The author gratefully acknowledges the anonymous reviewer for his/her insightful comments and thorough corrections that lead to the significant improvement of the quality of this manuscript. The author has checked the manuscript carefully and tried the best to address all the comments. Below, the italic is used for quoting the comments from the reviewer and following with the point-by-point responses.

#### General comments:

This paper introduces a new technique for estimating the covariance inflation factor needed to help mitigate the problem of filter divergence often encountered when using EnKF data assimilation methods. Their approach is novel in the sense that computes these estimates by minimizing an objective function based on the concept of generalized cross validation, a technique commonly used in the machine learning literature. There is considerable overlap between the fields of data assimilation and machine learning and I appreciate that the author is trying to bridge the gap between these two fields. In my opinion, there is much that we can learn from one another.

**Response:** Thank you for your review and comments.

However, the paper falls short of offering good comparisons for their new technique. Rather, it is more a proof-of-concept that this technique works better than the basic EnKF, which is known not to work well without inflation. There are a few additional questions that I would like to see answered:

1. How does it depend on the ensemble size and the number of observations?

**Response:** Thank you for your comment. Intuitively, for any ensemble based assimilation scheme, large ensemble size will lead to small analysis error but with expensive computational cost in the practical problems. The ensemble size in the practical land surface assimilation problem is usually several tens (Kirchgessner et al. 2014). The preferences of the proposed inflation method with respect to different ensemble size (10, 30 and 50) are evaluated and the results are listed in Table 1. It shows that, using a 10-member ensemble increases the analysis RMSE to about triple while using a 50-member ensemble reduces the analysis RMSE by 20%, relative to that using a

30-member ensemble. The forecast ensemble spread increase slightly form 10-member ensemble to 50-member ensemble. The GAI and GCV function values change sharply form 10-member ensemble to 30-member ensemble while become relatively stable from 30-member ensemble to 50-member ensemble. Ensembles less than 10 became unstable and no significant changes occurred for ensembles more than 50. Considering the computation cost in practical problems, a 30-member ensemble can be necessary to estimate statistically robust results.

To evaluate the preferences of the inflation method with respect to different number of observations, synthetic observations are generated at every other grid points and every 4 time steps. Hence, there are totally 20 observations at each observation step in this case. The assimilation results with ensemble size 10, 30 and 50 are listed in Table 2. It shows that, the GAI values are larger than those with 40-observation in all assimilation schemes. This may due to that, the denominator of the GAI statistic (Eq. (16)) is relative small in the 20-observation experiments. The forecast ensemble spread does not change much, while the GCV function and the RMSE values increase largely in the 20-observation experiments with respect to those in the 40-observation experiments illustrating that more observations will lead to less analysis error.

These are added in the revised version as section 3.3 (Influence of ensemble size and observation number).

### 2. How does it compare with other the inflation schemes mentioned? What are the computational tradeoffs?

**Response:** The comparisons with the constant inflated EnKF are added in the revised version, also following the second reviewer. The constant is particularly selected as the median of the estimated inflation factor by minimizing the GCV function. Besides small fluctuation, the mean GAI value of the constant inflated EnKF is 27.80%, which is smaller than that of the improved EnKF. The mean spread value of improved EnKF is 3.32, which is slightly larger than that of the constant inflated EnKF (3.25). It illustrates that the underestimation of forecast ensemble spread can be effectively compensated for the two EnKF schemes with forecast error inflation, while the improved EnKF is more effective than the constant inflated EnKF. The analysis RMSE, as well as the values of

the GCV functions, decrease sharply no matter which inflation scheme is adopted. However, the GCV function and the RMSE values of the improved EnKF are smaller than those of the constant inflated EnKF, indicating that the on-line estimate method performs better than the simple multiplicative inflation techniques with a constant.

