\mathrm{a}}) , \tag{18}$$

$$\hat{y}_t = h(\hat{x}_{t,\mathrm{b}}) . \tag{19}$$

Equations (15)–(19) show a general algorithm for the Gaussian nonlinear model and the nonlinear measurement function. The derivation of the Kalman gain K does not invoke any linear assumptions for the dynamical model or measurement function. If the observation is approximated as the true value, the $P_{\tilde{x}_\mathrm{b}\tilde{y}}$ in Eq (16) is the cross-covariance between the state and observation errors, and the $P_{\tilde{y}\tilde{y}}$ is the error covariance of the difference between the observation and its prediction $\hat{y}_t$. Additionally, in the case of nonlinear models, the statistical moments can be exactly calculated in a closed form only if the underlying distribution is Gaussian.

3. Application of the general Kalman filter form for the standard KF and EnKF

It is clear that the linear assumption is made for the measurement function to obtain Eq. (4), as indicated by the linear operator h. To deal with the nonlinear measurement function in the EnKF, HM2001 proposed Eqs. (11) and (12) to directly evaluate the nonlinear measurement functions. Apparently, there is a gap here, i.e., the left hand sides of Eqs. (11) and (12) need the linear measurement function h, whereas their right hand sides directly use the nonlinear function h. HM2001 realized that there was this gap and used the equivalence sign "≡" instead of the equality sign "=" in Eqs. (11) and (12). However, the equivalence is primarily based on intuition. It is necessary to examine the equivalence in a rigorous, statistical framework.

First, we re-examine the optimal Kalman gain, Eq. (4), using the general form of the Kalman gain, Eq. (16). When the dynamical model is linear, i.e., $x_t = \mathbf{M}x_{t-1} + \eta_{t-1}, \hat{x}_{t,\mathrm{b}} = \mathbf{M}\hat{x}_{t-1,\mathrm{a}}^\mathrm{T}, P_{t,\mathrm{b}} = \mathbf{M}P_{t-1,\mathrm{a}}\mathbf{M}^\mathrm{T} + Q$, where $Q = E(\eta_{t-1}\eta_{t-1}^\mathrm{T})$. When the measurement function is linear, i.e., $\hat{y}_t = \mathbf{H}\hat{x}_{t,\mathrm{b}}$,

$$\begin{aligned}\tilde{y}_t &= y_t - \hat{y}_t = \mathbf{H}x_t + \varepsilon_t - \mathbf{H}\hat{x}_{t,\mathrm{b}} = \mathbf{H}\tilde{x}_{t,\mathrm{b}} + \varepsilon_t ,\\ P_{\tilde{x}_\mathrm{b}\tilde{y}} &= P_{\tilde{x}_\mathrm{b}\tilde{x}_\mathrm{b}}\mathbf{H}^\mathrm{T} ,\\ P_{\tilde{y}\tilde{y}} &= \mathbf{H}P_{\tilde{x}_\mathrm{b}\tilde{x}_\mathrm{b}}\mathbf{H}^\mathrm{T} + R ,\end{aligned}$$

where $R = E(\varepsilon_t\varepsilon_t^\mathrm{T})$. Then, the optimal Kalman gain is

$$K = P_{\tilde{x}_\mathrm{b}\tilde{y}}P_{\tilde{y}\tilde{y}}^{-1} = P_{\tilde{x}_\mathrm{b}\tilde{x}_\mathrm{b}}\mathbf{H}^\mathrm{T}(\mathbf{H}P_{\tilde{x}_\mathrm{b}\tilde{x}_\mathrm{b}}\mathbf{H}^\mathrm{T} + R)^{-1} . \tag{20}$$

Equation (20) is identical to Eq. (4). Therefore, Eq. (4) used in the KF, EKF, and EnKF is a special case of Eq. (16), under the assumption of a linear measurement function.

We now examine Eqs. (11) and (12) of HM2001 that have been widely used to treat the nonlinear measurement function in the EnKF. Emphasis is placed on the comparison of Eqs. (4), (11), and (12) against Eq. (16).

