# Chapter 9: Ensemble based data assimilation

Typically there are two kinds of modeling techniques using either observed data (statistical modeling) or numerical models (numerical modeling). In this chapter, we will talk the modeling and simulation using both approaches, that is, the observations will be incorporated into numerical models for optimal modeling and simulation. In statistics, this is called state-space estimation. In the earth science, it is called data assimilation. For example, a strict definition of data assimilation in atmospheric and oceanic sciences is the process to estimate the state of a dynamic system such as atmospheric and oceanic flow by combining the observational and model forecast data (Talagrand 1997).

Intuitionally, one might think that an optimal simulation scheme is to directly replace model variables by observations during numerical integrations. Such a direct replacement is usually not correct since observations are not perfect and contain errors. A simple replacement will introduce observation errors into models, and ignore possible impact of observation errors on model behaviors, easily resulting in imbalance of model dynamics and physics. Thus, the application of observations into numerical models must consider both model and observation errors, which play a critical role in the assimilation process.

We will start to display the assimilation concept by a simple example. A detail introduction can be found in Kalnay (2003).

For an unknown true state value, denoted by $T_t$, there are two samples, denoted by $T_1$ (e.g. model simulation) and $T_2$ (observation), which have the errors $\epsilon_1$ and $\epsilon_2$, respectively. Thus, we have

$$\begin{aligned} T_1 &= T_t + \epsilon_1, \\ T_2 &= T_t + \epsilon_2. \end{aligned}$$

If the measurement or observation is unbiased, and the variances of errors are known, i.e.,

$$E(\epsilon_1) = E(\epsilon_2) = 0, \quad Var(\epsilon_1) = \sigma_1^2, \quad Var(\epsilon_2) = \sigma_2^2. \qquad (1)$$

The question here is to seek an optimal estimate, denoted by $T_a$ (called analysis in the assimilation field), for $T_t$ using $T_1$ and $T_2$. This optimal estimate is the central issue of data assimilation.

There are several methods for this solution, as demonstrated below.

# 1. The general framework of several assimilation approaches

## 1.1 Least square method

Denote $T_a = a_1 T_1 + a_2 T_2$. $T_a$ should be unbiased. i.e., $E(T_a) = E(T_t)$, so $a_1 E(T_1) + a_2 E(T_2) = E(T_t)$, and then $a_1 + a_2 = 1$, where (1) is invoked.

The best (optimal) estimate should satisfy the below condition:

$$\sigma_a^2 = E(T_a - T_t)^2 \to min.$$

Then,

$$\begin{aligned} \sigma_a^2 &= E[a_1 T_1 + a_2 T_2 - T_t]^2 = E[a_1(T_1 - T_t) + a_2(T_2 - T_t)]^2 \\ &= E(a_1^2 \epsilon_1^2 + a_2^2 \epsilon_2^2 + 2a_1 a_2 \epsilon_1 \epsilon_2) = a_1^2 \sigma_1^2 + (1 - a_1)^2 \sigma_2^2, \end{aligned}$$

here, we assumed that the errors of $T_1$ and $T_2$ are uncorrelated, i.e., $E(\epsilon_1 \epsilon_2) = 0$. Thus,

$$\frac{\partial \sigma_a^2}{\partial a_1} = 0 \to a_1 = \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2}.$$

Namely,

$$T_a = a_1 T_1 + (1 - a_1) T_2 = T_1 + \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2}(T_2 - T_1).$$

## 1.2 Variational approach

In general, assimilation methods can be classified into two categories: variational and sequential. Variational methods such as three-dimensional variational (3D-VAR) method and four-dimensional variational (4D-Var) method (Dimet and Talagrand 1986, Courtier et al. 1998) are batch methods, whereas sequential methods such as Kalman filter proposed by Kalman (1961) belong to the estimation theory. They both have had great success. The European Centre for Medium-Range Weather Forecasts (ECMWF) introduced the first 4D-VAR method into the operational global analysis system in November 1997 (Rabier et al. 2000, Mahfouf and Rabier 2000, Klinker et al. 2000). The ensemble Kalman filter (EnKF) was first introduced into the operational ensemble prediction system by Canadian Meteorological Centre (CMC) in January 2005 (Houtekamer et al. 2005).

Below we will demonstrate the idea of variational assimilation by the above example. First, a cost function should be defined for variational assimilation approach. For this simple example, we define the cost function as below:

$$J(T) = \frac{1}{2}\left[\frac{(T-T_1)^2}{\sigma_1^2} + \frac{(T-T_2)^2}{\sigma_2^2}\right], \quad (2)$$

$$T = a_1 T_1 + a_2 T_2. \quad (3)$$

The solution is to seek an analysis $T_a$, determined by $a_1$ and $a_2$, leading to the cost function minimum, i.e., $J(T_a) \rightarrow$ minimum. Obviously, we have

$$\frac{\partial J(T)}{\partial a_1} = 0; \quad \frac{\partial J(T)}{\partial a_2} = 0.$$

Substitute with (2), it is

$$\frac{\partial J(T)}{\partial a_1} = \frac{T-T_1}{\sigma_1^2}\frac{\partial T}{\partial a_1} + \frac{T-T_2}{\sigma_2^2}\frac{\partial T}{\partial a_1}; \quad (4)$$

Eq. (3) leads to $\frac{\partial T}{\partial a_1} = T_1$. Thus, the solution of (4), denoted by $T_a$, satisfies

$$T_a = \frac{\sigma_2^2}{\sigma_1^2+\sigma_2^2}T_1 + \frac{\sigma_1^2}{\sigma_1^2+\sigma_2^2}T_2. \quad (5)$$

The above is a simple example of the 3D variational assimilation approach, where we only consider the analysis error (cost function) for a time point. However, in many cases, we need to consider the error growth during a period, i.e., the sum of errors during the period, in the cost function (2). For example, the cost function of 4D-Var is defined as below:

$$J(T) = \frac{1}{2}\sum_{t=1}^{N}[\frac{(T(t) - T_1(t))^2}{\sigma_1^2} + \frac{(T(t) - T_2(t))^2}{\sigma_2^2}]. \qquad (6)$$

Meanwhile $T(t)$ follows a dynamical model, saying $T(t) = \int_{t_0}^{N} F\,(T(t))dt = M(T(t_0))$ ,where $F$ is a nonlinear dynamical model, $M$ is the integral operator, and $t_0$ is the initial time. Thus, the cost function value of (6) is only determined by the initial condition. Namely, the objective here is to seek optimal initial condition $T_0$ that enables (6) minimum, i.e., minimizing (6) subject to dynamical model $F$. This is a standard conditional extreme problem which can be solved by Lagrange Multiplier approach. However the complexity of dynamical model excludes the possibility to get the analytical solution. We have to solve the minimum problem by aid of numerical methods, e.g., Newton conjugate gradient method. All of numerical methods require the gradient value $\frac{\partial J}{\partial T_0}$ for solution.

Again, it is almost impossible for obtaining analytical solution of $\frac{\partial J}{\partial T_0}$ due to the complexity of $F$. Usually researchers get the gradient value numerically using an approach of tangent-linear and adjoint model. The details on tangent-linear and adjoint model can be found in relevant references as cited above. It should be noticed that it is very difficult, even intractable sometimes, to construct tangent-linear and adjoint model in some cases. Thus, more and more researchers have started to apply sequential assimilation methods instead of 4D-Var in recent years. Next we will introduce the concept of the sequential assimilation method using the above example.

## 1.3 Bayesian approach

Assume $T_1$ and $\sigma_1$ are the mean value and standard deviation of the model prediction, which implies a prior probability distribution of truth $T$,

$$p(T) = \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{(T_1-T)^2}{2\sigma_1^2}}.$$

Given the observation $T_2$ and its standard deviation $\sigma_2$, the posterior distribution of the truth can be expressed by Bayes' theorem:

$$p(T|T_2) = \frac{p(T_2|T)p(T)}{p(T_2)} \propto \frac{1}{\sqrt{2\pi}\sigma_2} e^{-\frac{(T_2-T)^2}{2\sigma_2^2}} \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{(T_1-T)^2}{2\sigma_1^2}}. \qquad (7)$$

$p(T_2)$ was ignored in (7) since it is independent of $T$, and usually plays as a normalization factor. The likelihood function $p(T_2|T)p(T)$ describes the probability that the observation becomes $T_2$ given an estimation of $T$. It is commonly assumed to be Gaussian $N(T, \sigma_2)$. The object here is to estimate the truth by maximizing the posteriori probability $p(T|T_2)$ (namely, we ask the truth to occur as much as possible - maximum probability). Maximizing $p(T|T_2)$ is equivalent to maximizing the logarithm of the right item of (7), i.e.,

$$\log(p(T|T_2)) = \log\left(\frac{1}{\sqrt{2\pi}\sigma_2}\right) - \frac{(T_2-T)^2}{2\sigma_2^2} + \log\left(\frac{1}{\sqrt{2\pi}\sigma_1}\right) - \frac{(T_1-T)^2}{2\sigma_1^2}\Big)$$
$$= \text{const} - \frac{1}{2}\left[\frac{(T-T_2)^2}{\sigma_2^2} + \frac{(T-T_1)^2}{\sigma_1^2}\right] \rightarrow \text{maximum.} \qquad (8)$$

Obviously, maximum of $p(T|T_2)$ occurs at the minimum of the second item of right side hand of (8), i.e., minimum of the cost function $J$ of (2). Thus, under the assumption of Gaussian distribution, maximizing a posterior probability (Bayesian approach) is equivalence to minimizing cost function (variational assimilation approach). Further, if the model $F$ is linear and the probability distribution is Gaussian, it can be proved that the Kalman filter is equivalent to 4D-Var adjoint assimilation method.

# 2. Optimal Interpolation (OI) and Kalman filter (KF)

## 2.1 Optimal Interpolation

The most special case in data assimilation is that the forecast model is linear and the errors are Gaussian. The solution among sequential methods to this case is provided by Kalman filter. Typically the Kalman filter applies to the below state-space model:

$$x_{t+1} = Mx_t + \eta_t, \qquad (9)$$
$$y_t = Hx_t + \zeta_t, \qquad (10)$$

where $M$ and $H$ are linear operator of model and measurement, respectively. The $x$ is model state and $y$ is the observation, and the subscript implies the time step. The $\eta_t$ and $\zeta_t$ are the model errors and observational errors, respectively, which have variance: $var(\eta_t) =< \eta_t, \eta_t^T >= Q, var(\eta_t) =< \zeta_t, \zeta_t^T >= R$. The objective here is to estimate model state $x$ using $y$, making it close to true state (unknown) as much as possible.