For the aspect of computational cost in minimizing the GCV function, the most expensive part is in computing the influence matrix  $\mathbf{A}_i(\lambda)$ . Since the matrix multiplication is commutative for the trace, the GCV function can be easily re-expressed as

$$GCV_{i}(\lambda) = \frac{p_{i}\mathbf{d}_{i}^{\mathrm{T}}\left(\mathbf{H}_{i}\lambda\mathbf{P}_{i}\mathbf{H}_{i}^{\mathrm{T}}+\mathbf{R}_{i}\right)^{-1}\mathbf{R}_{i}\left(\mathbf{H}_{i}\lambda\mathbf{P}_{i}\mathbf{H}_{i}^{\mathrm{T}}+\mathbf{R}_{i}\right)^{-1}\mathbf{d}_{i}}{\left[\mathrm{Tr}\left(\left(\mathbf{H}_{i}\lambda\mathbf{P}_{i}\mathbf{H}_{i}^{\mathrm{T}}+\mathbf{R}_{i}\right)^{-1}\mathbf{R}_{i}\right)\right]^{2}}$$
(1)

Since both of the numerator and denominator of the GCV function are scalars, the inverse matrix is only needed in  $(\mathbf{H}_i \lambda \mathbf{P}_i \mathbf{H}_i^{\mathrm{T}} + \mathbf{R}_i)^{-1}$ , which can be effectively calculated using the Sherman–Morrison–Woodbury formula (Golub; Loan 1996). Furthermore, the calculation of the inverse matrix and the multiplication are also indispensable for the conventional EnKF (Eq. (6)). There is no additional computation burden for the improved EnKF by minimizing the GCV function essentially. Therefore, the total computation of the improved EnKF is feasible.

#### 3. What does the time series of the inflation factor look like? Is it smooth?

**Response:** The time series of estimated inflation factors are shown in Figure 2 in the revised version, which vary between 1 and 6 with greatly majority. The median is 1.88, which is used in the comparison of the improved EnKF and the simple multiplicative inflation techniques like setting a constant inflation factor. This has been added to section 3.2 in the revised version.



Figure 2. The time series of estimated inflation factors by minimizing GCV function.

### 4. Does it prevent the problem of ensemble divergence?

**Response:** The ensemble analysis state members of the conventional EnKF, improved EnKF and constant inflated EnKF are shown in Figure 7, which indicates the uncertainty of the analysis state to some extent. The true trajectory obtained by numerical solution is also plotted. It illustrates that, there is a larger difference between the true trajectory and the ensemble analysis state members for the conventional EnKF than those for the improved EnKF and constant inflated EnKF. In additional, the analysis state is more consistent with the true trajectory for the improved EnKF than that for the constant inflated EnKF. Therefore, the forecast error inflation can lead more accurate analysis state than the constant inflated EnKF.



Figure 7. The ensemble analysis state members of the conventional EnKF (black line), the improved EnKF (blue line) and the constant inflated EnKF (red line). The green line refers to the true trajectory obtained by numerical solution.

I understand that some of these questions fall under the future work category. But I do think it should be explicitly stated that this paper is intended just to show proof-of-concept, and that a more thorough comparison will be forthcoming in the near future.

**Response:** Thank you for your comment. Some comparisons of these questions have been added in the revised version. The more thorough comparison and application will be conducted in the near future studies.

The paper also needs considerable grammatical revision. In my following comments, I have tried to be as explicit as possible in offering suggestions.

**Response:** Thank you for your comment. The grammars have been checked carefully and the language has been polished in the revised version.

#### Specific comments:

#### 1. P3 L3-13:

The author implicitly assumes the existence of a 'true' underlying state of the system. While this assumption is common, it is still an assumption. Also, be careful about saying: "are more close to the true state than either of them..." and "can be technically easily obtained by minimizing a cost function...". The former is not necessarily true, the latter depends on what you mean by 'easy'. While it is easy enough to run an optimization algorithm to minimize the cost function, you have no guarantees that the solution is unique when the models are nonlinear. Finding the most appropriate analysis state (i.e the global minimum) is a much more difficult problem.

**Response:** Thank you for your comments. It is true that the existence of a "true" state is a common assumption and finding the global minimum is a very difficult problem. This paragraph has been written as follows:

For a state variable in the geophysical research fields, the common assumption is the existence of a "true" underlying state of the system. Data assimilation is a powerful mechanism to estimate the true trajectory, based on the effective combination of the dynamical forecast system (such as a numerical model) and the observations (Miller et al.