When the noise is additive, the nonlinear state-space equation [Eq. (1)] becomes

$$\begin{aligned}x_t &= M(x_{t-1}) + \eta_{t-1} ,\\ y_t &= h(x_t) + \varepsilon_t ,\end{aligned}$$

The assumption of additive noise is commonly used for the assimilation in Gaussian-based systems. For a non-additive noise system (e.g., multiplicative noise), Gaussian-based assimilation methods, such as the EnKF, are often invalid.

We started from Eq. (16), i.e., $K = P_{\tilde{x}_\mathrm{b}\tilde{y}}P_{\tilde{y}\tilde{y}}-1$. If the estimate is unbiased and the ensemble size L is infinite, we can use the ensemble mean to represent the true value, i.e.,

$$\left.\begin{aligned}x_t &= E(\hat{x}_{i,t,\mathrm{b}}) + \eta_t = \bar{\hat{x}}_{t,\mathrm{b}} + \eta_t\\ y_t &= h(\bar{\hat{x}}_{t,\mathrm{b}}) + \varepsilon_t\end{aligned}\right. , \tag{21}$$

where E[·] denotes the expectation, i is the ensemble index and the overbar represents the mean over all the ensemble members. The terms η_t and ς_t were added due to the random nature of the true states:

$$\begin{aligned}P_{\tilde{x}_\mathrm{b}\tilde{y}} &= E[(\hat{x}_{i,t,\mathrm{b}} - x_t)(\hat{y}_{i,t} - y_t)^\mathrm{T}]\\ &= E[\hat{x}_{i,t,\mathrm{b}} - E(\hat{x}_{i,t,\mathrm{b}}) - \eta_t][h(\hat{x}_{i,t,\mathrm{b}}) - h(E(\hat{x}_{i,t,\mathrm{b}})) - \varepsilon_t]^\mathrm{T} .\end{aligned}$$

For a realistic ensemble system with finite ensemble size, $P_{\tilde{x}_\mathrm{b}\tilde{y}}$ can be written as:

$$P_{\tilde{x}_\mathrm{b}\tilde{y}} = \frac{1}{L-1}\sum_{i=1}^{L}(\hat{x}_{i,t,\mathrm{b}} - \bar{\hat{x}}_{t,\mathrm{b}})[h(\hat{x}_{i,t,\mathrm{b}}) - h(\bar{\hat{x}}_{t,\mathrm{b}})]^\mathrm{T} . \tag{22}$$

Similarly,

$$\begin{aligned}P_{\tilde{x}_\mathrm{b}\tilde{x}_\mathrm{b}} &= E[(\hat{x}_{i,t,\mathrm{b}} - x_t)(\hat{x}_{i,t,\mathrm{b}} - x_t)]^\mathrm{T}\\ &= E[\hat{x}_{i,t,\mathrm{b}} - E(\hat{x}_{i,t,\mathrm{b}}) - \eta_t][\hat{x}_{i,t,\mathrm{b}} - E(\hat{x}_{i,t,\mathrm{b}}) - \eta_t]^\mathrm{T}\\ &= \frac{1}{L-1}\sum_{i=1}^{L}(\hat{x}_{i,t,\mathrm{b}} - \bar{\hat{x}}_{t,\mathrm{b}})(\hat{x}_{i,t,\mathrm{b}} - \bar{\hat{x}}_{t,\mathrm{b}})^\mathrm{T} + Q , \qquad (23)\\ P_{\tilde{y}\tilde{y}} &= E[(\hat{y}_{i,t} - y_t)(\hat{y}_{i,t} - y_t)^\mathrm{T}]\end{aligned}$$

$$
\begin{aligned}
&= E[h(\hat{x}^b_{i,t}) - h(\overline{\hat{x}}^b_t) - \varepsilon_t][h(\hat{x}^b_{i,t}) - h(\overline{\hat{x}}^b_t) - \varepsilon_t]^{\mathrm{T}} \\
&= E[(h(\hat{x}^b_{i,t}) - h(\overline{\hat{x}}^b_t))(h(\hat{x}^b_{i,t}) - h(\overline{\hat{x}}^b_t))^{\mathrm{T}} + R\,, \\
P_{\tilde{y}\tilde{y}} &= \frac{1}{L-1}\sum_{i=1}^{L}[h(\hat{x}_{i,t,\mathrm{b}}) - h(\overline{\hat{x}}_{t,\mathrm{b}})][h(\hat{x}_{i,t,\mathrm{b}}) - h(\overline{\hat{x}}_{t,\mathrm{b}})]^{\mathrm{T}} + R\,.
\end{aligned} \tag{24}
$$