Assuming the estimate of model state $x^a$ at a time step is a linear combination of model forecast $x^b$ and observation $y^o$ , i.e., the filter itself is linear, so

$$x^a = x^b + K[y^o - Hx^b]. \qquad (11)$$

Eq. (11) is the standard expression of Kalman filter. $K$ is called Kalman gain which determines the optimal estimate. $y^o - Hx^b$ is also call as the innovation. Before deriving the $K$, we denote the covariance matrix of the analysis error $\epsilon^a$ by $P^a$ , i.e., $P^a =< \epsilon^a, (\epsilon^a)^T >$ where $\epsilon^a = x^a - x^{tr}$ and $x^{tr}$ is the true value of model state. Similarly, observed errors and forecast errors are defined by $\epsilon^o = y^o - Hx^{tr}$ and $\epsilon^b = x^b - x^{tr}$ , respectively. It should be noticed that the forecast error $\epsilon_b$ is different from the model error $\zeta_t$ that is a systematic bias. Also, denote

$$B = < \epsilon^b, (\epsilon^b)^T > ------ \text{background(forecast)errorcovariance},$$
$$R = < \epsilon^o, (\epsilon^o)^T > ------ \text{Observationerrorcovariance}.$$

Assuming the observation error is not related to forecast error, so

$$< \epsilon^b, (\epsilon^o)^T >=< \epsilon^o, (\epsilon^b)^T >= 0.$$

Clearly, we ask the $K$ that can lead to $P^a$ minimum. Subtracting $x^{tr}$ on both sides of eq. (11) leads to the below equation:

$$x^a - x^{tr} = x^b - x^{tr} + K[y^o - Hx^b + Hx^{tr} - Hx^{tr}]. \qquad (12)$$

Namely,

$$\epsilon^a = \epsilon^b + K(\epsilon^o - H\epsilon^b), \qquad (13)$$

and

$$\begin{aligned} P^a = & \quad E[\epsilon^b + K(\epsilon^o - H\epsilon^b)][\epsilon^b + K(\epsilon^o - H\epsilon^b)]^T \\ = & \quad E[\epsilon^b + K(\epsilon^o - H\epsilon^b)][(\epsilon^b)^T + (\epsilon^o - H\epsilon^b)^T K^T] \\ = & \quad E[\epsilon^b(\epsilon^b)^T + \epsilon^b(\epsilon^o - H\epsilon^b)^T K^T + K(\epsilon^o - H\epsilon^b)(\epsilon^b)^T \\ & \quad + K(\epsilon^o - H\epsilon^b)(\epsilon^o - H\epsilon^b)^T K^T] \\ = & \quad B - BH^T K^T - KHB + K(R + HBH^T)K^T \\ = & \quad B - BH^T K^T - K(BH^T)^T + K(R + HBH^T)K^T. \end{aligned} \qquad (14)$$

Here we used $B = B^T$. The optimal estimate asks the trace of $P^a$ minimum, namely,

$$\frac{\partial[trace(P^a)]}{\partial K} = 0,$$

so

$$-2BH^T + 2K(R + HBH^T) = 0,$$

$$K = BH^T(HBH^T + R)^{-1}. \qquad (15)$$

Substitute into (14),

$$\begin{aligned} P^a = & \quad B - BH^T K^T - K(BH^T)^T + K(R + HBH^T)K^T \\ = & \quad B - BH^T K^T - KHB + BH^T(HBH^T + R)^{-1}(R + HBH^T)K^T \\ = & \quad B - KHB = (I - KH)B, \end{aligned}$$

where we invoked the below properties:

$$\frac{\partial Ax}{\partial x^T} = \frac{\partial x^T A}{\partial x} = A,$$
$$\frac{\partial x^T Ax}{\partial x} = x^T(A + A^T),$$
$$\frac{\partial A^T x}{\partial x} = \frac{\partial x^T A^T}{\partial x^T} = A^T,$$
$$\frac{\partial(trace[xAx^T])}{\partial x} = 2xA,$$
$$\frac{\partial(trace[xA])}{\partial x} = \frac{\partial(trace[Ax^T])}{\partial x} = A.$$

Thus we have the optimal estimate filter:

$$x^a = x^b + K[y^o - Hx^b], \quad (16)$$
$$K = BH^T(HBH^T + R)^{-1}, \quad (17)$$
$$P^a = (I - KH)B. \quad (18)$$

In the estimate (16) - (18), if the background error covariance $B$ is prescribed, the estimate is called optimal interpolation. The OI does not involve state equation (9) and $B$ is unchanged during the entire assimilation process.

## 2.2 Kalman filter

Now, we consider $B$ in (17) change with the assimilation cycle. This is more realistic since the model prediction errors should be expected to decrease with the assimilation.

From eq. (9), we have

$$x_{t+1}^{tr} = Mx_t^{tr} + \eta_t, \quad (19)$$
$$x_{t+1}^{b} = E(Mx_t^a + \eta_t) = Mx_t^a. \quad (20)$$

Eq (19) indicates that even the true value is input at a time step, model can't get a true value for next step due to model bias $\eta_t$. Eq (20) shows a standard procedure for the model prediction of next step starting from the analysis of previous step.

Subtracting (19) from (20) produces:

$$\epsilon_{t+1}^b = M\epsilon_t^a - \eta_t, \quad (21)$$

$$\begin{aligned} B_{t+1} &= E(\epsilon_{t+1}^b(\epsilon_{t+1}^b)^T) \\ &= E[(M\epsilon_t^a + \eta_t)(M\epsilon_t^a + \eta_t)^T] = MB_tM^T + Q. \end{aligned} \quad (22)$$

The above equation considers the evolution of the background (prediction) error covariance with the time, controlled by the dynamical model operator $M$. The eqs. (16)- (20) plus the above equation constitutes the framework of Kalman filter for eq. (9), namely

$$\begin{aligned} x_t^a &= x_t^b + K[y^o - Hx_t^b], && (23)\\ K &= B_tH^T(HB_tH^T + R)^{-1}, && (24)\\ P_t^a &= (I - KH)B_t, && (25)\\ x_{t+1}^b &= Mx_t^a, && (26)\\ B_{t+1} &= MP_t^aM^T + Q. && (27) \end{aligned}$$

One Kalman filter cycle is consist of two parts, namely, one analysis step (Eqs. (23) - (25)) and one prediction step (Eqs. (26) - (27)). The analysis state $x_t^a$ and covariance $B_t^a$ are treated as initial conditions for the prediction step, until the next observation is available. Sometimes, $B_t$ is also denoted by $P_t^f$ in Kalman filter literatures. The detailed procedure of Kalman filter is like below:

1. $Q$ and $R$ are specified. For convenience, $Q$ and $R$ are usually assumed to be diagonal matrix. An initial value of $B$ is given, e.g., $B_0 = Q$;
2. $K$ is calculated using (24);
3. The analysis $x^a$ is obtained using (23);
4. prediction (background) error covariance $B$ is updated to $P^a$ using (25);
5. The model (9) is integrated forward using (26), and the prediction error covariance for next step is computed using (27);
6. Repeat step 2 to step 5 till the end of the assimilation period. So, KF is a recursive algorithm.

## 2.3 Extended Kalman filter (EKF)

In deriving Eqs. (13) and (22), we assume the state model $M$ and measurement model $H$ are both linear. Further, we also assume the error has Gaussian distribution. Therefore, classic KF only works for linear models and Gaussian distribution. If the dynamical model and measurement model are not linear, we cannot directly apply for KF. Instead, linearization must be performed prior to applying for KF. The linearized version of KF is called extended KF (EKF), which solves the below state-space estimate problem:

$$\begin{aligned} x_{t+1} &= f(x_t, \eta_t), \\ y_t &= h(x_t, \zeta_t), \end{aligned} \qquad (28)$$

where $f$ and $h$ are nonlinear models. Assume the error is additive noise, i.e.,

$$\begin{aligned} x_{t+1} &= f(x_t) + \eta_t, \\ y_t &= h(x_t) + \zeta_t. \end{aligned} \qquad (29)$$

The filter is still assumed to be "linear", i.e.,

$$x^a = x^b + K[y^o - h(x^b)].$$

Actually, it is not a linear combination of the forecast $x^b$ and observation $y^o$ if $h$ is not linear. However, we just extend the formulation of Eq (11), and apply it intuitively in nonlinear cases. Ignoring high order terms, the following holds approximately

$$h(x + \delta x) = h(x) + \frac{\partial h}{\partial x}\delta x = h(x) + H\delta x, \qquad (30)$$

where $H$ is the linearization of $h$, and $H_{i,j} = \frac{\partial h_i}{\partial x_j}$. So

$$y^o - h(x^b) = y^o - h(x^{tr} + x^b - x^{tr}) = y^o - h(x^{tr}) - H(x^b - x^{tr}) = \epsilon^o - H\epsilon^b, \qquad (31)$$

$$x^a = x^b + K(\epsilon^o - H\epsilon^b). \qquad (32)$$

Eq (32) is identical to Eq (11). Similarly, subtracting $x^{tr}$ on both sides of eq (32) leads to the below equation:

$$\epsilon^a = \epsilon^b + K(\epsilon^o - H\epsilon^b), \qquad (33)$$

which is the same as eq. (13). Following the same derivation as that for eq (13), we can obtain the equations similar to (16) to (18). Therefore, if the measurement model $h$ is nonlinear, the KF can be still applied with a linearization of $h$.

Similar to (19) and (20), the state model is as below:

$$x_{t+1}^{tr} = f(x_t^{tr}) + \eta_t, \quad (34)$$
$$x_{t+1}^{b} = E(f(x_t^a) + \eta_t) = f(x_t^a). \quad (35)$$

Subtracting (34) from (35) produces:

$$\begin{aligned} \epsilon_{t+1}^b &= f(x_t^a) - f(x_t^{tr}) - \eta_t = f(x_t^a) - f(x_t^{tr} - x_t^a + x_t^a) - \eta_t \\ &= f(x_t^a) - f(x_t^a - \epsilon_t^a) - \eta_t = M\epsilon_t^a - \eta_t \end{aligned} \quad (36)$$

where $M_{i,j} = \frac{\partial f_i}{\partial x_j}$.

Comparing (21) with (36) reveals that (22) still works here. Thus, the EKF can be summarized as below:

$$x_t^a = x_t^b + K[y^o - h(x_t^b)], \quad (37)$$
$$K = B_t H^T (H B_t H^T + R)^{-1}, \quad (38)$$
$$P_t^a = (I - KH)B_t, \quad (39)$$
$$x_{t+1}^b = f(x_t^a), \quad (40)$$
$$B_{t+1} = M P_t^a M^T + Q, \quad (41)$$
$$M_{i,j} = \frac{\partial f_i}{\partial x_j}, \quad (42)$$
$$H_{i,j} = \frac{\partial h_i}{\partial x_j}. \quad (43)$$

The procedure to perform EKF is similar to that for KF, as listed above. The disparities and similarities between EKF and KF include i) Kalman gain $K$ has the same form for both, especially the linear or linearized measurement model should be used; ii) the update equation of model error covariance has the same form, with linear and linearized state model used; iii) forecast model is different, with KF using linear eq. (26) and EKF using nonlinear model (40); iv) the filtering algorithm is different, linear measurement model $H$ used in KF (eq. (23)) and nonlinear model $h$

in EKF (eq. (37)). It should be noticed that EKF is only an approximate KF for nonlinear state model.

# 3. Ensemble Kalman filter (EnKF)

## 3.1 Basics of EnKF

A challenge in EKF is to update background (prediction) error covariance by (39) and (41), which requires the linearization of nonlinear model. The linearization of nonlinear model is often difficult technically, and even intractable in some cases, e.g. non-continuous functions existing in models. Another drawback of EKF is to neglect the contributions from higher-order statistical moments in calculating the error covariance.