1994). The result of data assimilation is an analysis state, which is usually a better estimate of the state variable with fully considering all of the information provided by the model forecasts and observations. Actually, the analysis state can be generally treated as the weighted average of the model forecasts and observations, while the weights are approximately proportional to the inverse of the corresponding covariance matrices (Talagrand 1997). Therefore, the performance of a data assimilation method significantly relies on whether the error covariance matrices are estimated accurately. If this is the case, it can be attributed to a fairly technical aspect and can be accomplished with the fast development of supercomputers (Reichle 2008), although finding the global minimum is a much difficult problem when the models are nonlinear.

## 2. *P5 L1*: Would leave-one-out cross validation be applicable to data assimilation, where the data is a time-series?

**Response:** Since EnKF is a sequential assimilation method, the observations at current step (40-dimensioal vector in the experiments of this manuscript) are assimilated to the forecast model for a given assimilation step. Therefore the cross validation could also be applicable.

3. P5 L4-16: Why is Generalized Cross Validation better? What makes it generalized? What are these "favorable properties" of "consistency of the relative loss"? I understand it has not been used much in data assimilation, but I think this should be more explicitly motivated, as it is the core method of this article.

**Response:** The Cross Validation is a general procedure that can be applied to estimate tuning parameters in a wide variety of problems, which aims at minimizing the estimated error at the observation grid point. This criterion has been widely used in the linear regression and smoothing spline fields (Allen 1974; Gu; Wahba 1991; Wahba; Wold. 1975; Wahba et al. 1995). For the problem of estimating the inflation factor in this study, the objective function based on Cross Validation principle is (the detailed derivation is listed in Appendix A)

$$V_{i}(\lambda) = \frac{1}{p_{i}} \sum_{k=1}^{p_{i}} \frac{\left(\tilde{\mathbf{y}}_{i,k}^{o} - \left(\mathbf{R}_{i}^{-1/2}\mathbf{H}_{i}\mathbf{x}_{i}^{a}\right)_{k}\right)^{2}}{\left(1 - a_{k,k}\right)^{2}}$$
(2)

where  $a_{k,k}$  is the element at the site pair (k, k) of the influence matrix  $\mathbf{A}_i(\lambda)$ . Substituting  $a_{k,k}$  by the average  $\frac{1}{p_i} \sum_{k=1}^{p_i} a_{k,k} = \frac{1}{p_i} \operatorname{Tr}(\mathbf{A}_i(\lambda))$  can get the following objective function of Generalized Cross Validation

$$GCV_{i}(\lambda) = \frac{\frac{1}{p_{i}} \mathbf{d}_{i}^{\mathrm{T}} \mathbf{R}_{i}^{-1/2} \left( \mathbf{I}_{p_{i}} - \mathbf{A}_{i}(\lambda) \right)^{2} \mathbf{R}_{i}^{-1/2} \mathbf{d}_{i}}{\left[ \frac{1}{p_{i}} \mathrm{Tr} \left( \mathbf{I}_{p_{i}} - \mathbf{A}_{i}(\lambda) \right) \right]^{2}}$$
(3)

It is easy to see that the GCV criterion is a weighted version. Originally proposed to reduce the computational burden, GCV is one of a number of criteria which all involve an adjustment to the average mean-squared-error over the training set (Craven; Wahba 1979).

4. P5 L17-19: I don't understand these statements. What does it mean to be "inflated properly"? How does it "reassign the weights"? The segway to analysis sensitivity does not follow logically to me.

**Response:** Since the analysis state can be treated as the weighted average of model forecasts and observations, the weight approximately proportional to the inverse of the corresponding error covariance matrix. In the covariance inflation scheme, the forecast error matrix is multiplied by an appropriate inflation factor. Usually the inflation factor is larger than 1. Too small or too large inflation factor will cause the analysis state still over relies on model forecasts or observations. Therefore the inflation factor should be estimated accurately. This is what means "inflated properly" in the manuscript.

Once the inflation factor is estimated appropriately, the forecast error covariance matrix will be improved in the EnKF with inflation scheme. Then the weights of model forecasts and observations in the analysis state will be adjusted. This is what means "reassign the weights".

These explanations have been written in the revised version.

# 5. P9 L9: Please specifically state how you actually compute lambda\_i. I assume you minimize the GCV as an objective function?

**Response:** Yes, this has been specifically stated in the revised version.

## 6. P10: If S^f=I-S^o=I-A\_i, then can't the GCV\_i function be interpreted as minimizing the normalized forecast sensitivity?