Here, the assumption is that the noise terms ε_t and η_t have zero mean and are uncorrelated with other variables. The variances of η_t and ε_t are Q and R, respectively. Equation (23) represents the forecast error covariance estimated by the ensemble member. Compared to the standard EnKF [Eq. (9)], there appears to be one more item Q on the left hand side of Eq. (23). The absence of Q in the standard EnKF algorithm is because the forecast error is being defined with respect to the ensemble mean rather than to the true state. Thus, the random nature of the true states is ignored. The standard EnKF often systematically underestimates the error covariance and requires an inflation scheme to "adjust" the estimated error covariance.

The Kalman gain is written as

$$
\begin{aligned}
K &= P_{\tilde{x}_b\tilde{y}}P^{-1}_{\tilde{y}\tilde{y}} \\
&= \frac{1}{L-1}\sum_{i=1}^{L}(\hat{x}_{i,t,\mathrm{b}} - \overline{\hat{x}}_{t,\mathrm{b}})[(h(\hat{x}_{i,t,\mathrm{b}}) - h(\overline{\hat{x}}_{t,\mathrm{b}})]^{\mathrm{T}} \\
&\quad * \left\{\frac{1}{L-1}\sum_{m=1}^{L}[h(\hat{x}_{i,t,\mathrm{b}}) - h(\overline{\hat{x}}_{t,\mathrm{b}})][h(\hat{x}_{i,t,\mathrm{b}}) - h(\overline{\hat{x}}_{t,\mathrm{b}})]^{\mathrm{T}} + R\right\}^{-1}.
\end{aligned} \tag{25}
$$

A comparison of Eqs. (11) and (12) with Eqs. (22) and (24) reveals that they are completely equivalent, if Eq. (13) holds true. From the linearization point of view, Eq. (13) holds true only if Eq. (14) also holds true. Conversely, when Eqs. (22) and (24) are used instead of Eqs. (11) and (12) in the EnKF, the modified Kalman gain form should be more rigorous in the statistical framework, which is equivalent to the general Kalman gain form, Eq. (16), without demanding any assumption of linearization. Clearly, when the noise is non-additive, the equivalence is no longer valid. However, in case of non-additive noise, all Kalman-based filters are invalid due to the non-Gaussian nature of the systems. Recently, Ambadan and Tang (2011) discussed the assimilation of a nonlinear system in a multiplicative noise environment and found that the intrinsic properties of the multiplicative noise challenge the current EnKF algorithms.

In the above derivations, we used the forecast measurement to represent the true measurement, i.e., $y_t = h(\overline{\hat{x}}_{t,\mathrm{b}}) + \varepsilon_t$, as indicated in Eqs. (24) and (25). One important assumption here is the unbiased nature of the forecast $(\hat{x}_{t,\mathrm{b}})$, i.e., the ensemble mean instead of the unknown true state. This unbiased assumption results in the prediction error of measurement, which may be serious in some cases. One solution used to reduce the impact of the unbiased assumption on the estimate of the Kalman gain is to directly use the actual observation $y_{t,\mathrm{o}}$ to represent the true measurement; namely

$$
y_t = y_{t,\mathrm{o}} + \varepsilon_t. \tag{26}
$$

Thus, the Kalman gain can be written as

$$
\begin{aligned}
K &= P_{\tilde{x}_b\tilde{y}}P^{-1}_{\tilde{y}\tilde{y}} \\
&= \frac{1}{L-1}\sum_{i=1}^{L}(\hat{x}_{i,t,\mathrm{b}} - \overline{\hat{x}}_{t,\mathrm{b}})[(h(\hat{x}_{i,t,\mathrm{b}}) - y_{t,\mathrm{o}} - \varepsilon_t]^{\mathrm{T}} \\
&\quad * \left\{\frac{1}{L-1}\sum_{m=1}^{L}[h(\hat{x}_{i,t,\mathrm{b}}) - y_{t,\mathrm{o}} - \varepsilon_t][h(\hat{x}_{i,t,\mathrm{b}}) - y_{t,\mathrm{o}} - \varepsilon_t]^{\mathrm{T}}\right\}^{-1}.
\end{aligned} \tag{27}
$$