To avoid the linearization of nonlinear model, the ensemble Kalman filter (EnKF) was introduced by Evensen et al. (Evensen 1994; Houtekamer and Mitchell 1998), in which the prediction (background) error covariance $B$ of (38) are estimated approximately using an ensemble of model forecasts. The main concept behind the formulation of the EnKF is that if the dynamical model is expressed as a stochastic differential equation, the prediction error statistics, which are described by the Fokker-Flank equation, can be estimated using ensemble integrations (Evensen 1994, 1997); thus, the error covariance matrix $B$ can be calculated by integrating the ensemble of model states. The EnKF can overcome the EKF drawback that neglects the contributions from higher-order statistical moments in calculating the error covariance. The major strengths of the EnKF include the following: (i) there is no need to calculate the tangent linear model or Jacobian of nonlinear models, which is extremely difficult for ocean (or atmosphere) general circulation models (GCMs); (ii) the covariance matrix is propagated in time via fully nonlinear model equations (no linear approximation as in the EKF); and (iii) it is well suited to modern parallel computers (cluster computing) (Keppenne 2000). EnKF has attracted a broad attention and been widely used in atmospheric and oceanic data assimilation.

Simply saying, EnKF used the below formula to replace (38) and neglected (41) - (43) in EKF while other equations are kept the same, i. e,

$$B = \frac{1}{N-1}\sum_{i=1}^{N}(x_i^b - \overline{x^b})(x_i^b - \overline{x^b})^T, \qquad (44)$$

where $x_i^b$ represents the $i$-th member of the forecast ensemble of system state vector at step $t$, and $N$ is the ensemble size. The use of (44) avoids processing the $M$, the linearized operator of nonlinear model. In eq. (38), the measurement function $H$ is still linear or linearized, which causes concern. To avoid the linearization of nonlinear measurement function, Houtekamer and Mitchell (2001) and Hamill (2006) wrote Kalman gain (38) by

$$BH^T \equiv \frac{1}{N-1}\sum_{i=1}^{N}[x_i^b - \overline{x^b}][h(x_i^b) - \overline{h(x^b)}]^T, \qquad (45)$$

$$HBH^T \equiv \frac{1}{N-1}\sum_{i=1}^{N}[h(x_i^b) - \overline{h(x^b)}][h(x_i^b) - \overline{h(x^b)}]^T, \qquad (46)$$

where $\overline{h(x^b)} = \frac{1}{N}\sum_{i=1}^{N} h(x_i^b)$. Eq. (45) and (46) allow direct evaluation of the nonlinear measurement function $h$ in calculating Kalman gain. However, (45) and (46) have not been proven mathematically, and only were given intuitionally. Amabadan and Tang (2009), Tang and Amabadan (2009) and Tang et al (2014) argued that (45) and (46) approximately hold if and only if

$$\overline{h(x^b)} = h(\overline{x^b}), \qquad (47)$$

$$x_i^b - \overline{x^b} = \varepsilon^i \text{ is small for } i = 1,2,\ldots,N. \qquad (48)$$

Under the conditions of (47) and (48), Tang et al (2014) argued (45) and (46) actually linearize the nonlinear measurement functions $H$ to $h$. Therefore, direct application of the nonlinear measurement function in (45) and (46) in fact imposes an implicit linearization process using ensemble members. In next section, we will see that (45) and (46) can be modified under a rigorous framework

Thus, the equations and procedure of EnKF are summarized as below:

$$x_i^a = x_i^b + K[y^o + \varepsilon^i - h(x_i^b)], \quad (49)$$

$$B = \frac{1}{N-1}\sum_{i=1}^{N}(x_i^b - \overline{x^b})(x_i^b - \overline{x^b})^T, \quad (50)$$

$$K = BH^T(HBH^T + R)^{-1}, \quad (51)$$

$$BH^T \equiv \frac{1}{N-1}\sum_{i=1}^{N}[x_i^b - \overline{x^b}][h(x_i^b) - \overline{h(x^b)}]^T, \quad (52)$$

$$HBH^T \equiv \frac{1}{N-1}\sum_{i=1}^{N}[h(x_i^b) - \overline{h(x^b)}][h(x_i^b) - \overline{h(x^b)}]^T, \quad (53)$$

$$P^a = (I - KH)B, \quad (54)$$

$$x_{i,t+1} = f(x_i^a + \gamma_i). \quad (55)$$

1. put perturbations on initial conditions and integrate the model, i.e., $x_{i,1} = f(x_0 + \gamma_i)$ where $i = 1,2\ldots,N$ (ensemble size) and $x_0$ is the initial condition;

2. using (51), (52) and (53) to calculate Kalman gain $K$;

3. calculate analysis using (49) after $K$ is obtained. It should be noted that each ensemble member produces an analysis; the average of all analyses ($N$) can be obtained;

4. using (55) to obtain new ensemble members for next round analysis. Here $\gamma_i$ is perturbation on the $i$-th member.

5. repeat Step 2 to Step 5 until the end of assimilation period.

6. It should be noted that the observation should be treated as a random variable with the mean equal to 0 and covariance equal to $R =< \varepsilon\varepsilon^T >$. This is why there is $\varepsilon_i$ in (49). Simply, $\varepsilon_i$ is often drawn from a normal distribution $\varepsilon_i \sim N(0, R)$

From the above procedure, we find that eq. (50) is not directly applied here. Instead, we use (52) and (53) to calculate $K$. This is because i) (51) and (52) avoid the linearization of nonlinear model; ii) avoid the explicit expression of matrix $B$, which is often very large and cannot be written in current computer sources in many

realistic problems. This should be noticed that (51) and (52) avoid writing B directly. The measurement function $h$, projecting model space (dimension) to observation space (dimension), greatly reduces the number of dimension.

## 3.2 Some remarks on EnKF with large dimensional problems

### Initial perturbation

The success of EnKF highly depends on the quality of ensemble members produced by initial perturbations. It is impractical to represent all possible types of errors within the ensemble because of the computational cost, the method of generating initial perturbations must be chosen judiciously. i) The first issue is the amplitude of initial perturbations. Usually the following two factors are considered when selecting the amplitude of initial perturbations: the amplitude of observation error and the amplitude of model errors induced by model parameters and uncertainty in model physics. If a model is perfect, the amplitude of the perturbations should be the same as the amplitude of observation errors. This combined error is used to determine the amplitude of perturbations. ii) When the perturbation amplitude is determined, the practical initial perturbation field generating each ensemble member could be constructed by a normalized pseudorandom field multiplied by the prescribed amplitude. Considering the spatial coherence, the pseudorandom field is red-noise as proposed by Evensen (2003), summarized as below:

1. Calculate the statistical characteristics for the pseudorandom field to meet its variance of 1 and mean of 0.

$$e^{-1} = \frac{\sum^{l,p} e^{-2(k_l^2 + r_p^2)/\sigma^2} \cos(k_l r_h)}{\sum^{l,p} e^{-2(k_l^2 + r_p^2)/\sigma^2}}, \qquad (56)$$

where $k_l = \frac{2\pi l}{x_n} = \frac{2\pi l}{N\Delta x}$; $r_p = \frac{2\pi p}{y_m} = \frac{2\pi p}{M\Delta y}$, $N$ and $M$ are the number of grid points in $x$-axis (lon.) and $y$-axis (lat.). For example, if your model domain is 114*42, $N = 114$ and $M = 42$. The $l$ and $p$ are wave-number, changing from 1 to the maximum value of $N/2$ and $M/2$. $\Delta x$ and $\Delta y$ are the interval of two adjacent

points, often set to 1. $r_h$ is the de-correlation length. The purpose of (56) is to derive the $\sigma^2$ for the other feature:

$$c^2 = \frac{1}{\Delta k \sum^{l,p} e^{-2(k_l^2+r_p^2)/\sigma^2}}. \qquad (57)$$

2. After $c$ and $\sigma^2$ are obtained, we can construct a 2-dimension pseudorandom field:

$$W(x_n, y_m) = \sum^{l,p} \frac{c}{\sqrt{\Delta k}} e^{-\frac{(k_l^2+r_p^2)}{\sigma^2}} e^{2\pi i \varphi(l,p)} e^{i(k_l x_n + r_p y_m)} \Delta k. \qquad (58)$$

3. While $x_n, y_m$ cover the whole domain, (58) produce a $n * m$ 2-dimensional random filed with spatial coherence structure and the variance of 1 and mean of 0. If the realistic uncertainty (error) has an amplitude $\beta$, the perturbation should be $\beta W$ . Similarly, (58) is often used for the error perturbation $\gamma_i$ used in (55).

Sometimes, we need to consider the vertical coherence of pseudorandom fields between adjacent levels in oceanic models. A simple method for this purpose is to construct the pseudorandom field at the $k$th level $\varepsilon_k$ by following equation:

$$\varepsilon_k = \alpha \varepsilon_{k-1} + \sqrt{1-\alpha^2} W_k, \qquad (59)$$

where $W_k$ $(k = 1, \ldots, L)$ is the pseudorandom field at the $k$th level without considering vertical coherence, constructed using the above method. Initially, for the surface perturbation ($k = 1$), the vertical coherence is not considered, i.e., $= 0$ , since $\varepsilon_{k-1}$ does not exist. Eq. (59) indicates that a practical pseudorandom at the $k$th level ($\varepsilon_k$ ) is composed of $W_k$ and $\varepsilon_{k-1}$ . As such the $\varepsilon_k$ is correlated with $\varepsilon_{k-1}$, i.e., the practical pseudorandom fields of two adjacent levels ( $\varepsilon_{k-1}$ and $\varepsilon_k$ ) are coherent with each other. Their correlation or coherent structure is determined by the coefficient $\alpha \in [0,1]$. Eq. (59) generates a sequence that is white in the vertical direction if $\alpha = 0$ (i.e., $\varepsilon_k = W_k$ ), but a sequence that is perfect correlated in vertical if $\alpha = 1$ (i.e., $\varepsilon_k = \varepsilon_{k-1}$ ). Eq. (59) is also often used to construct random fields that is

temporally coherent, for example, a continuous random noise that has coherence in time , as used for $\gamma_i$ in (55) (Evensen 2003). The random noise $\gamma_i$ in (55) can also be replaced by the random noise imposed in model forcing. For example, the random noise is continuously added to wind forcing for oceanic models. Even for some atmospheric models with transition processes, there are inherent random noises making $\gamma_i$ not necessary. One important criteria for $\gamma_i$ and the amplitude $\beta$ is to examine ensemble spread by some sensitivity experiments.

## The computational cost of Kalman gain

The Kalman gain, as expressed by (51), has dimension of $m * m$, where $m$ is the number of model variables of observation. In many realistic problems, $m$ is a very large number ($m \gg N$, the ensemble size), making the inversion very expensive.