**Response:** The GCV function can be interpreted like this, because the aim of inflation scheme is increasing the observation weight appropriately. Since the sensitivities of analysis state to the model forecasts and observations are complementary, it will decrease the normalized forecast sensitivity.

This has been added to the revised version.

#### 7. P14 L2: Any motivation for setting the ensemble size at 30?

**Response:** The ensemble size in the practical land surface assimilation problem is usually several tens (Kirchgessner et al. 2014). Too large ensemble size will significantly increase the computational cost. Therefore the ensemble size in this study in selected as 30 to evaluate the performance of the assimilation method, which will be applied in the practical problem in the future.

The explanation has been added in the revised version. Also following your general comment 1, the inflation scheme with different ensemble size (10, 30 and 50) is investigated. Please see the response to the general comment 1.

# 8. P14 L15: Are there other examples in the literature to compare this correlation coefficient to? Should ideally it be as close to 1 as possible?

**Response:** There some comparisons between the analysis RMSE and the objective function, such as (Liang et al. 2012; Zheng 2009). This correlation coefficient is an indicator that can show whether the choice of the objective function is appropriate. In the ideal case, it is as close to 1 as possible.

9. P15 L22: Can you be more precise than this: "seems to be a good objective function"?

**Response:** The sentence has been changed to "The assimilation results show that, inflating the conventional EnKF using the factor estimated by minimizing the GCV function can indeed reduce the analysis RMSE".

#### **Technical corrections:**

1. Title: An estimate of **the** inflation factor and analysis sensitivity in **the** ensemble Kalman filter

**Response:** The correction has been followed.

### 2. P2 L7: Why does it "need" to be inflated? What happens otherwise?

**Response:** Otherwise the sampling covariance matrix of perturbed forecast states will underestimate the true forecast error covariance matrix, due to the limited ensemble size and large model error. This can eventually result in the divergence of the filter.

This has been added to the abstract of the revised version.

3. P2 L10: I would say the method is "tested" not "validated". Validation to me implies a more thorough comparison.

My suggestion for the abstract:

The Ensemble Kalman Filter is a widely used ensemble based assimilation method, which estimates the forecast error covariance matrix using a Monte Carlo approach that involves an ensemble of short-term forecasts. While the accuracy of the forecast error covariance matrix is crucial for achieving accurate forecasts, the estimate given by the EnKF needs to be improved using inflation techniques. Otherwise...?

In this study, the forecast error covariance inflation factor is estimated using a generalized cross-validation technique. The improved EnKF assimilation scheme is tested with the atmosphere-like Lorenz-96 model with spatially correlated observations, and is shown to reduce both the analysis error and its sensitivity to the observations.

**Response:** Thank you for your suggestion. The abstract of the revised version has been rewritten as follows:

The Ensemble Kalman Filter is a widely used ensemble based assimilation method,

which estimates the forecast error covariance matrix using a Monte Carlo approach that involves an ensemble of short-term forecasts. While the accuracy of the forecast error covariance matrix is crucial for achieving accurate forecasts, the estimate given by the EnKF needs to be improved using inflation techniques. Otherwise the sampling covariance matrix of perturbed forecast states will underestimate the true forecast error covariance matrix, due to the limited ensemble size and large model error. This can eventually result in the divergence of the filter.

In this study, the forecast error covariance inflation factor is estimated using a generalized cross-validation technique. The improved EnKF assimilation scheme is tested with the atmosphere-like Lorenz-96 model with spatially correlated observations, and is shown to reduce both the analysis error and its sensitivity to the observations.

### 4. P3 L3-13: This paragraph needs some revision. See scientific comment 1 above.

**Response:** This paragraph has been written in the revised version. Please see the "Response" to the scientific comment 1 above.

5. P4 L1: What does it mean "gradually important"? I also think this needs a more motivation about what why inflation is used. Assume the reader has never used an EnKF before.

**Response:** It means researchers realize that, the covariance inflation is becoming more and more important. The following texts have been added in the revised version.

Covariance inflation, as a technique used to mitigate filter divergence by inflating the empirical covariance in EnKF, can increase the weight of the observation in the analysis state (Xu et al. 2013). Actually, it will perturb the subspace spanned by the ensemble vectors and better capture the sub-growing directions that may be missed in the original ensemble (Yang et al. 2015).