One important disparity between Eqs. (27) and (25) is the disappearance of R in Eq. (27). However, it is implicitly represented by the perturbed observation. In other words, the observation should be randomly perturbed when applying the general form of the Kalman gain.

In the above discussion, we only assume that the model forecast is unbiased, i.e., $x_t = E(\hat{x}_{i,t,\mathrm{b}}) + \eta_t$. If we further assume that the forecast of the measurement model is unbiased and random, i.e.,

$$
y_t = E(\hat{y}_{i,t}) + \varepsilon_t = E(h(\hat{x}_{i,t,\mathrm{b}})) + \varepsilon_t\,, \tag{28}
$$

we have

$$
\begin{aligned}
P_{\tilde{x}_b\tilde{y}} &= E[(\hat{x}_{t,\mathrm{b}} - x_t)(\hat{y}_t - y_t)^{\mathrm{T}}] \\
&= E[\hat{x}_{i,t,\mathrm{b}} - E(\hat{x}_{i,t,\mathrm{b}}) - \eta_t][h(\hat{x}_{i,t,\mathrm{b}}) - E(h(\hat{x}_{i,t,\mathrm{b}})) - \varepsilon_t]^{\mathrm{T}} \\
&= \frac{1}{L-1}\sum_{i=1}^{L}[\hat{x}_{i,t,\mathrm{b}} - \overline{\hat{x}}_{i,t,\mathrm{b}}][h(\hat{x}_{t,\mathrm{b}}) - \overline{h(\hat{x}_{i.t,\mathrm{b}})}]^{\mathrm{T}}\,,
\end{aligned} \tag{29}
$$

$$
\begin{aligned}
P_{\tilde{y}\tilde{y}} &= E[(\hat{y}_t - y_t)(\hat{y}_t - y_t)^{\mathrm{T}}] \\
&= E[h(\hat{x}_{i,t,\mathrm{b}}) - E(h(\hat{x}_{i,t,\mathrm{b}})) - \varepsilon_t][h(\hat{x}_{i,t,\mathrm{b}}) - E(h(\hat{x}_{i,t,\mathrm{b}})) - \varepsilon_t]^{\mathrm{T}} \\
&= \frac{1}{L-1}\sum_{i=1}^{L}[(h(\hat{x}_{i,t,\mathrm{b}}) - \overline{h(\hat{x}_{i,t,\mathrm{b}})})(h(\hat{x}_{i,t,\mathrm{b}}) - \overline{h(\hat{x}_{i,t,\mathrm{b}})})^{\mathrm{T}} + R\,.
\end{aligned} \tag{30}
$$

So we can see that Eqs. (29) and (30) are identical to Eqs. (11) and (12). Thus, another interpretation of Eqs. (11) and (12) is the application of the unbiased assumption to the measurement forecast, under which the linearization assumption, Eq. (13), can be removed. The assumption of Eq. (13) can clearly be seen as equivalent to the assumption of the unbiased nature of the measurement forecast. Thus, Eqs. (11) and (12) have a rigorous statistical foundation when the unbiased assumption is applied to both the model forecast and the measurement forecast.

In summary, there are three schemes used to estimate the Kalman gain in the EnKF while the measurement function is nonlinear. The similarity, disparity, and theoretical accuracy of the estimates are summarized in Table 1. Clearly, when the observation is appropriately perturbed, Scheme 3 should have the smallest estimated errors, followed by Scheme 2 and Scheme 1.

4. Application of modified Kalman gain to the simple Lorenz model

In this section, we use the 3-component Lorenz model to examine several of the aforementioned algorithms. This

Table 1. Three Schemes for the optimal Kalman gain in the EnKF.

