

Nonlinear Processes in Geophysics

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Title: On improving ensemble transform Kalman filter assimilation with nonlinear observational operator

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We thank the two anonymous reviewers for the very helpful and insightful comments that lead to significant improvement of the quality of this manuscript. We have tried our best to address all the comments. Below we use boldface to indicate the comments from the reviewers and the associate editor, and italics for our responses.

To reviewer 1

Recommendation: Accept subject to Minor Revision

The manuscript discusses two novel approximations to deal with nonlinear observation operators in the context of the ETKF. The problem has central relevance in geophysical data assimilation where Earth observations are often derived from nonlinear relation. The proposed approach leads to a new way to compute the inflation factor required to adjust the forecast error covariance matrix in most ensemble-based scheme. To the best of my knowledge the method introduced by the authors is new and it is well outlined in the context of state-of-the-art procedures against which it is compared numerically.

The manuscript is quite well written and relatively easy to follow; it is somehow long in the mathematical derivation but the authors have rightly cut the formalism into appendices in order to make the read of the main text easier.

My overall opinion is therefore positive and I think this study is worth to be published after minor modifications that I list below.

Response: *Thank you for your thorough review of our manuscript and we appreciate your encouraging comments.*

1. Page 545, line 19. Typos: Burgerss) Burgers

Response: *We have corrected this typo.*

2. Page 545, lines 22 - 25. It is unclear why the linear approximation on \mathcal{H} should affect the error covariance evolution and not just the analysis step.

Response: *This is partly due to that inflation on error covariance matrix plays an important role in error covariance evolution. All existing estimations of inflation factors are related to the observation operator. If the tangent-linear operator is used to approximate a strongly nonlinear observation operator, the inflation factor can be incorrectly estimated. That can affect the estimation of error covariance evolution.*

3. Page 548, lines 5 - 10. I suggest the authors to improve notation. In fact while the number in the brackets for the state vector is time, it is the observation in h . Furthermore h is an operator which is applied to the state vector and using the notation $h(1)$ is confusing.

Response: *The notation has been changed to $H_i = \{h_{1,i}, h_{2,i} \cdots, h_{p,i}\}^T$, $\mathbf{x}_i^t = \{X_{1,i}^t, X_{2,i}^t, \dots, X_{n,i}^t\}^T$ and $\mathbf{y}_i^o = \{y_{1,i}^o, y_{2,i}^o, \dots, y_{p,i}^o\}^T$.*

4. Page 554, lines 20 - 24. Along with model error, other factors may affect the consistency between F-RMSE and F-Spread, namely the nonlinearities and the sampling error. The authors mention them later in the text; I suggest them to do it at this point too.

Response: *Thanks for the comment. In the last paragraph of section 2.3, we have added the sentence “Beside model error, the nonlinearities and the sampling error may also affect the consistency between F-RMSE and F-Spread as it is discussed later in this paper.”.*

5. Page 556, Eq. (32). The authors state the observations are spatially correlated.

From Eq. (32) this is not clear, since the observation at point k , only depends on the state vector at the same point. Does the spatial correlation of the observation error come from the state vector in (32) ?. Please clarify.

Response: *The spatial correlation of the observation errors come from Eq. (33).*

6. Page 557, line 4. I suggest the authors to include also the main equation characterizing the ETKF for consistency with the other listed methods. These equations should be Eq. (12) and (13) I guess.

Response: *Following this comment, the expression for ETKF is modified to “Traditional ETKF in linear approximation (Eq. (12)) and optimization (Eq. (10))”.*

7. Page 557, lines 4 - 9. The comparison would be more self-consistent if an algorithm having SS in the inflation and nonlinear in the optimization would be at hand. I suggest the authors to either add such an algorithm among those under comparison or at least discussing it in the text.