6. P4 L1-15: Past tense seems more appropriate here: "tune" > tuned, "select" > selected.

**Response:** The words have been changed.

#### 7. P4 L5: However, such methods are very empirical and subjective.

**Response:** The correction has been followed.

### 8. P4 L8: How does moment estimation "facilitate the calculation"?

**Response:** The moment estimation just obtains the estimated inflation factor by solving an equation of the innovation statistic and its realization. It does not need expensive calculation such as the determinant of high dimensional matrix in the maximum likelihood estimation. Therefore the moment estimation can facilitate the calculation.

9. P4 L10: "obtain a better estimate of the inflation factor, but..."

**Response:** The correction has been followed.

10. P4 L16: The idea of cross validation was first introduced in linear regression and spline smoothing.

**Response:** The correction has been followed.

11. P4 L20: In cross validation, the data is divided into subsets, some of which are used for modeling and analysis while others are used for verification and validation.Response: Thank you for your suggestion. The correction has been followed.

*12. P5 L21: "sources"* 

**Response:** The word has been changed.

13. P5 L22: Replace "The quantity can be introduced..." with: "In the context of statistical data assimilation, this quantity describes the sensitivity of the analysis to the observations, which is complementary..."

**Response:** Thank you for your suggestion. The sentence has been replaced.

14. P6 L3: This study focuses on methodology that can be potentially applied to geophysical applications of data assimilation in the near future.

**Response:** The correction has been followed.

15. P6 L14: dynamical forecast model

**Response:** The correction has been followed.

*16. P7 L4: series of analysis states***Response:** The word has been corrected.

17. P8 L16: "The multiplicative inflation"Response: "The" has been deleted.

18. P8 L18: by estimating the inflation factors \lambda\_iResponse: The correction has been followed.

19. P9 L16: In the EnKF, "can be treated" > isResponse: The correction has been followed.

20. P9 L17: and forecast. That is,Response: The correction has been followed.

21. P10 L14: detailed proofResponse: The word has been corrected.

22. P10 L14-15: Why quotes? Should there be a reference?**Response:** Yes, the references (Gu 2002; Pena; Yohai 1991) have been added.

23. P10 L15: "degrees of freedom for the signal"Response: The correction has been followed.

24. P10 L16: Reference for its interpretation as "amount of information"? Is this heuristic or in an information theoretic sense?

Response: The phrase "amount of information" is in an information theoretic sense. The

reference (Ellison et al. 2009) has been added.

25. P11 L5: ... states usually underestimate the true forecast...Response: The correction has been followed.

26. P11 L6-10: This will cause the analysis to over rely on the forecast state, excluding useful information from the observations. This is captured by the fact that for the conventional EnKF scheme the GAI values are rather small. Adjusting the inflation of the forecast error covariance matrix alleviates this problem to some extent, as will be shown in the following simulations.

**Response:** Thank you for your suggestion. The correction has been followed.

27. P11 L22: I would say Numerical ExperimentsResponse: The correction has been followed.

28. P12 L2: validated > testedResponse: The word has been changed.

29. P12 L4: performancesResponse: The word has been changed.

30. P12 L12: Cyclic boundary conditionsResponse: The correction has been followed.

31. P12 L13: to beResponse: The words have been deleted.

32. P12 L15: are analogous toResponse: The correction has been followed.

33. P12 L18: performances

**Response:** The word has been changed.

34. P12 L20: The time step for generating the numerical solution is set at 0.05 non-dimensional units, which is roughly...

**Response:** The correction has been followed.

*35. P13 L1: I would maybe move this sentence up, before you discuss the time step.* **Response:** The sentence has been moved to the front of this paragraph.

36. P13 L10: correlate, which is common in applications involving remote sensing and radiance data.

**Response:** The correction has been followed.

37. P13 L20-22: Modifying the forcing strength F changes the model forecast considerably. For values of F larger than 3 the system is chaotic. To simulate model error, the forcing term for the forecast is set to 7, while using F=8 to generate the 'true' state.