A simple procedure is to rewrite the Kalman gain $K$, as below:

$$K = \tilde{x}\tilde{x}^T H^T (H\tilde{x}\tilde{x}^T H^T + \varepsilon\varepsilon^T)^{-1}, \qquad (60)$$

where $\tilde{x}$ indicates the model ensemble predictions removed the ensemble mean ($\tilde{x}_i = [x_i^b - \overline{x^b}]$, for $i = 1,2,\ldots,L$ ). $R = \frac{1}{N}\varepsilon\varepsilon^T$ was invoked here. If we assume the ensemble prediction error ( $x^b - \overline{x^{tr}} \approx x^b - \overline{x^b} = \tilde{x}$ ) is not correlated to observation error, i.e., $\tilde{x}\varepsilon^T = 0$ , the following is valid (Evensen 2003),

$$(H\tilde{x}\tilde{x}^T H^T + \varepsilon\varepsilon^T) = (H\tilde{x} + \varepsilon)(H\tilde{x} + \varepsilon)^T, \qquad (61)$$

where $(H\tilde{x} + \varepsilon)$ has dimension $m * N$. Usually ensemble size $N$ is much less than $m$. Using (singular value decomposition) SVD technique, we have

$$(H\tilde{x} + \varepsilon) = U\Sigma V^T.$$

The Eq. (61) then becomes

$$(H\tilde{x}\tilde{x}^T H^T + \varepsilon\varepsilon^T) = U\Sigma V^T V\Sigma^T U = U\Sigma\Sigma^T U^T = U\Lambda U^T.$$

So,

$$(H\tilde{x}\tilde{x}^T H^T + \varepsilon\varepsilon^T)^{-1} = U\Lambda^{-1}U^T, \qquad (62)$$

where $U$ and $\Lambda$ are the eigenvector and the square of eigenvalues of $(H\tilde{x} + \varepsilon)$. There are $N$ non-zero eigenvalues for $(H\tilde{x} + \varepsilon)$, therefore the dimension is not large, allowing us to efficiently compute the inversion for a global analysis in most practical situations.

## Stochastic EnKF and deterministic EnKF

In EnKF introduced in the previous section, the observation assimilated into dynamical model should be treated to be stochastic variable, as expressed by $y^o + \varepsilon^i$ in (49). It is a must if the classic EnKF algorithm, as expressed by (49) – (55), is used. It has been proven that if the EnKF assimilates deterministic observations (i.e., observation $y^o$ not changed at each ensemble member), the analysis error covariance will be systematically underestimated, typically leading to filter divergence, as indicated by below (Houtekamer and Mitchell 1998; Burgers et al. 1998):

$$P^{a*} = (I - KH)B(I - KH)^T \qquad (63)$$

Eq. (63) gives the analysis error covariance if the observed is not perturbed. Comparing (63) with (54), a theoretically unbiased estimate, $P^{a*}$ is always less than $P^a$.

However, the perturbed observation approach (i.e., $y^o + \varepsilon^i$) introduces an additional source of sampling error that reduces analysis error covariance accuracy and increases the probability of understanding analysis error covariance (Whitaker and Hamill 2002; Tippett et al. 2003). Thus an approach that only uses a single observation realization but avoids systematical underestimation of analysis error covariance was pursued. There are several approaches to implement this goal, as summarized by Tippett et al. (2003). Below, we will introduce an approach developed by Whitaker and Hamill (2002), called Ensemble square-root filter (EnSRF).

Denote the deviation of analysis from the analysis mean by $\tilde{x}^a = x^a - \overline{x}^a$ . It is easy to write

$$\tilde{x}^a = \tilde{x}^b + \widetilde{K}[\tilde{y}^o - H\tilde{x}^b], \qquad (64)$$

where $\tilde{y}^o = y^o - \overline{y}^o$. If a single observation realization is assimilated in all ensemble members, $\tilde{y}^o = 0$ and

$$\tilde{x}^a = \tilde{x}^b - \widetilde{K}H\tilde{x}^b = \left(I - \widetilde{K}H\right)\tilde{x}^b,$$

$$P^{a*} = (I - \widetilde{K}H)B(I - \widetilde{K}H)^T.$$

We seek a definition for $\widetilde{K}$ that will result in an ensemble whose analysis error covariance satisfies (54), i.e.,

$$(I - \widetilde{K}H)B(I - \widetilde{K}H)^T = (I - KH)B. \qquad (65)$$

The solution of (65) is

$$\widetilde{K} = (1 + \sqrt{\frac{R}{HBH^T + R}})^{-1}K. \qquad (66)$$

Therefore, EnSRF is summarized as below:

$$\overline{x}^a = \overline{x^b} + K\left[y^o - H\overline{x^b}\right], \quad (67)$$

$$\tilde{x}^a = \tilde{x}^b - \tilde{K}H\tilde{x}^b, \quad (68)$$

$$x^a = \overline{x}^a + \tilde{x}^a, \quad (69)$$

$$B = \frac{1}{N-1}\sum_{i=1}^{N}(x_i^b - \overline{x^b})(x_i^b - \overline{x^b})^T, \quad (70)$$

$$K = BH^T(HBH^T + R)^{-1}, \quad (71)$$

$$\tilde{K} = (1 + \sqrt{\frac{R}{HBH^T + R}})^{-1}K, \quad (72)$$

$$BH^T = \frac{1}{N-1}\sum_{i=1}^{N}[x_i^b - \overline{x^b}][h(x_i^b) - \overline{h(x^b)}]^T, \quad (73)$$

$$HBH^T = \frac{1}{N-1}\sum_{i=1}^{N}[h(x_i^b) - \overline{h(x^b)}][h(x_i^b) - \overline{h(x^b)}]^T, \quad (74)$$

$$P^a = (I - \tilde{K}H)B, \quad (75)$$

$$x_{i,t+1}^f = F(x_i^a + \gamma_i). \quad (76)$$

It should be noted that there are two Kalman Gains used in EnSRF, the original $K$ for ensemble analysis mean, and a new $\tilde{K}$ for deviation of analysis from the analysis mean. Eq. (67) indicates that one single observation realization of classic EnKF has the same ensemble analysis mean as stochastic observations or EnSRF.

Initially, the term EnKF refers, in particular, to the stochastic ensemble Kalman filter, which requires perturbing the observations. Subsequently, several deterministic EnKFs that avoid the use of perturbed observations were developed, e.g., the ETKF (Bishop et. al., 2001), the EAKF (Anderson, 2001), and the EnSRF. These filter designs are labelled as variants of the EnKF because they are also based on the Kalman filtering formula and ensemble representations.

## Inflation approach

The forecast error covariance is defined by (44):

$$B = \frac{1}{N-1}\sum_{i=1}^{N}(x_i^b - \overline{x^b})(x_i^b - \overline{x^b})^T = \frac{1}{N-1}\tilde{X} * \tilde{X}^T \quad (77)$$

Eq. (77) is an approximation to $B$ using forecast ensemble. Due to limited computational source, the ensemble size $N$ is often restricted to a small value for many realistic issues. A small ensemble size may cause a very small ensemble spread, causing the approximation of $B$ by (77) is seriously underestimated. To solve this problem, the $B$ is multiplied by a inflator factor $\lambda$ (slightly greater than 1). $\lambda$ is empirically determined, such as some sensitivity experiments, with the typical value of 1.01. The $\lambda B$ is used to replace $B$ in EnKF formula (49) – (55). This approach is equivalent to the below approach:

$$x_i^b = \lambda(x_i^b - \overline{x^b}) + \overline{x^b}.$$

## Localization of EnKF

When EnKF is applied to high-dimensional atmospheric and oceanic models, the limited ensemble size will cause the estimated correlations to be noisy (Houtekamer and Mitchell, 1998). When the ensemble size is insufficient, it will produce spurious correlations between distant locations in the background covariance matrix $B$. Unless they are suppressed, these spurious correlations will cause observations from one location to affect the analysis in locations an arbitrarily large distance away, in an essentially random manner (Hunt et al., 2007). This need to be remedied by the localization method.

Another reason for using localization is that the treatment of localization artificially reduces the spatial domain of influence of observations during the update. The localization dramatically reduces the necessary ensemble size, which is very important for operational systems. Two most common distance-based localization methods used in practice are local analysis and covariance localization.

Using local analysis, only measurements located within a certain distance from a grid point will impact the analysis in this grid point. This allows for an algorithm where the analysis is computed grid point by grid point. It was found that severe localization could lead to imbalance, but with large enough radius of influence (de-correlation length) for the measurements, this was not a problem. Hunt et al. (2007)

use the local analysis method in their ETKF algorithm, developed a local ensemble transform Kalman filter (LETKF).

To eliminate the small background error covariance associated with remote observations, Houtekamer and Mitchell (2001) uses a Schur (element wise) product of a correlation function with local support and the covariance of the background error calculated from the ensemble. That is, the matrix $B$ in eq. (70) is replaced by $\rho \circ B$, where "$\circ$" represents the elementwise product and the elements $\rho$ relates to the distance of the grid point to the observation $r$ as below :

$$\rho(r) = \left(1 + \alpha r + \frac{\alpha^2 r^2}{3}\right) e^{-\alpha r}. \qquad (78)$$

Here, $\alpha$ is a scalar parameter. To the author's knowledge, this is the first case that the covariance localization is used in EnKF.

Nowadays, a typical covariance localization approach is to represent prior covariances using an element-wise product of ensemble covariance and a correlation function with compact support (Gaspari and Cohn 1999). Anderson (2009) applied this approach to the Data Assimilation Research Test bed system, which has been used for realistic cases.

## Nonlinear Measurement function

It is clear that the linear assumption is made for the measurement function to obtain Eq. (51), as indicated by the linear operator H. To deal with the nonlinear measurement function in the EnKF, HM2001 proposed Eqs. (52) and (53) to directly evaluate the nonlinear measurement functions. As discussed in last section, there is a gap here, i.e., the lhs (left hand side) of Eqs. (52) and (53) need the linear measurement function H, whereas their rhs (right hand sides) directly uses the nonlinear function h. HM2001 realized this gap and used the equivalence sign "≡"

instead of the equality sign "=" in Eqs. (52) and (53). However, the equivalence is primarily based on intuition. Tang et al (2014) examined the equivalence in a rigorous, statistical framework. Based on the general form of Kalman Gain that will be discussed in next section, they derived a statistical estimation for Kalman gain, i.e.,

$$K = P_{\hat{x}_b\hat{y}} P_{\hat{y}\hat{y}} = \frac{1}{N-1}\sum_{i=1}^{L}(\hat{x}_{i,t}^b - \bar{\hat{x}}_t^b)[(H(\hat{x}_{i,t}^b) - H(\bar{\hat{x}}_t^b)]^T$$

$$* \{\frac{1}{N-1}\sum_{m=1}^{L}[H(\hat{x}_{i,t}^b) - H(\bar{\hat{x}}_t^b)][H(\hat{x}_{i,t}^b) - H(\bar{\hat{x}}_t^b)]^T + R\}^{-1}$$

A comparison of Eqs. (51), (52) and (53) with the above equation reveal that they are completely equivalent, if Eq. (47) holds true. From the linearization point of view, Eq. (47) holds true if and only if Eq. (48) also holds true. Conversely, the above equation were used instead of Eqs. (51) - (53) in the EnKF, the modified Kalman gain form should have been more rigorous in the statistical framework, which is equivalent to the general Kalman gain forms (83) –(84), 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 theoretically invalid due to the non-Gaussian nature of the systems.

