Reply to comment on "Sigma-Point Kalman Filter Data Assimilation Methods for Strongly Nonlinear Systems"

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1. Introduction

Drs. Hamill et al. (2009, hereafter "H09") presented a critique of our recent work (Ambadan and Tang 2009, hereafter "AT09"). In their comment, two core points are that i) AT09 incorrectly stated the nature of measurement function; ii) AT09 should use more appropriate experimental designs, especially *a state-of-the art* EnKF as a reference benchmark in comparison with "Sigma-point" Kalman filter (SPKF)". While we thank Drs Hamill et. al for their constructive criticism, we would like to clarify the two issues.

2. Nature of measurement function in EnKF

For the purpose of presentation, we start from the standard EnKF formulation, as follows (Hamill 2006):

$$\mathbf{x}_{\mathrm{t}}^{\mathrm{a}} = \mathbf{x}_{\mathrm{t}}^{\mathrm{b}} + \mathbf{K}(\mathbf{y}_t - h(\mathbf{x}_{\mathrm{t}}^{\mathrm{b}})) \quad (1)$$

$$\mathbf{K} = \mathbf{P}_{\mathrm{t}}^{\mathrm{b}}\mathbf{H}^T(\mathbf{H}\mathbf{P}_{\mathrm{t}}^{\mathrm{b}}\mathbf{H}^T + \mathbf{R})^{-1} \quad (2)$$

$$\mathbf{P}_{\mathrm{t}}^{\mathrm{a}} = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}_{\mathrm{t}}^{\mathrm{b}} \quad (3)$$

where $\mathbf{P}_{\mathrm{t}}^{\mathrm{b}}$ is the forecast error covariance matrix; $\mathbf{x}_{\mathrm{t}}^{\mathrm{b}}$ represents the system state vector at step t; $\mathbf{R}$ is the observation error covariance matrix, and h is a nonlinear measurement function. $\mathbf{H}$ is the Jacobian matrix of h, i.e., the linearized measurement operator. The forecast error covariance matrix $\mathbf{P}_{\mathrm{t}}^{\mathrm{b}}$ at time step t is approximated using a finite set of model state ensemble (say M) given by,

$$\mathbf{P}^{\mathrm{b}} = \frac{1}{M-1}\sum_{i=1}^{M}(\mathbf{x}_i^b - \overline{\mathbf{x}^b})(\mathbf{x}_i^b - \overline{\mathbf{x}^b})^T \quad (4)$$

Apparently, the $\mathbf{H}$ used in Kalman gain (2) is a linearized operator, thus imposing the assumption of the linearization of nonlinear measurement function in the standard EnKF formulation. The linearization can be done either by analytical analysis like EKF (Extended Kalman Filter) or by ensemble members, as proposed by (Houtekamer and Mitchell 2001; Hamill 2006). The latter is often implicit and might not be very straightforward, deserving further analysis.

In Houtekamer and Mitchell (2001) and Hamill (2006), Kalman gain (2) was written by

$$\mathbf{P}^{\mathrm{b}}\mathbf{H}^T = \frac{1}{M}\sum_{i=1}^{M}(\mathbf{x}_i^b - \overline{\mathbf{x}^{\mathbf{b}}})(h(\mathbf{x}_i^b) - \overline{h(\mathbf{x}^{\mathbf{b}})})^T \tag{5}$$

$$\mathbf{HP}^{\mathrm{b}}\mathbf{H}^T = \frac{1}{M}\sum_{i=1}^{M}(h(\mathbf{x}_i^b) - \overline{h(x^b)})(h(\mathbf{x}_i^b) - \overline{h(\mathbf{x}^b)})^T \tag{6}$$

Where $\overline{h(\mathbf{x}^b)} = \frac{1}{M}\sum_{i=1}^{M} h(\mathbf{x}_i^b)$

(5) and (6) allow direct evaluation of the nonlinear measurement function *h* in calculating Kalman gain. Mathematically, (5) and (6) approximately hold if and only if

$$\overline{h(\mathbf{x}^b)} = h(\overline{\mathbf{x}^{\mathbf{b}}}) \tag{7}$$

$$\mathbf{x}_i^b - \overline{\mathbf{x}^b} = \boldsymbol{\varepsilon}_i, \quad \text{Norm}\,(\boldsymbol{\varepsilon}_{\mathrm{i}}) \text{ is small for i} = 1, 2\,..., \text{M} \tag{8}$$

Under the conditions of (7) and (8), (5) and (6) actually linearize the nonlinear measurement functions *h to* **H**. Therefore, direct application of the nonlinear measurement function in (5) and (6) in fact imposes an implicit linearization process using ensemble members.