Response: *Following this comment, we investigated the second-order approximation method for estimating inflation factors while using the nonlinear optimization scheme. The corresponding A-RMSE is 2.20 for the forcing parameter $F=12$ and parameter of observation operator $\alpha=0.1$, which is larger than that of method TN and smaller than that of method NN. We have added this discussion in the fourth paragraph of section 4.1 in the revised version.*

8. Figure 1 and 2. Please improve the quality of the figures by using colors or thicker lines. Also, I strongly suggest the authors to include a similar figure showing A-RMSE for the algorithms under comparison as a function of α . This will further fortify the result in Fig. 2 and the overall results in general.

Response: *Thanks for your suggestion. We have used colors in Figure1 and thicker lines in Figure 2. Also, A-RMSE as a function of α for the different schemes is shown in the Figure 1(b) of the revised version. It shows that all the schemes have the same A-RMSE with $\alpha=0$ (i.e. the observation operator is linear), indicating that*

there is no difference among them. For each scheme, the A-RMSE increases as the parameter α increases from 0 to 0.1. The magnitude relation of all schemes is basically consistent with that in Figure 1(a). The larger the parameter α is, the bigger difference the different schemes have.

9. Page 557, lines 23 - 28. The authors should include some hints on the physical interpretation of L in terms of the state-estimation accuracy. This will help to fully interpret the results in Table 1.

Response: *The interpretation “The function represents the second-order distance of the squared innovation statistic ($\mathbf{d}_i \mathbf{d}_i^T$) to its expectation. Generally speaking, for a more accurate assimilation scheme, the realization of $\mathbf{d}_i \mathbf{d}_i^T$ should be closer to its expectation and therefore the value of the objective function should be smaller.” is added in the corresponding paragraph.*

10. Page 558, lines 1 - 2. It is not strictly true that a smaller error corresponds to a smaller value of the objective function L: see SS.

Response: *We have changed the expression to “In the majority of the cases”.*

11. Page 560, line 6. I would change”... may be more appropriate ...” into”... may also be appropriate ...”. Moreover inflation of the background is also useful when the system is highly chaotic and the ensemble size too small. Multiplicative inflation of the background in fact does not change the range of the matrix which can be desirable if the ensemble members have correctly catch the dynamics instabilities.

Response: *Thanks for your suggestion. We have changed the expression.*

12. Page 560, lines 9 - 12. I understand that everything is based on the equality: $\langle \mathbf{d} \mathbf{d}^T \rangle = \mathbf{H} \mathbf{P} \mathbf{H}^T + \mathbf{R}$, where \mathbf{d} is the innovation vector, \mathbf{P} the forecast error covariance matrix and $\langle . \rangle$ the expectation operator. If my understanding is

correct, I suggest the authors to include this in the text. A good place might be when the objective function is introduced.

Response: *In the cases of nonlinear observation operator, the mean value of $\mathbf{d}_i \mathbf{d}_i^T$ is*

$$E(\mathbf{d}_i \mathbf{d}_i^T) = E \left[\left(\mathbf{R}_i^{-1/2} (\mathbf{y}_i^o - H_i(\mathbf{x}_i^t)) + \mathbf{R}_i^{-1/2} (H_i(\mathbf{x}_i^t) - H_i(\mathbf{x}_i^f)) \right) \left(\mathbf{R}_i^{-1/2} (\mathbf{y}_i^o - H_i(\mathbf{x}_i^t)) + \mathbf{R}_i^{-1/2} (H_i(\mathbf{x}_i^t) - H_i(\mathbf{x}_i^f)) \right)^T \right]. \quad (\text{A2})$$

Especially, if the observation operator is a linear matrix (\mathbf{H}_i), Eq. (A2) can be simplified to

$$E(\mathbf{d}_i \mathbf{d}_i^T) = \mathbf{R}_i^{-1/2} \mathbf{H}_i \mathbf{P} \mathbf{H}_i^T \mathbf{R}_i^{-1/2} + \mathbf{I}, \quad (\text{A3})$$

where \mathbf{I} is the $p_i \times p_i$ identity matrix. We have added this in Appendix A in the revised version.