## 4. General form of ensemble-based filters for Gaussian models

In proceeding sections, we introduced Kalman based filters. Originally Kalman filter applies linear model and linear measurement function. Further, EKF and EnKF were developed to address nonlinear models. However the measurement functions are still assumed to be linear. Eqs. (52) and (53) can directly evaluate nonlinear measurement functions but they were proposed intuitionally and not proven yet. In this section, we will present a general form for nonlinear measurement function, and further prove eqs. (52) and (53) mathematically using the general form.

For generality, we assume the below model:

$$\begin{aligned} x_{t+1} &= f(x_t, \eta_t), \\ y_t &= h(x_t, \zeta_t), \end{aligned} \qquad (79)$$

where $f$ and $h$ are nonlinear operator of model and measurement. The $x$ is model state and $y$ is the observation. The $\eta_t$ and $\zeta_t$ are the model errors and observed errors, respectively, which have variance: $var(\eta_t) =< \eta_t, \eta_t^T >= Q$, $var(\zeta_t) =< \zeta_t, \zeta_t^T >= R$. Assuming the estimate of model state $x^a$ at a time step is a linear combination of model forecast $x^b$ and observation $y^o$ , i.e., the filter itself is linear, so

$$x^a = x^b + K[y^o - h(x^b)]. \qquad (80)$$

Denote $\hat{x}^a = x^t - x^a$, $\hat{x}^b = x^t - x^b$, $\hat{y} = y^o - h(x^b)$. We have

$$\hat{x}^a = \hat{x}^b - K\hat{y}, \qquad (81)$$

$$\begin{aligned} P^a = E[\hat{x}^a(\hat{x}^a)^T] = E[(\hat{x}^b - K\hat{y})(\hat{x}^b - K\hat{y})^T] \\ = E[\hat{x}^b(\hat{x}^b)^T - \hat{x}^b\hat{y}^T K^T - K\hat{y}(\hat{x}^b)^T + K\hat{y}\hat{y}^T K^T] \end{aligned}$$

$$P^a = P^b - P_{\hat{x}\hat{y}}K^T - KP_{\hat{y}\hat{x}} + KP_{\hat{y}\hat{y}}K^T.$$

The optimal estimate asks the trace of $P^a$ minimum, namely,

$$\begin{aligned} \frac{\partial[trace(P^a)]}{\partial K} &= 0 \\ -P_{\hat{x}\hat{y}} - P_{\hat{y}\hat{x}} + 2KP_{\hat{y}\hat{y}} &= 0 \\ K &= P_{\hat{x}\hat{y}}P_{yy}^{-1} \\ P^a &= P^b - KP_{\hat{x}\hat{y}} \end{aligned}$$

where we invoked the below properties:

$$\begin{aligned} \frac{\partial(trace[xAx^T])}{\partial x} &= x(A + A^T) = 2xA, \\ \frac{\partial(trace[xA^T])}{\partial x} &= \frac{\partial(trace[Ax^T])}{\partial x} = A^T = A. \end{aligned}$$

Thus we have the optimal estimate filter:

$$
\begin{aligned}
x_t^a &= x_t^b + K\left[y^o - h\left(x_t^b\right)\right], && (82)\\
K &= P_{\hat{x}\hat{y}} P_{yy}^{-1}, && (83)\\
P_t^a &= P_t^b - K P_{\hat{x}\hat{y}}, && (84)
\end{aligned}
$$

$$
\begin{aligned}
x_{t+1}^b &= E[f(x_t^a, \eta_t)] = E[f(x_t^a)],\\
y_t &= E\left[h\left(x_t^b, \zeta_t\right)\right] = E\left[h\left(x_t^b\right)\right].
\end{aligned} \qquad (85)
$$

Eqs. (82)-(85) give a general algorithm for Gaussian nonlinear model and nonlinear measurement function. It is also assumed that the noise is additive in eq. (85). The first term of eq. (83) can be interpreted as the cross-covariance $P_{\hat{x}\hat{y}}$ between the state and observation errors, and the remaining expression can be interpreted as the error covariance $P_{\hat{y}\hat{y}}$ of the difference between model observation and observation itself. Here, $\hat{y}$ is defined as the error between the noisy observation $y^o$ and its prediction $h(x^b)$.

If the model is linear, obviously

$$
\begin{aligned}
x_{t+1}^b &= M x_t^a + \eta_t,\\
B_{t+1} &= M P_t^a M^T + Q.
\end{aligned}
$$

If the measurement function is linear, i.e.,

$$
\begin{aligned}
\hat{y} &= y^o - h(x^b, \zeta) = y^o - Hx^b + \zeta = Hx^t - Hx^b + \zeta = H\hat{x}^b + \zeta,\\
P_{\hat{x}\hat{y}} &= P_{\hat{x}\hat{x}} H^T,\\
P_{\hat{y}\hat{y}} &= H P_{\hat{x}\hat{x}} H^T + R.
\end{aligned}
$$

So, Kalman gain

$$
K = P_{\hat{x}\hat{x}} H^T \left(H P_{\hat{x}\hat{x}} H^T + R\right)^{-1}. \qquad (86)
$$

Eq. (86) is identical to eq. (51). Therefore, eq. (51), or KF, EKF and EnKF, is a special case of eq. (86) under the assumption of linear measurement function.

In the standard KF the state error covariance is updated at each analysis cycle during the measurement update process. Updating the error covariance matrix is important because it represents the change in forecast error covariance when a measurement is performed. The EnKF implementation does not require the covariance update equation because it can directly calculate the updated error covariance matrix from a set of ensemble members. Evensen (2003) has derived the analysis covariance equation, which is consistent with the standard KF error covariance to update eq. (39). But the true representation of the updated error covariance requires a large ensemble size, which is often computationally infeasible.

The general form of the Kalma gain makes use of the reformulated error covariance. In a broad sense, the above algorithm implicitly uses the prior covariance update equation (or the analysis error covariance matrix) to calculate the forecast error covariance. Thus, the above algorithm is fully consistent with the time update and measurement update formulation of the Kalman filter algorithm. On this basis, one can develop a new type of Kalman filter which chooses the ensemble members deterministically in such a way that they can capture the statistical moments of the nonlinear model accurately. In the next subsection we will discuss the new type of Kalman filter, called Sigma-point Kalman filter, based on the above algorithm.

# 5. Sigma-Point Kalman filters (SPKF)

## 5.1 Basics of SPKF

EnKF was developed in order to overcome the linearization of nonlinear models. As introduced earlier, the idea behind EnKF is to 'integrate' Fokker-Plank equation using ensemble technique to estimate the forecast error covariance. Theoretically if the ensemble size is infinite, the estimate approaches the true value. However in reality, we can only use finite ensemble size, even very small size for many problems, leading to truncation errors. Thus, some concerns exist such as: how to wisely generate finite samples for the optimal estimate of prediction error covariance; how much the least ensemble size is for an efficient estimate of error

covariance; and how much the true error covariance can be taken into account in the EnKF, given an ensemble size. In this section, we will introduce a new ensemble technique for EnKF, which is called Sigma-point Kalman filter (SPKF).

The so-called sigma-point approach is based on deterministic sampling of state distribution to calculate the approximate covariance matrices for the standard Kalman filter equations. The family of SPKF algorithms includes the unscented Kalman filter (UKF; Julier et al. 1995; Wan and van der Merwe 2000), the central difference Kalman filter (CDKF; Ito and Xiong 2000), and their square root versions (van der Merwe and Wan 2001a,b). Another interpretation of the sigma-point approach is that it implicitly performs a statistical linearization (Gelb 1974) of the nonlinear model through a weighted statistical linear regression (WSLR) to calculate the covariance matrices (van der Merwe and Wan 2001a,b; van der Merwe et al. 2004). In SPKF, the model linearization is done through a linear regression between a number of points (called sigma points) drawn from a prior distribution of a random variable rather than through a truncated Taylor series expansion at a single point (van der Merwe et al. 2004). It has been found that this linearization is much more accurate than a truncated Taylor series linearization (van der Merwe and Wan 2001a). Eqs. (82) - (85) construct a core of SPKF. A central issue here is how to generate the optimal ensemble members for applying these equations. There are two basic approaches aforementioned, UKF and CDKF. For an $L$-dimensional dynamical system represented by a set of discretized state space equations of (79), it has been proven that $2L + 1$ ensemble members, constructed by UKF or CDKF, can precisely estimate the mean and covariance. We ignore the theoretical proof and only outline the UKF scheme as below.

Denote $2L + 1$ sigma-points at time $k$ for producing ensemble members by $\chi_k = [\chi_{k,0}, \chi_{k,1}^{+}, \ldots, \chi_{k,L}^{+}, \chi_{k,1}^{-}, \ldots, \chi_{k,L}^{-}]$, which is defined according to the following expressions:

$$\chi_{k,0} = \overline{X}_k^a, \quad (87)$$

$$\chi_{k,i}^{+} = \overline{X}_k^a + [c\sqrt{P_{X,k}^a}]_i, \quad (88)$$

$$\chi_{k,i}^{-} = \overline{X}_k^a - [c\sqrt{P_{X,k}^a}]_i, \quad (89)$$

where $L = N_x + N_\eta + N_\zeta$ is the sum of the dimensions of model states, model noise and measurement noise. The augmented state vector $X = [x; \eta; \zeta]$ is a $L$-dimensional vector. $\sqrt{P_{X,k}^a}$ is the covariance of the augmented state vector (analysis) at the previous step. $[\sqrt{P_{X,k}^a}]_i$ is the $i$th row (column) of the weighted matrix square root of the covariance matrix ($L$ dimension). $c$ is a scale parameter which will be specified later. The key point here is to produce $(2L + 1)$ ensemble members by integrating model with $2L + 1$ initial conditions of (87)-(89); by these ensemble members the filter (82)-(84) will be performed.

The procedure is summarized as below:

1. Initially, perturb a small amount, denoted by $\tilde{x}_0$ on initial condition $x_0$, using Evensen (2003) method; also randomly generate perturbation for $q$ and $r$, drawn from normal distributions of $N(0, Q)$ and $N(0, R)$. Thus, we can construct the augmented state vector and corresponding covariance ($k = 0$);

$$\overline{X}_0^a = [x_0; 0; 0],$$
$$P_0^x = \tilde{x}_0 \tilde{x}_0^T,$$
$$P_{X,0} = \begin{pmatrix} P_0^x & 0 & 0 \\ 0 & Q & 0 \\ 0 & 0 & R \end{pmatrix}.$$

2. From the above formula, we can calculate sigma-points using (87) - (89). Note that each set of sigma-points, denoted by $\chi_k$, has dimension $L$, e. g., the $i$th sigma-point can be expressed by $\chi_{k,i} = [x_{k,i}; \eta_{k,i}; \zeta_{k,i}]$.

3. Using the $2L + 1$ sigma-points to integrates state-space model. For the $i$th sigma-point, we have ($x_{k+1,i}^f = f(x_{k,i}, \eta_{k,i})$. When $i$ varies from 1 to $2L + 1$, we produce $2L + 1$ ensemble members, from which analysis mean and covariance

will be obtained, which are in turn used to produce sigma-points for next step $(k+1)$, to form a recursive algorithm.