Scheme name	Equations	Assumptions	Sources of estimated errors
Scheme 1 (HM2001)	(10), (11) and (12)	(1) An unbiased assumption for the model prediction; (2) The noise is additive; (3) An implicit assumption for linearization of measurement function, or an unbiased assumption for measurement prediction; (4) Forecasted observation instead of raw observation	Assumptions (i)–(iv)
Scheme 2	(25)	(1) An unbiased assumption for model prediction; (2) The noise is additive; (3) Forecasted observation instead of raw observation;	Assumptions (i)–(iii)
Scheme 3	(27)	(1) An unbiased assumption for model prediction; (2) The noise is additive; (3) Perturbed raw observation is directly used.	Assumptions (i)–(ii)

model consists of three ordinary differential equations:

$$\begin{aligned} \frac{dx_1}{dt} &= \sigma(x_2 - x_1) + \eta_1 \\ \frac{dx_2}{dt} &= \rho x_1 - x_2 - x_1 x_3 + \eta_2 \ , \\ \frac{dx_3}{dt} &= x_1 x_2 - \beta x_3 + \eta_3 \end{aligned} \tag{31}$$

where $(x_i, \eta_i)(i = 1, 2, 3)$ are the model state variable and random noise, respectively, and $\Lambda = (\sigma, \rho, \beta)$ are model parameters.

In our test experiment, we focused on the parameter estimate, where the parameters are treated as special states for estimation, which can be written as

$$\begin{aligned} \Lambda_t &= \Lambda_{t-1} + \eta_{t-1} \\ y_t &= h((x_i)_t, \Lambda_t) + \varepsilon_t \end{aligned} \ , \tag{32}$$

where the measurement function is the nonlinear model h. The true data were produced by integrating Eq. (31) with parameters (α, ρ, β) of (10.0, 28.0 and 8/3), and initial conditions of 1.5088, -1.531, and 25.46; the integration interval was 0.01. These sets are the same as in Miller et al. (1994).

For this experiment, the state observations were generated by adding Gaussian noise $\mathrm{N}(0, \sqrt{2})$ to the model integrations (i.e., perturbed observations used in assimilation), as in Miller et al. (1994) and Evensen (1997). To make a fair comparison between the filters, the unknown parameter, ρ, was initially set to zero. Additionally, the observation interval was 25; thus, the observations were assimilated every 25 time steps. In the experiment, the errors of the model and the observation were assumed to be uncorrelated in space and time.

We assumed that the parameter ρ is uncertain, so it needed to be estimated. Figure 1 presents the estimations using the three schemes, with an ensemble size of 100 for each. Figure 1a shows the parameter estimation using the standard EnKF scheme (Scheme 1), and Figs. 1b and c show the modified approaches described in Table 1 (Schemes 2 and 3). The parameter estimates in all three schemes approach the true value after some time steps, but Scheme 3 has a relatively slow convergence compared to Schemes 1 and 2, probably because the observation noise ς used in Eq. (27) is too large[a], leading to a long training time. The modified EnKF schemes have better estimations than the standard EnKF, with the best values from Scheme 3, consistent with the theoretical analysis shown in Table 1.

An interesting feature in Figure 1 is that the performances of both Schemes 1 and 2 start to degrade after around 600 time steps, especially for Scheme 1, as indicated by an increasing divergence of the estimated parameter away from the true value. This is most probably due to the variation of nonlinearity of the dynamical system (phase transition) during the assimilation period. Figure 2 shows the model integration (true states) over 1000 time steps. As can be seen, the nonlinearity of the system increases with the time steps and the model states seem to become chaotic after around 600 time steps. Unlike Schemes 1 and 2, Scheme 3 seems little affected by the variation of nonlinearity. This is probably because by perturbing the observation, we used observed information to calculate the covariance matrix instead of evaluating $\overline{h(\hat{x}_\mathrm{b})}$ (Scheme 1) or $h(\overline{\hat{x}_\mathrm{b}})$ (Scheme 2), alleviating the impact of nonlinearity on the estimation. Thus, Scheme 3 has a relatively steady performance and relatively little impact from the variation in nonlinearity.