**Response:** Thank you for your suggestion. The correction has been followed.

38. P14 L5-7: The increase in GAI from 10% for the conventional EnKF to 30% for the EnKF with forecast error inflation indicates that the latter relies more on the observations. This is important because...

**Response:** Following your correction, the sentences have been rewritten as follows: The increase in GAI from 10% for the conventional EnKF to 30% for the EnKF with forecast error inflation indicates that the latter relies more on the observations. This is important because the observation can play a more significant role in combining it with the model forecast to generate the analysis state.

39. P14 L8: To evaluate the resulting estimate, ...

**Response:** The correction has been followed.

40. P14 L10-11. ... values of the GCV functions decrease sharply ... right?Response: Yes. The typo has been corrected.

41. P14 L12: I don't understand this statement. Did you mean to say "The variance of the analysis"?

Response: The mean in the manuscript is "The variability of the analysis".

42. P14 L15: ... which indicates that the GCV function is a good criterion to estimate the inflation factor.

**Response:** The correction has been followed.

43. P15 L3-6: Accurate estimates of the forecast error covariance matrix are crucial to the success of any data assimilation scheme. In the conventional EnKF ... Response: The correction has been followed.

44. P15 L7-8: But limited ensemble size and large model error often cause it to be underestimated. This produces an analysis state that over relies on the forecast and excludes the observations, which can eventually cause the filter to diverge. **Response:** The correction has been followed.

45. P15 L10: Begin new paragraph with this sentence. The use of multiplicative covariance inflation techniques can mitigate this problem to some extent. Several methods have been proposed in the literature, each with different assumptions. For instance, the moment...

**Response:** Thank you for your suggestion. The correction has been followed.

46. P15 L16: ... but requires computing high dimensional matrix determinants.Response: The correction has been followed.

47. P15 L18: but is limited to spatially independent ...Response: The correction has been followed.

#### 48. P15 L19: is estimated using generalized cross validation.

**Response:** The correction has been followed.

49. P16 L2-7: These sentences are perhaps better suited for the introduction, say on p5. **Response:** Following your suggestion, these sentences have been moved to the introduction section.

50. P16 L11: ... compared with the conventional EnKF scheme.Response: The correction has been followed.

51. P16 L13: This suggests that this method of minimizing the GCV works well for estimating the inflation factor.

**Response:** The sentence has been corrected.

52. P16 L15: What do you mean by "varieties"?

**Response:** The word has been deleted and the sentence is changed to "The analysis sensitivities in the proposed approach and in the conventional EnKF scheme..."

53. P16 L16: "The influence matrix..." this does not need to be restated.Response: The sentence has been deleted.

54. P16 L19-22: The time-averaged GAI statistic increases from about 10% in the conventional EnKF scheme to about 30% using the proposed inflation method. This illustrates that the inflation mitigates the problem of the analysis depending excessively on the forecast and excluding the observations.

**Response:** Thank you for your suggestion. The correction has been followed.

55. P17 L1-2: What do you mean they are "more reasonable"?

**Response:** In the conventional EnKF the analysis over relies on the forecast state and excludes useful information form the observation (The GAI statistic is only about 10%).

Adjusting the inflation of the forecast error covariance matrix in EnKF can increase the GAI to about 30%. Therefore more information form the observation is contained in the analysis.

56. P17 L3: It is also worth noting that the inflation...Response: The correction has been followed.

57. P17 L4-5: Forcing all components of the state vector to use the same inflation factor could systematically overinflate the ensemble variances ...Response: The correction has been followed.

58. P17 L7: Start a new paragraph here. The examples shown here using the Lorenz-96 model illustrate the feasibility of this approach for using GCV as a metric to estimate the covariance inflation factor.

**Response:** Thank you for your suggestion. The correction has been followed.

#### Comments on Figures:

1. Figures 1 and 2 are not really that instructive for me.

**Response:** Figures 1 shows the detailed procedure of the assimilation scheme. The flowchart is elaborated exhaustively in section 2.1 and 2.2. Figure 2 has been deleted in the revised version.

2. Figures 3-5 would benefit from using different colors to distinguish between the traces.**Response:** All figures of assimilation results have been plotted using different colors.

Again, thanks for your constructive comments and thorough corrections.

The references in this reply are listed as follows (Some of them are already in the original manuscript and some are newly added in the revised version).

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