Supposed we have $2L+1$ ensembles, the analysis mean and the covariance are calculated as follows

$$\overline{x}^f_{k+1} = \sum_{i=0}^{2L} w_i^{(m)} x^f_{k+1,i}, \quad (90)$$

$$(P^f_{xx})_{k+1} = \sum_{i=0}^{2L} w_i^{(c)} [x^f_{k+1,i} - \overline{x}^f_{k+1}][x^f_{k+1,i} - \overline{x}^f_{k+1}]^T, \quad (91)$$

$$y^f_{k+1,i} = h\left(x^f_{k+1,i}, \zeta_{k+1,i}\right), \quad (92)$$

$$\overline{y}^f_{k+1} = \sum_{i=0}^{2L} w_i^{(m)} y^f_{k+1,i}, \quad (93)$$

$$(P_{yy})_{k+1} = \sum_{i=0}^{2L} w_i^{(c)} [y^f_{k+1,i} - \overline{y}^f_{k+1}][y^f_{k+1,i} - \overline{y}^f_{k+1}]^T, \quad (94)$$

$$(P_{xy})_{k+1} = \sum_{i=0}^{2L} w_i^{(c)} [x^f_{k+1,i} - \overline{x}^f_{k+1}][y^f_{k+1,i} - \overline{y}^f_{k+1}]^T, \quad (95)$$

$$K_{k+1} = P_{xy}P_{yy}^{-1}, \quad (96)$$

$$\overline{x}^a_{k+1} = \overline{x}^f_{k+1} + K_{k+1}\left[y_{k+1} - \overline{y}^f_{k+1}\right], \quad (97)$$

$$P^a_{k+1} = (P^f_{xx})_{k+1} - K_{k+1}P_{yy}K^T_{k+1}, \quad (98)$$

where

$$c = \sqrt{L+\lambda},$$

$$w_0^{(m)} = \frac{\lambda}{L+\lambda},$$

$$w_0^{(c)} = \frac{\lambda}{L+\lambda} + 1 - \alpha^2 + \beta,$$

$$w_i^{(m)} = w_i^{(c)} = \frac{1}{2(L+\lambda)}, i = 1,2,\ldots 2L$$

$$\lambda = \alpha^2(L+\kappa) - L,$$

$\alpha$ and $\kappa$ are tuning parameters. $0 < \alpha < 1$ and $\kappa \geq 0$. Often $\kappa$ is chosen 0 as default value; and $\beta = 2$.

4. From $P_{k+1}^{a}$, as well choosing random perturbation for model noise $\eta$ and observation noise $\zeta$, drawn from Gaussian distribution of $N(0, Q)$ and $N(0, R)$, we calculate sigma-points using eqs. (87)-(89), and repeat Step 2 and so on until the assimilation is completed for the entire period.

## 5.2 Remarks of SPKF

1. SPKF was introduced into the earth sciences recently (e.g., Ambadan and Tang, 2009; Luo and Moroz 2009). The main differences between SPKF and EnKF include i) SPKF chooses the ensemble members deterministically while EnKF uses random perturbation to generate ensemble members; ii) the number of sigma-points is a fixed value as $2L + 1$, while the ensemble size in EnKF is prespecified; iii) SPKF uses eq. (98) to update the error covariance matrix, while EnKF does not update explicitly the error covariance matrix; iv) sigma-points are calculated using eqs. (87)-(89) every time when the observation is available, while the ensemble members in EnKF only perturbed in the intial time. Recent application of SPKF on a realistic oceanic model indicates that the SPKF is better than the EnKF in the similar level of computational cost (Tang et al. 2014)

2. In SPKF, the number of sigma-points is $2L + 1$, here $L$ is the dimension of the augmented state vector $X = [x; \eta; \zeta]$, i.e., $L = N_x + N_\eta + N_\zeta$ is the sum of model state, model noise and observation noise. Usually $L$ is the order $10^3$ - $10^4$, so the computational expense is a huge challenge in SPKF for realistic problems. A solution is to use the truncated singular value decomposition (TSVD) to reduce the sigma-points. As seen from the eqs. (87) - (89), the $P_{X,k}^{a}$ is a $L * L$ matrix, thus the dimension of $P_{X,k}^{a}$ determines the ensemble size. Supposed that $P_{X,k}^{a}$ can be expressed as

$$P_{X,k}^{a} = E_{X,k}^{a} \Sigma_k (E_{X,k}^{a})^T, \qquad (99)$$

where $\Sigma_k = diag(\sigma_k^1, \sigma_k^2, \ldots, \sigma_k^L)$ is a diagonal matrix of eigenvalues which are sorted in descending order, i.e., $\sigma_k^1 \geq \sigma_k^2 \geq \ldots \geq \sigma_k^L$ , and $E_{X,k}^a = [e_{X,k,1}^a, e_{X,k,2}^a, \ldots, e_{X,k,L}^a]$. Truncating the first $m$ modes, so we can write the sigma-points (87)-(89) as below:

$$\chi_{k,0} = \overline{X}_k^a \quad (100)$$

$$\chi_{k,i}^+ = \overline{X}_k^a + c\sqrt{\sigma_k^i} e_{X,k,i}^a \quad (101)$$

$$\chi_{k,i}^- = \overline{X}_k^a - c\sqrt{\sigma_k^i} e_{X,k,i}^a \quad (102)$$

$i = 1,2,\ldots,m$. Thus the ensemble size becomes $2 * m + 1$. Some fast SVD algorithms can be used here such as Lanczos and block Lanczos (Chapter 9 of Golub and Loan). The application of the truncated SVD was also found in (Hansen 1987; Ehrendorfer and Tribbia 1997).

3. Further simplification of $P_{X,k}^a$ based on its definition (or Cholesky decomposition), i.e., $P_{X,k}^a = A_{X,k}^a * (A_{X,k}^a)^T$, where $A_{X,k}^a$ is the data which has subtracted the ensemble mean. Thus, eqs. (87)-(89) can be written as follows

$$\chi_{k,0} = \overline{X}_k^a \quad (103)$$

$$\chi_{k,i}^+ = \overline{X}_k^a + (cA_{X,k}^a)_i \quad (104)$$

$$\chi_{k,i}^- = \overline{X}_k^a - (cA_{X,k}^a)_i \quad (105)$$

where $(cA_{X,k}^a)_i = [x_k^a; \eta_k; \zeta_k]_i, i = 1,2,\ldots,L$, $(x_k^a)_i = (x_k^f)_i + K_k[y_k - y_k^f]$. Eqs. (103)-(105) transfer the covariance matrix $P_{X,k}^a$ to data matrix $A_{X,k}^a$ in constructing sigma-points. The largest advantage is to avoid explicit expression of $P_{X,k}^a$, which could be a very large matrix beyond memory of current computers. However (103)-(105) cannot reduce the ensemble size (2L+1). A solution is to decompose such as Principal Component Analysis, as used in (Ambadan and Tang, 2009). Further discussions on optimal construction of sigma-points should be conducted for a realistic application of SPKF.

4. Again, we look at Sigma-point generation, i.e., eqs (100)-(102) or (103)-(105). As we defined, an augmented matrix is applied here: $= [x; \eta; \zeta]$ . Without losing the generality, we only take eqs (103) - (105) and rewrite them as below:

$$\begin{bmatrix} x_{k,0} \\ \eta_{k,0} \\ \zeta_{k,0} \end{bmatrix} = \begin{bmatrix} \overline{x}_{k,0} \\ 0 \\ 0 \end{bmatrix} \qquad (106)$$

$$\begin{bmatrix} x_{k,i} \\ \eta_{k,i} \\ \zeta_{k,i} \end{bmatrix} = \begin{bmatrix} \overline{x}_{k,0} \\ 0 \\ 0 \end{bmatrix} + c \begin{bmatrix} x^a_{k,i} \\ \eta_{k,i} \\ \zeta_{k,i} \end{bmatrix} \qquad (107)$$

Similarly, we can write (105) using individual variables. From eqs. (106) and (107), we can draw,

- Noise and model state analysis in constructing sigma-points at $k$ step are independent. It should be noted that $x^a_k$ is from eq. (97) and noise are draw from a Gaussian distribution. If we assume that noise is taken randomly each time, $x^a_k$ is only relevant to noise which is drawn at time step $k$, and independent with model noise and observation noise drawn for analysis of the time step $k+1$, thus, $P_{X,k}$ is a diagonal block matrix, i.e.,

$$P_{X,k} = \begin{pmatrix} P^x_k & 0 & 0 \\ 0 & Q & 0 \\ 0 & 0 & R \end{pmatrix} \qquad (108)$$

- There are not update equations for noise so they are randomly taken from Gaussian distribution, i.e., the index $i$ in $\eta_i$ and $\zeta_i$ actually does not have meaning. Thus, it should be a reasonable assumption that the $\eta_i$ and $\zeta_i$ ,used for constructing sigma-points at time step $k+1$, is not related to $P_{X,k}$ (time step of $k$), as argued above. Thus, (108) always hold unless the noise is designed considering the temporal coherence such as red noise in time.

- Based on above, the actual ensemble size is $2N_x + 1$, not $2L + 1$. This is because neither model noise nor observation noise can produce ensemble alone. Model error $\eta_i$ and $x_{k,i}^f$ must jointly together to produce ensemble members with$N_x$.

  Let us see this in details: at the initial time, initial perturbation on model states, plus drawn noise for model errors and measurement errors are with mean and variance as follows

$$\overline{X}_0^a = [x_0; 0; 0], \quad P_{X,0} = \begin{pmatrix} P_0^x & 0 & 0 \\ 0 & Q & 0 \\ 0 & 0 & R \end{pmatrix}.$$

  Theoretically there are $2(N_x + N_\eta + N_\zeta) + 1$ ensembles, denoted by the $i$ th column of $P_{X,0}$ ( $i = 1, \ldots, N_x$ ; $Nx + 1, \ldots, N_x + N_\eta$ ; $N_x + N_\eta + 1, \ldots, N_x + N_\eta + N_\zeta$) and formula (87) - (89). However, at the $i$th column, the elements of the row, indicating the model inputs $(x, \eta, \zeta)$ , only have the non-zero values of $N_x$. Obviously, the sigma-points of zero-values makes the update equation $\chi_{k+1,i} = f(\chi_{k,i})$ invalid, thus, the actual ensemble size is $2N_x + 1$.

5. When truncation technique is applied to reduce the ensemble size, the ensemble spread might be shrunk due to relatively small ensemble size. Like EnKF, an inflation approach of SPKF might be helpful. It is interested in developing such a scheme for SPKF.

6. Again, we can localize SPKF, like localized EnKF, to solve memory and computation issues.

7. All of the remarks of SPKF are from the authors' thinking and understanding. It is interesting to further test and validate these ideas and properties using simple models.