For many realistic atmospheric and oceanic estimation problems, especially for model state estimation, (7) and (8) approximately hold since the nonlinearity of the measurement function *h* might not be strong and perturbation growth is relatively small. However in some cases where either condition is not held, (5) and (6) could cause large errors in estimating the Kalman gain. To demonstrate this, we now consider an example of a one-dimensional nonlinear model with a nonlinear measurement function, as shown below:

State-space model: $x_{k+1} = x_k^2 + q_k$ $q_k \sim N(0, Q)$

Measurement model $y_k = \sin(x_k) + r_k$ $r_k \sim N(0, R)$

At step k, we have an analysis of the model state, denoted by x_k^a. In the next assimilation cycle, the $\mathbf{P}^b\mathbf{H}^T$ and $\mathbf{HP}^b\mathbf{H}^T$ are required to calculate for the Kalman gain. Here we use two approaches: one is to directly calculate them since **H** is known and the other is to use (5) and (6). The ensemble is generated by perturbing x_k^a with random numbers drawn from a normal distribution with mean zero and variance 0.1. Initially x_k^a is arbitrarily set to 10, and ensemble size is 10000. A small perturbation and a large ensemble size will help obtain a relatively stable analysis.

Table 1: Comparison between LHS and RHS of (5) and (6)

x_k^a	Ensemble size	LHS of (5)	RHS of (5)	LHS of (6)	RHS of (6)
10	10000	3.62	0.48	3.22	0.49

As shown in Table 1, when the measurement function is a nonlinear sine function, (5) and (6) produce large errors. In other words, (5) and (6) hold only if the linearization conditions (7) and (8) are satisfied. The nonlinearity of the measurement functions may exist in some realistic problems, especially in the estimation of model parameters. In the EnKF framework, the parameter estimation is typically processed by defining the parameter as a special or specific system state. This makes the measurement function mapping the observation of real system states to the parameter space to be nonlinear.

Mathematically, a good solution for this issue is to re-formulize the Kalman Gain. As shown by Eq (9) in AT09, the Kalman gain can be expressed:

$$\mathbf{K} = \mathbf{P}_{x,\tilde{y}} \mathbf{P}_{\tilde{y}}^{-1} \qquad (9)$$

Here, $\tilde{y}$ is defined as the error between the noisy observation and its prediction given by $\tilde{\mathbf{y}} = \mathbf{y}_t - h(\mathbf{x}_t^b)$. (9) avoids the use of the Jacobian while retaining consistency and accuracy, which allows strong nonlinear measurement functions such as the parameter estimates of strongly nonlinear Lorenz 63 and Lorenz 96 models (Ambadan and Tang 2009b)

3. Reference benchmark used in comparison

The general focus of AT09 was to introduce the SPKFs to atmospheric assimilation community. The SPKF concepts were originally derived by Julier et al. 1995, and subsequently developed by many researchers as mentioned in AT09. The so called SPKF and its square-root variants were originated in the signal processing community. The SPKF is based on deterministic sampling approach whereas EnKF is based on random sampling of ensembles. The essential difference between SPKF and EnKF is the perturbation for generating ensemble and the formulation of Kalman gain. As an early introductory work, AT09 performed two basic SPKF filters: unscented Kalman filter and central difference Kalman filter. For the sake of comparison in the same line, we chose the standard EnKF, rather than some recently developed derivatives of EnKF such as the Local Ensemble Transform Kalman Filter (LETKF, Hunt et al. 2007) or Ensemble Square-Root Filters (EnSRF, Tippett et al 2003). It should be noted that the L63 experimental settings were very similar to those in Evensen (1997).

We agree with H09 that these *state-of-the-art* EnKFs can effectively improve the assimilation analysis. It is our motivation that the AT09 can bring SPKF to the attention of the atmospheric assimilation community, making further development and application of SPKF in the field of atmospheric assimilation. It might be more appropriate to compare a *state-of-the-art* EnKF, as mentioned in H09, with a similar SPKF, which is being pursued.

4. Conclusion

In current EnKF formulation, the measurement function is implicitly assumed to be linear or locally linearized. The direct application of nonlinear measurement operators in current EnKF formulation, as proposed in Houtekamer and Mitchell (2001) and Hamill (2006), is actually an implicit linearization through ensemble members. In some cases, the implicit linearization of nonlinear operators might lead to large errors of Kalman gain. An alternative treatment of nonlinear measurement function is to re-formulize Kalman gain used in SPKF as presented in AT09.

We agree with H09 that the *state-of-the-art* EnKFs can lead to better assimilation analysis than a standard EnKF used in AT09. However we think a parallel comparison between EnKF and SPKF in the same line, as performed in AT09, should be allowed. We expect a comparison between a *state-of-the-art* EnKF and *a state-of-the-art* SPKF in the near future.

5. References:

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