Figure 3 shows $\overline{h(\hat{x}_{i,\mathrm{b}})} - h(\overline{\hat{x}_\mathrm{b}})$ for x, y and z, which is the source of difference between Schemes 2 and 1 shown in Figs. 1a and b. The difference is rather small in this case and thus Scheme 2 is only slightly better than Scheme 1 in Fig. 1. In cases when $\overline{h(\hat{x}_{i,\mathrm{b}})} - h(\overline{\hat{x}_\mathrm{b}})$ is large, the two schemes may have significant differences.

5. Summary and discussion

For atmospheric and oceanic data assimilation systems, the measurement function may be nonlinear. In this paper, we explored several schemes for calculating the optimal Kalman gain when the measurement function is nonlinear, including a widely used scheme in the standard EnKF. Emphasis was placed on a comprehensive interpretation of the current algorithm and an extension of it in a rigorous statistical framework.

[a]The noise variance is arbitrarily set to 2.

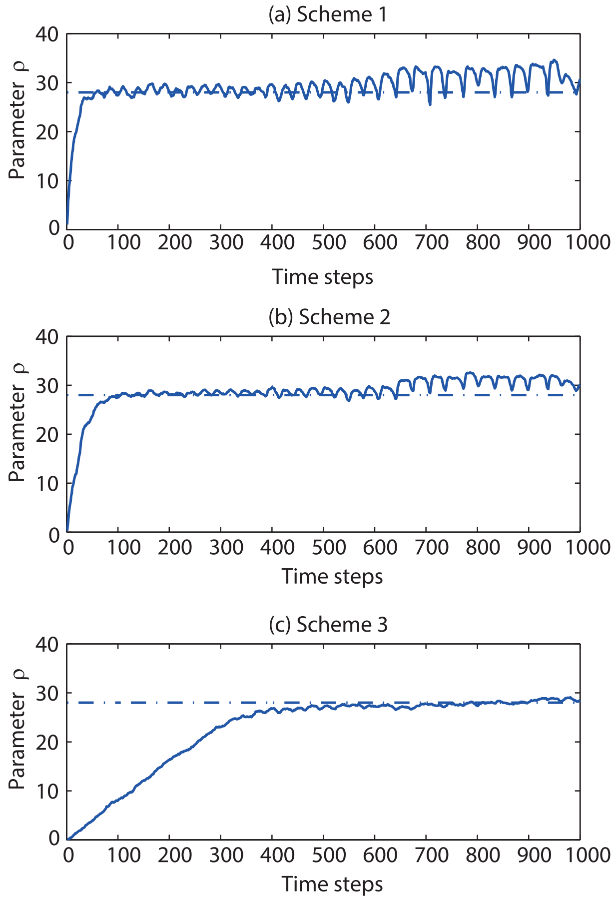

Fig. 1. Parameter ρ estimate by the three Kalman gain schemes. The dashed line is the true parameter, and the solid line is the estimated parameter.

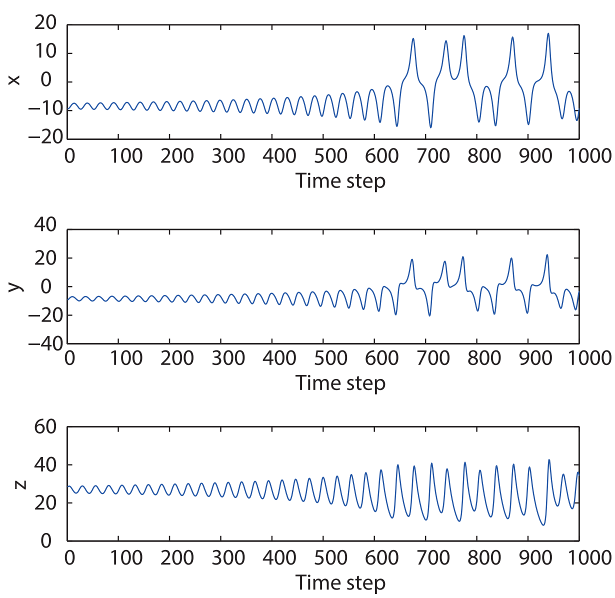

Fig. 2. The evolution of model states during the first 1000 time steps.