# 6. Beyond Kalman filters: Particle Filter and its derivatives

## 6.1 Standard particle filter

We have introduced the Kalman filter (KF), extended Kalman filter (EKF), ensemble Kalman filter (EnKF) and sigma-point Kalman filter (SPKF) in previous sections. All of those filters belong to the sequential data assimilation method, i.e., observation data is assimilated into the model system as soon as it is available. The Bayesian estimation theory provide a general framework of the sequential data assimilation methods. If we assume the state space model is

$$\begin{aligned} x_{t+1} &= f(x_t, \eta_t) \\ y_t &= h(x_t, \zeta_t) \end{aligned}$$

the analysis step of a Bayesian-based assimilation method is deduced by Bayes' theorem:

$$p(x_t|y_t) = \frac{p(y_t|x_t)p(x_t)}{p(y_t)}, \qquad (109)$$

where $p(y_t)$ plays as a normalization factor.

Recalling section 1.3, eq. (7) actually assumes that the prior probability density function $p(x_t)$ and the likelihood function $p(y_t|x_t)$ are Gaussian distribution functions, and thus the posterior probability density function $p(x_t|y_t)$ is also a Gaussian. Based on the Gaussian assumption, the cost function of 3D-Var (i.e., eq. (2)) can be derived, and it is equivalent to the Kalman filter (23) - (27). All the Kalman-based filters (e.g., EKF, EnKF, EnSRF, SPKF, etc. ) contain the inherent Gaussian assumption, and they are derived and validated for Gaussian systems in theory. However, this Gaussian assumption is often not held for nonlinear systems. Even for an initial Gaussian error, it often becomes non-Gaussian while propagating forward with nonlinear models.

The particle filter (PF) is a sequential data assimilation method which is able to deal with the nonlinear, non-Gaussian state estimation problem. Like EnKF, PF also uses

an ensemble, but it is used to approximately estimate the full probability density function rather than only the error covariance $B$. An ensemble member is also referred to as a particle in PF literatures.

Suppose the prior probability density is the sum of Dirac-Delta functions

$$p(x_t) = \sum_{i=1}^{N} \delta\left(x_t - x_t^i\right), \qquad (110)$$

where $\{x_t^i, i = 1,2,\dots,N\}$ are particles drawn from $p(x_t)$. The posterior probability density is derived by applying the Bayes' theorem (109) directly, that is

$$p(x_t|y_t) \propto p(y_t|x_t)p(x_t) = \sum_{i=1}^{N} w_{t,i}\,\delta\left(x_t - x_t^i\right), \qquad (111)$$

in which $w_{t,i} \propto p(y_t|x_t^i)$, a normalization step is required to make $\{w_{t,i}, i = 1,2,\dots,N\}$ sum up to 1. If we assume the likelihood function is Gaussian, $w_{t,i}$ can be computed by

$$p(y_t|x_t^i) = \frac{1}{\sqrt{2\pi}}\exp\{[y_t - h(x_t^i)]R^{-1}[y_t - h(x_t^i)]^T\}. \qquad (112)$$

Or else we can use any specified probability density function of $p(y_t|x_t)$ to compute the likelihood.

With the posterior probability density function $p(x_t|y_t)$, the analysis value and covariance can be computed by

$$\overline{x_t} = \int x * p(x|y_t)dx = \sum_{i=1}^{N} w_{t,i}x_t^i, \qquad (113)$$

$$var(x_t) = \int x^2 * p(x|y_t)dx - \overline{x_t}^2 = \sum_{i=1}^{N} w_{t,i}(x_t^i)^2 - \overline{x_t}^2, \qquad (114)$$

and higher order moments of the posterior state can also be estimated.

Before stepping forward to next stage, a resampling step is required to make each particle with uniform weight. A typical resampling strategy is the Sequential Importance Resampling (SIR), which removes particles with very small weights and duplicates those with large weights. A detailed algorithm of SIR can be found in (Arulampalam et al., 2002). The resampling algorithm gives the indices and number of copies of those particles which should be duplicated, i.e.,

$$1,2,\dots,\mathrm{N} \xrightarrow{SIR} \mathrm{s}_1,\mathrm{s}_2,\dots,\mathrm{s}_\mathrm{N} \qquad (115)$$

$$\mathrm{s}_\mathrm{i} \in 1,2,\dots,N.$$

After the resampling step, the ensemble is with members equally-weighted as $\{x_t^{s_i}, i = 1,2,\dots,N\}$, and thus eqs. (110) - (112) can be repeated for the next analysis stage.

In summarize, the algorithm of standard particle filter is below:

1. generate the initial ensemble $\{x_0^i, i = 1,2,\dots,N\}$ as EnKF does.
2. integrate the model until the observation is available.
3. using eq. (112) to compute the weight for each particle, and normalize them.
4. using eq. (113) to obtain the analysis; using eq. (114) to obtain the covariance if necessary.
5. apply the resampling algorithm to derive the resampling indices (eq. (115)), and derive the new ensemble $\{x_t^{s_i}, i = 1,2,\dots,N\}$.
6. repeat step 2 to step 5 until the end of assimilation period.

The standard particle filter (Gordon, 1993) is also known as the bootstrap particle filter or SIR particle filter.

## 6.2 Variants of PF

The particle filter is a highly promising technique because it does not invoke any Gaussian assumptions. It has been widely used and studied in many other fields. The PF estimates the full probability density function of the forecasted state based on an ensemble of states with different weights. However, the PF suffers from the problem of filter degeneracy, i.e., the procedure collapses to a very small number of highly weighted particles among a horde of almost useless particles carrying a tiny proportion of the probability mass. Even if resampling techniques are used, the degeneracy cannot be completely avoided with limited ensemble size. The number of particles must grow substantially with the dimension of the system to avoid degeneracy (Bengtsson, 2003; Synder, 2007), a requirement that is apparently too costly for large models such as GCMs. Various efforts have been made to resolve this issue, as documented in an excellent overview (Van Leeuwen, 2009).

Several strategies are often employed to address the problem of filter degeneracy in applications of the particle filter. For example, Papadakis et al. (2010) proposed a weighted ensemble Kalman filter (WEnKF), which uses an ensemble-based Kalman filter as the proposal density, from which the particles are drawn. Van Leeuwen et al. developed a fully nonlinear particle filter by exploiting the freedom of the proposal transition density, which ensures not only that all particles ultimately occupy high-probability regions of state space but also that most of the particles have similar weights. The implicit particle filter uses gradient descent minimization combined with random maps to find the region of high probability, avoiding the calculation of Hessians. Luo et al. have proposed an efficient particle filter that uses residual nudging to prevent the residual norm of the state estimates from exceeding a pre-specified threshold. These particle filters were very recently proposed and have attracted broad attention in the community of atmos./ocean. data assimilation. Below we will briefly introduce the equivalent weights particle filter (EWPF) by Van Leeuwen (2011).

The equivalent weights particle filter is a fully nonlinear data assimilation method which works in a two-stage process. It uses the proposal density to ensure that the particles have almost equivalent weights, by which the filter degeneracy can be avoided.

In the standard PF, the particles at time step $t$ are propagated by the original model, i.e., $x_{t+1}^i = f(x_t^i) + \eta_t$, which implies that the particles at time step $t+1$ are drawn from the transition density $p(x_{t+1}|x_t)$. In that case, the weight of each $x_{t+1}^i$ varies greatly, and filter degeneracy is very likely to happen.

In EWPF, another transition density, call the proposal density, is introduced. The proposal density depends on the future observation $y_{t+1}$ and all previous particles $\{x_t^i, i = 1,2,\dots,N\}$. With the help of proposal density, the particle $x_t^i$ is propagated using a different model

$$x_{t+1}^i = g\left(x_t^i, y_{t+1}\right) + \eta_t. \qquad (116)$$

The model $g$ can be anything, for instance, one can add a relaxation term and change random forcing:

$$x_{k+1}^i = f\left(x_k^i\right) + \eta_k^i + A\left(y_{t+1} - H\left(x_k^i\right)\right), \quad k = 1,\dots,p(k) \qquad (117)$$

where $p(k)$ is a function of the time between observations, and each $k$ implies each model step without observation. The $A$ is a relaxation term which will "drag" the particle towards future observation. In Browne et al. (2015), it is given by

$$A = p(k)QH^T R^{-1}, \qquad (118)$$

where the matrices $Q$ and $R$ correspond to the model error covariance and observation error covariance respectively.

The second stage of EWPF involves updating each particle at the observation time $t+1$ via the formula

$$x_{t+1}^i = f(x_t^i) + \alpha_i QH^T(HQH^T + R)^{-1}(y_{t+1} - H(f(x_t^i))) + \eta_t^i, \qquad (119)$$

where $\alpha_i$ are scalers computed so as to make the weights of the particles equal. Using the expression for weights and setting all weights equal to a target weight (e.g., $1/N$)

$$w_i = p\left(y_{t+1}\middle|x_{t+1}^i(\alpha_i)\right) = w_{target},$$

$\alpha_i$ can be solved by numerical methods.

Eqs. (117) - (119) show an example of how to construct the proposal model $g$ in (116), it can also be done by running 4D-var on each particle (implicit particle filter), or using the EnKF as proposal density. Those methods refer to Morzfeld et al. (2012) and Papadakis et al. (2010).

## 6.3 Remarks of PF

### Combined method of EnKF and PF

The ensemble Kalman particle filter (EnKPF) is a combination of EnKF and the SIR particle filter. It was recently introduced to address non-Gaussian features in data assimilation for highly nonlinear systems, by providing a continuous interpolation between the EnKF and SIR-PF analysis schemes (Frei and Kunsch, 2013).

As stated above, both EnKF and PF methods are based on the Bayesian estimation theory, but they approximate the probability density function of the state in different ways. The EnKF only approximates the mean and covariance of the state through a series of equally weighted ensemble members. And the particle filter considers the weights of the ensemble members according to the likelihoods. The EnKF contains the Gaussian assumption but requires small ensemble size to prevent filter degeneracy, which is in contrast with the PF.

The EnKPF takes advantage of both methods by combining the analysis schemes of the EnKF and the SIR-PF using a controllable index (i.e., tuning) parameter. In contrast with both the EnKF and the SIR-PF, the analysis scheme of the EnKPF not only updates the ensemble members but also considers the weights.

Assume that the forecast ensemble $x_i^f, i = 1,2, \dots, N$ and the observation data $y$ are available and that the forecast covariance $P^f$ can be calculated using the ensemble, the analysis scheme of EnKPF is given below:

1. Choose $\gamma \in [0,1]$ and apply the EnKF which is based on the inflated observation error covariance $R/\gamma$ as follows:

$$K_1(\gamma) = P^f H^T (HP^f H^T + R/\gamma)^{-1} = \gamma P^f H^T (\gamma H P^f H^T + R)^{-1}, \quad (120)$$

$$v_i = x_i^f + K_1(\gamma)(y - Hx_i^f), \quad (121)$$

$$Q = \frac{1}{\gamma} K_1(\gamma) R K_1(\gamma)^T. \quad (122)$$

2. Compute the weights $w_i$ for each updated member $v_i$ as follows:

$$w_i = \phi\left(y; Hv_i, \frac{R}{1-\gamma} + HQH^T\right), \quad (123)$$

3. and normalize the weights by $\hat{w}_i = w_i / \sum_{i=1}^N w_i$, in which $\phi$ is the probability density function of a Gaussian.