13. Page 561, lines 1 - 8. This paragraph is important but not clearly written.

Please rephrase the description of the experiments with a fixed-tuned inflation.

Response: *Following this comment, the paragraph is modified to “In many practical experiments, the inflation factor is constant in time and is chosen by trial and error to give the assimilation with the most favourable statistics (e.g. Anderson and Anderson 1999). For testing the fixed-tuned inflation method, suppose $\mathbf{x}_i^a(\lambda)$ and $\mathbf{x}_i^f(\lambda)$ are the analysis state and forecast state using time invariant inflation factor λ . Then the*

statistics $\sum_{i=1}^N \sqrt{\frac{1}{p_i} \|\mathbf{y}_i^o - H_i(\mathbf{x}_i^a(\lambda))\|^2}$ and $\sum_{i=1}^N \sqrt{\frac{1}{p_i} \|\mathbf{y}_i^o - H_i(\mathbf{x}_i^f(\lambda))\|^2}$ are minimized to tune the λ

respectively. When Eq (10) is minimized to estimate the weights of perturbed analysis states, the corresponding A-RMSEs of the two fixed-tuned methods are estimated as 2.97 and 2.85 respectively which are larger than that of method SS (2.29). The ratios of F-RMSE to F-Spread are estimated as 3.14 and 3.45 respectively which are also larger than 1.80 of method SS (see Table 2). All these facts indicate than the empirical estimation method for the inflation factor is not as good as method SS.”

14. Page 578, Table 1. I suggest the authors to include the ratio between F-RMSE

over A-RMSE. This will help quantifying the relative improvement gained at the analysis and the average error growth during the forecast. For instance, these ratios would reveal the large error reduction obtained by TN at the analysis.

Response: *Thanks for your suggestion. We have added the ratios between F-RMSEs over A-RMSEs to Table1, which can be considered as a measurement of the improvement gained at the analysis step. All the ratios are larger than 1, which indicate that the analysis state is better than the forecast state. Among all methods, the ratio is largest for the method TN, which indicates the largest error reduction at the analysis step.*

To reviewer 2

General comments

This paper addresses some issues associated with Ensemble Transform Kalman Filter (ETKF) in applications to nonlinear observation operators. In particular, the paper proposes the use of second-order Taylor expansion in approximation of nonlinear observation operator to improve error covariance inflation in ETKF. The proposed methodology is applied to the Lorenz 40-variable model.

Overall, the paper clearly describes the improvements and demonstrates the benefit of introducing the second order information. Most of the mathematical description is focused on the improvements of the error covariance inflation methodology for the ETKF.

Response: *Thank you for your thorough review of our manuscript and we appreciate your encouraging comments.*

Specific comments

1) Introduction: Although the title of the paper indicates it is focusing on the ETKF applications and improvements, it would be beneficial to describe the treatment of nonlinearity in general ensemble data assimilation outside of ETKF, including the Maximum Likelihood Ensemble Filter (Zupanski 2005) and the particle filters (van Leeuwen 2009).

Response: *Following this comment, we have added the following sentences in the third paragraph of the introduction: “In general ensemble data assimilation, Maximum Likelihood Ensemble Filter (MLEF) minimizes a cost function that depends on a general nonlinear observation operator to estimate the state vector, which is equivalent to maximize the likelihood of the posterior probability distribution (Zupanski, 2005). Particle filter uses a set of weighted random samples (particles) to approximate the posterior probability distribution that may depend on a nonlinear observation operator (Leeuwen, 2009).”*

Also, the proposed methodology implicitly assumes the use of incremental minimization

(e.g. a form of truncated Newton method), with outer and inner loops. This should be clearly stated, since this is only one possible approach to iterative minimization, with many more efficient methods available in mathematical optimization and control theory.