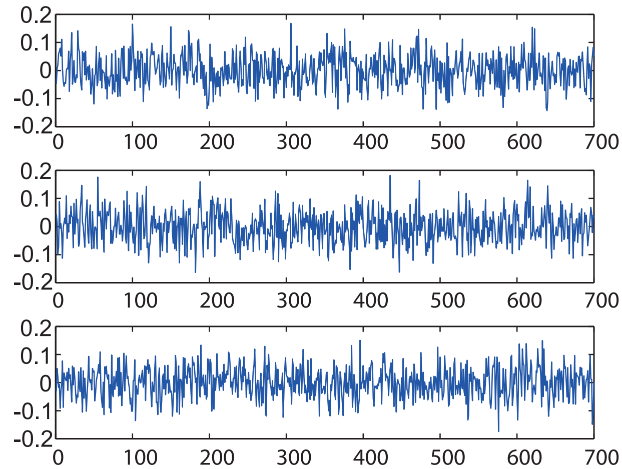

Fig. 3. $\overline{h(\hat{x}_i^b)} - h(\overline{\hat{x}^b})$ for x (upper panel), y (middle panel), and z (bottom panel) of the Lorenz model. h is the nonlinear Lorenz model itself.

When the measurement function h is nonlinear, the current EnKF algorithm contains an implicit assumption; the forecast of the measurement function $h(\hat{x}_b)$ is unbiased or the mean of the forecast $(\overline{h(\hat{x}_b)})$ equals the forecast of the mean $(h(\overline{\hat{x}_b}))$. While the forecast of model state $\hat{x}_b$ is assumed to be unbiased, the two assumptions are actually equivalent. Another interpretation for the latter is the implicit assumption of the linearization process, under which $\overline{h(\hat{x}_b)}$ approximates $h(\overline{\hat{x}_b})$ as $\hat{x}_b$ gets close to $\overline{\hat{x}_b}$. Based on the general form of the Kalman gain and some statistical derivations, we presented two modified Kalman gain algorithms. Compared to the current Kalman gain algorithm, the modified ones remove the above assumptions; thus, they can lead to smaller estimated errors. This outcome was confirmed by an actual example, where we used the simple Lorenz 3-component model as the test. The parameter estimate of this simple Lorenz model is designed with a highly nonlinear measurement function. The three Kalman gain algorithms were applied to estimate the model parameters. The results showed that the modified algorithms lead to a better estimate than the current algorithm in such a simple dynamical system.

A prerequisite for the Kalman filters is the Gaussian distribution of model and observation errors, under which the KF provides an optimal estimate for the state-space equation [Eq. (2)]. The Gaussian assumption reflects the fact that the KF is designed based on minimizing the analysis error variance (i.e., trace of error covariance), which ignores the higher-order moments. For a non-Gaussian system, the solution by the KF is not optimal. The EKF, EnKF, and SPKF use the same optimality criterion in their algorithms. For a nonlinear state-space system, the Gaussian assumption is often violated, even when the initial noise is Gaussian, because a nonlinear transformation of the Gaussian process is often non-Gaussian. In his seminal paper, Kalman (1960) confined the filter to linear systems and linear measurement functions. Thus, the EKF and EnKF are only an approximation to the optimal estimate of the nonlinear state-space equation [Eq.

(1)]. Such an approximation can provide at least a practical solution for many realistic problems, as indicated by the broad application of the EnKF in atmospheric and oceanic assimilation. However, one should take care in interpreting the EnKF estimates when they are applied to nonlinear state models or nonlinear measurement functions.

Care should also be taken when understanding and interpreting the outcomes. The statistical derivation is rigorous but some assumptions were made in this manuscript, like the unbiased assumption of the ensemble mean estimate, although they are also held in the classic EnKF. Furthermore, the outcomes from the statistical derivation were verified only by the parameter estimate of a simple 3-component dynamical system, where the measurement function is rather artificial in this context. A further test and validation is required using more complex systems. Nevertheless, the theoretical analyses and experiment results presented in this paper suggest that the development of the Kalman gain algorithm described here is on the right track, providing possible better assimilation schemes for realistic models when the measurement functions are nonlinear.

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