4. Calculate the resampling index $s(i)$ for each member $v_i$ according to $\hat{w}_i$ using the SIR algorithm, then set

$$x_i^u = v_{s(i)} + K_1(\gamma)\frac{\epsilon_{1,i}}{\sqrt{\gamma}}, \quad (124)$$

5. where $\epsilon_{1,i}$ is a random observation error drawn from the Gaussian $\mathbf{N}(0, R)$.

6. Compute $K_2(1-\gamma) = (1-\gamma)QH^T[(1-\gamma)HQH^T + R]^{-1}$, generate $\epsilon_{2,i}$ from $\mathbf{N}(0, R)$ and EnKF with the inflated observation error again as follows:

$$x_i^a = x_i^u + K_2(1-\gamma)\left[y + \frac{\epsilon_{2,i}}{\sqrt{1-\gamma}} - Hx_i^u\right]. \quad (125)$$

The $\gamma$ can be determined recursively to match the optimal performance of EnKPF. More details of EnKPF can be found in (Frei and Kunsch, 2013; Shen and Tang, 2015).

## Localization in PF

Previous sections have introduced the localization technique in EnKF, which greatly improves the performance of EnKF in high-dimensional models. The advantages of localization motivate the search for a localization procedure in particle filtering.

Van Leeuwen (2009) had a deep discussion on this topic. He argued that one can calculate the weights locally, but it is not easy for resampling. In the resampling step low-weight particles are abandoned and high-weight particles are duplicated. However, with local weights, different particles are selected in different parts of the domain. The problem is that we have to have continuous (in space) model fields to propagate forward in time with the model. Just constructing a new particle that consists of one particle in one part of the model domain and another particle in another domain will lead to problems at the boundary between these two (Van Leeuwen, 2009).

The problem of spatial discontinuity makes the localization in particle filter not feasible currently. Most of the advanced particle filters (e.g. EWPF, implicit particle filter) are using the idea of global weight, i.e., the weight for each member is a scalar.

However, there are still some attempts on the localization in particle filter. For example, Poterjoy (2015) developed the localized particle filter (LPF) which updates particles locally using ideas borrowed from EnKF. The paper (Poterjoy, 2016) has demonstrated some advantage of the new filter over EnKF, especially when the observation networks consist of densely spaced measurements that relate nonlinearly to the model state. This is a very interesting work about the particle filter, it also has a potential to work with large atmos./ocean. data assimilation systems.

## Reference

Ambadan, J. T., & Tang, Y. (2009), Sigma-point Kalman filter data assimilation methods for strongly nonlinear systems. Journal of the Atmospheric Sciences, 66(2), 261-285.

Anderson, J. L. (2001). An ensemble adjustment Kalman filter for data assimilation. Monthly weather review, 129(12), 2884-2903.

Anderson, J. L. (2009). Ensemble Kalman filters for large geophysical applications. Control Systems, IEEE, 29(3), 66-82.

Arulampalam, M. S., Maskell, S., Gordon, N., & Clapp, T. (2002). A tutorial on particle filters for online nonlinear/non-Gaussian Bayesian tracking. Signal Processing, IEEE Transactions on, 50(2), 174-188.

Bengtsson, T., Snyder, C., & Nychka, D. (2003). Toward a nonlinear ensemble filter for high-dimensional systems. Journal of Geophysical Research, 108(D24), 8775.

Bishop, C. H., Etherton, B. J., & Majumdar, S. J. (2001). Adaptive sampling with the ensemble transform Kalman filter. Part I: Theoretical aspects. Monthly weather review, 129(3), 420-436.

Browne, P. A., & Van Leeuwen, P. J. (2015). Twin experiments with the equivalent weights particle filter and HadCM3. Quarterly Journal of the Royal Meteorological Society, 141(693), 3399-3414.

Burgers, G., van Leeuwen, P. J., & Evensen, G. (1998). Analysis scheme in the ensemble Kalman filter. Monthly weather review, 126(6), 1719-1724.

Courtier, P., Andersson, E., Heckley, W., Vasiljevic, D., Hamrud, M., Hollingsworth, A., Pailleux, J. (1998). The ECMWF implementation of three-dimensional variational assimilation (3D‐Var). I: Formulation. Quarterly Journal of the Royal Meteorological Society, 124(550), 1783-1807.

Ehrendorfer, M., & Tribbia, J. J. (1997). Optimal prediction of forecast error covariance through singular vectors. Journal of the Atmospheric Sciences, 52(2), 286-313.

Evensen, G. (1994). Sequential data assimilation with a nonlinear quasi‐geostrophic model using Monte Carlo methods to forecast error statistics. Journal of Geophysical Research: Oceans (1978–2012), 99(C5), 10143-10162.

Evensen, G. (1997). Advanced data assimilation for strongly nonlinear dynamics. Monthly Weather Review, 125(6), 1342-1354.

Evensen, G. (2003). The ensemble Kalman filter: Theoretical formulation and practical implementation. Ocean dynamics, 53(4), 343-367.

Frei, M., & Künsch, H. R. (2013). Bridging the ensemble Kalman and particle filters. Biometrika, 100(4), 781-800.

Gaspari, G., & Cohn, S. (1999). Construction of correlation functions in two and three dimensions. Quarterly Journal of the Royal Meteorological Society, 125(554), 723-757.

Gelb, A. (1974). Applied optimal estimation: MIT press.

Golub, G. H., & van Loan, C. F. (2012). Matrix computations (Vol. 3): JHU Press.

Gordon, N. J., Salmond, D. J., & Smith, A. F. (1993). Novel approach to nonlinear/non-Gaussian Bayesian state estimation. Paper presented at the IEE Proceedings F (Radar and Signal Processing).

Hamill, T. M. (2006). Ensemble-based atmospheric data assimilation. Predictability of Weather and Climate: Cambridge University Press.

Houtekamer, P. L., & Mitchell, H. L. (1998). Data assimilation using an ensemble Kalman filter technique. Monthly Weather Review, 126(3), 796-811.

Houtekamer, P. L., & Mitchell, H. L. (2001). A sequential ensemble Kalman filter for atmospheric data assimilation. Monthly Weather Review, 129(1), 123-137.

Houtekamer, P. L., Mitchell, H. L., Pellerin, G., Buehner, M., Charron, M., Spacek, L., & Hansen, B. (2005). Atmospheric data assimilation with an ensemble Kalman filter: Results with real observations. Monthly Weather Review, 133(3), 604-620.

Hunt, B. R., Kostelich, E. J., & Szunyogh, I. (2007). Efficient data assimilation for spatiotemporal chaos: A local ensemble transform Kalman filter. Physica D: Nonlinear Phenomena, 230(1), 112-126.

Ito, K., & Xiong, K. (2000). Gaussian filters for nonlinear filtering problems. IEEE T. Automat. Contr., 45(5), 910-927.

Julier, S. J., Uhlmann, J. K., & Durrant-Whyte, H. F. (1995). A new approach for filtering nonlinear systems. American Control Conference, Proceedings of, 3, 1628-1632.

Kalman, R. E. (1960). A new approach to linear filtering and prediction problems. Journal of basic Engineering, 82(1), 35-45.

Kalnay, E. (2003). Atmospheric modeling, data assimilation, and predictability: Cambridge university press.

Keppenne, C. L. (2000). Data assimilation into a primitive-equation model with a parallel ensemble kalman filter. Monthly weather review, 128, 1971-1981.

Klinker, E., Rabier, F., Kelly, G., & Mahfouf, J. F. (2000). The ECMWF operational implementation of four‐dimensional variational assimilation. III: Experimental

results and diagnostics with operational configuration. Quarterly Journal of the Royal Meteorological Society, 126(564), 1191-1215.

Le Dimet, F. X., & Talagrand, O. (1986). Variational algorithms for analysis and assimilation of meteorological observations: theoretical aspects. Tellus A, 38(2), 97-110.

Luo, X., & Moroz, I. M. (2009). Ensemble Kalman filter with the unscented transform. Physica D: Nonlinear Phenomena, 238(5), 549-562.

Luo, X., & Hoteit, I. (2014). Efficient particle filtering through residual nudging. Quarterly Journal of the Royal Meteorological Society, 140(679), 557-572.

Mahfouf, J. F., & Rabier, F. (2000). The ECMWF operational implementation of four‐dimensional variational assimilation. II: Experimental results with improved physics. Quarterly Journal of the Royal Meteorological Society, 126(564), 1171-1190.

Morzfeld, M., Tu, X., Atkins, E., & Chorin, A. J. (2012). A random map implementation of implicit filters. Journal of Computational Physics, 231(4), 2049-2066.

Papadakis, N., Mémin, E., Cuzol, A., & Gengembre, N. (2010). Data assimilation with the weighted ensemble Kalman filter. Tellus A, 62(5), 673-697.

Poterjoy, J. (2016). A localized particle filter for high-dimensional nonlinear systems. Monthly weather review, 144(1), 59-76.

Rabier, F., Järvinen, H., Klinker, E., Mahfouf, J. F., & Simmons, A. (2000). The ECMWF operational implementation of four‐dimensional variational assimilation. I: Experimental results with simplified physics. Quarterly Journal of the Royal Meteorological Society, 126(564), 1143-1170.

Snyder, C., Bengtsson, T., Bickel, P., & Anderson, J. (2008). Obstacles to high-dimensional particle filtering. Monthly Weather Review, 136(12), 4629-4640.

Talagrand, O. (1997). Assimilation of observations, an introduction. JOURNAL-METEOROLOGICAL SOCIETY OF JAPAN SERIES 2, 75, 81-99.

Tang, Y and J. Amabadan, 2009: Reply to comment on "Sigma-point Kalman Filters for the assimilation of strongly nonlinear systems". J. Atmos. Sci., Vol 66(11), 3501-3503

Tang, Y., J. Ambadan, D. Chen, 2014: A modification of Kalman Gain for Nonlinear measurement function in Ensemble-Kalman filter, Advance in Atmospheric Sciences, doi: 10.1007/s00376-013-3117

Tippett, M. K., Anderson, J. L., Bishop, C. H., Hamill, T. M., & Whitaker, J. S. (2003). Ensemble square root filters*. Monthly Weather Review, 131(7), 1485-1490.

Van Der Merwe, R. (2004). Sigma-point Kalman filters for probabilistic inference in dynamic state-space models. Oregon Health & Science University.

Van Der Merwe, R., & Wan, E. (2001). Efficient derivative-free kalman filters for online learning. Paper presented at the Proceedings of ESANN, Bruges.

Van Der Merwe, R., & Wan, E. (2001). The square-root unscented kalman filter for state and parameter estimation. Paper presented at the Proceedings of the International Conference on Acoustics, Speech, and Signal Processing, Salt Lake City, Utah.

van Leeuwen, P. J. (2009). Particle filtering in geophysical systems. Monthly Weather Review, 137(12), 4089-4114.

van Leeuwen, P. J. (2011). Efficient nonlinear data-assimilation in geophysical fluid dynamics. Computers & Fluids, 46(1), 52-58.

Wan, E., & Van Der Merwe, R. (2000). The unscented kalman filter for nonlinear estimation. Paper presented at the Adaptive Systems for Signal Processing, Communications, and Control Symposium 2000.

Whitaker, J. S., & Hamill, T. M. (2002). Ensemble data assimilation without perturbed observations. Monthly Weather Review, 130(7), 1913-1924.