Response: *Following this comment, the sentences “It is worthwhile to point out that the proposed methodology implicitly assumes the use of incremental minimization with outer and inner loops. There may be other efficient methods available in mathematical optimization and control theory.” are added in the six paragraph of the introduction.*

2) Impact of higher order nonlinear Taylor approximation: The utility of the nonlinear difference between observation operators (e.g., Eq.(7)) is not adequately presented. For general nonlinear or even non-smooth radiative transfer operators (Steward et al. 2012), the utility of higher-order elements in Taylor expansion may be questionable. Also, the development of the second order term may be time consuming and difficult in case of complex observation operators, and this aspect should also be discussed. I believe that the paper would benefit if these issues are also addressed in discussion.

Response: *Thanks for the valuable comments. In the revised version, we discussed these caveats in the third paragraph of section 4.3.*

3) Realistic applications: Since the ultimate goal of data assimilation is to be applied with realistic high-dimensional systems and observations, the conclusion should include some discussion of the outlooks into the applicability of the proposed improvements of ETKF in realistic situations.

Response: *The following sentences are added in the conclusion section “The proposed method is computationally feasible to assimilate satellite observations with radiative transfer models as the nonlinear observation operators (see Appendix E) which are broadly used in atmospheric, ocean and land data assimilations.”*

References:

van Leeuwen, P. J., 2009: Particle Filtering in Geophysical Systems. *Mon. Wea. Rev.*, 137, 4089–4114.

Steward, J. L., I. M. Navon, M. Zupanski, and N. Karmita, 2012: Impact of Non-Smooth Observation Operators on Variational and Sequential Data Assimilation for a Limited-Area Shallow-Water Equation Model. *Quart. J. Roy. Meteorol. Soc.*, 138, 323-339.

Zupanski, M., 2005: Maximum Likelihood Ensemble Filter: Theoretical Aspects. *Mon. Wea. Rev.*, 133, 1710–1726.

Response: *These references are added in the revised version.*

Technical corrections

4) Abstract, line 8: **This statement is not correct. Iterative minimization with advanced Hessian preconditioning would require very few minimization iterations (1-2).**

Response: *In the revised version, the sentence is changed to “One problem in the minimization of a nonlinear objective function similar to 4D-Var is that the nonlinear operator and its tangent-linear operator have to be iteratively calculated if the Hessian is not preconditioned or the Hessian has to be calculated several times. This may be computationally expensive.”*

5) Introduction, p.544, L.24: **“... satellite radiance data : : :”**

Response: Comment is followed.

6) Introduction, p.546, L.3-5: **Not clear what the sentence wants to say. Given that degrees of freedom of the ensemble forecast error covariance are governed by the number of ensembles, it is only natural to define the minimization space in the ensemble domain. The way to deal with insufficient degrees of freedom is to consider hybrid variational-ensemble error covariance, which is outside of the paper’s considerations.**

Response: *Following this comment, the sentence is deleted in the revised version.*

7) Introduction, p.547, L.7-10: **Linearization typically doubles the number of operations, and thus increases the computational cost (e.g. $\text{del}(x*y)=x*\text{del}(y)+y*\text{del}(x)$). This should also be taken into account when discussing the cost.**

Response: *The computational cost is discussed in Appendix E. In the revised version, the paragraph “On the other hand, computing the first and second derivatives requires additional number of operations, but it is manageable.” is added in the end of Appendix E.*

8) Section 2.2.2: Mathematical derivation should be followed by a brief verbal description of the meaning and implications of equations, as this is the main novelty of this paper.

Response: *We have added more descriptions of the mathematical derivation in section 2.2.2.*

9) p. 562, L.13: Although it is true that most observation operators are localized, there are some that are not. How would this impact the computation of the second order term?

Response: *In the revised version, we discussed these problems in the fourth paragraph of section 4.2 as follows “For the observation operators which are not localized, the computation of the second-order term may be complex.”*