Introduction

The authors would like to express their gratitude for referees' critique of our manuscript. We believe that in formulating our responses, we have developed additional insights to the problem, and its extensions to future work, which we intend to discuss in our revised manuscript. However, before entering into details we would like to reiterate the purpose of this work: we have contributed a rigorous proof of phenomenon, demonstrating one of the underlying mechanisms that determine the role of covariance inflation in reduced rank Kalman filters, in a formulation characteristic of the standard ensemble Kalman filter. We have not, however, made any claim to providing a practical, computationally efficient, means of correcting for this phenomenon. Similar to how we view the seminal work of AUS as a theoretical framework for understanding the properties of ensemble based covariances in the presence of chaotic dynamics (and in the absence of model error), the derivation of KF-AUSE is meant to be used as a theoretical explanation for the empirically observed properties of ensemble based covariances in the presence of chaotic dynamics and additive model errors. This is emphasized already in the original submission throughout sections 3.4 and section 5, and specifically in: (i) lines 5 - 16, page 12; (ii) the discussion in page 13; (iii) lines 8 - 18, page 16; (iv) lines 3 - 5, page 18; (v) lines 14 - 19 page 19; (vi) lines 1 - 4 page 20; (vii) and lines 5 - 13, page 21. It is in the context of the above discussion, in which we have presented our results, that we will respond to the referees' comments.

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1 Responses to referee 1

Comment(I)

Referee:

"The difference between covariant and Backward Lyapunov vectors is already known but the authors treat this subtle point in a very precise way and this is surely a merit for the paper."

Response:

We are very grateful that the referee has appreciated this subtlety, which we wanted to emphasize in lines 26 - 33 of page 9 and lines 1 - 15 of page 10. We believe that, although this is a fine distinction, explaining the equivalences and differences in the span and orthogonal compliments of the two sets of vectors has important consequences in designing filtering techniques used to treat the effects of dynamical upwelling.

Comment(II)

Referee:

"The authors of a recent paper Palatella, Luigi, and Fabio Grasso. "The EKF-AUS-NL algorithm implemented with- out the linear tangent model and in presence of parametric model error." SoftwareX 7 (2018): 28-33. show a possible way to manage model error in the framework of EKF-AUS filters in a very low dimensional model. In particular they suggest that a new direction in the phase-space should be filtered for each degree of freedom of model error. Their approach is obviously unfeasible in high dimensional model, so I think that the approach followed by the authors of the manuscript under examination is important and worth of publication on NPG."

Response:

We appreciate the referee highlighting this recent publication and we will discuss it in our review of recent literature in the conclusion of our manuscript.

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2 Responses to referee 2

2.1 Major comments

Comment(I)

Referee:

"'In numerical experiments with a nonlinear model, I cite the authors: 'At each observation time, before observations are given, the true trajectory is perturbed by additive Gaussian noise with a prescribed covariance Q, fixed in time'. This set-up is for an additional observational error rather than a model error for a nonlinear case. Instead the "true" solution should be obtained from a stochastic nonlinear model integrated by the Euler-Maruyama scheme, for example."'

Response:

We apologize for not being sufficiently clear in explaining our nonlinear experimental set up, which is mathematically consistent with the model error scenario for discrete, nonlinear maps. To reiterate, at each observation time, before observations are given, the true trajectory is perturbed (in model space) by additive Gaussian noise with a prescribed covariance $\mathbf{Q}$, fixed in time. Define the nonlinear map $\mathbf{\Psi}(t_0,t_1):\mathbb{R}^n \rightarrow \mathbb{R}^n$ be the flow map, generated from the Lorenz-96 equations

$$L^m(\mathbf{x}) = -x^{m-2}x^{m-1} + x^{m-1}x^{m+1} - x^m + F, \tag{1}$$

that takes the model state from time t_0 to t_1. Then, noting that $\mathbf{\Psi}(t,t+\delta) = \mathbf{\Psi}(s,s+\delta)$ for all t and s, we will define $\mathbf{\Psi}_\delta \triangleq \mathbf{\Psi}(0,\delta)$. In our experiments, the "truth" is thus evolved via the equation,

$$\mathbf{x}_{k+1} = \mathbf{\Psi}_\delta(\mathbf{x}_k) + \mathbf{w}_{k+1}, \qquad \mathbf{w}_{k+1} \sim N(\mathbf{0},\mathbf{Q}) \tag{2}$$

while the mean trajectory of the "model" state is given by the deterministic evolution, $\mathbf{x}^{\mathrm{b}}_{k+1} = \mathbf{\Psi}_\delta(\mathbf{x}^{\mathrm{b}}_k)$. In our experimental design, the extended Kalman filter estimates the state of the nonlinear "true" state, perturbed by the noise $\mathbf{w}_k$, Eq. (2), and $\mathbf{M}_k$ (the linear propagator for the covariance forward evolution) is derived by the map $\nabla\mathbf{\Psi}_\delta\big|_{\mathbf{x}^{\mathrm{b}}_k}$. This experimental configuration is mathematically consistent with the extended Kalman filter for a discrete nonlinear map with model error, and is a standard formulation for model error twin experiments, utilized by e.g, Mitchell and Carrassi (2015); Sakov et al. (2018), with the configuration using the circulant covariance matrix, $\mathbf{Q}$, drawn specifically from Raanes et al. (2015). The interval between observations δ controls the nonlinearity of the map, where our chosen configuration can be considered weakly-nonlinear. We will include the above expanded discussion in our revision.

Regarding the use of stochastic differential equations (SDEs), we supply these simulations here in our response, but we decline from including these results in the revision. In particular, we do not believe they add substantial additional value to our manuscript as:

- the results are almost identical to those derived from the discrete EKF configuration;
- their presentation requires significant additional explanation, as many readers are unfamiliar with mathematically robust simulations of SDEs;
- there is not as simple an interpretation of the local Lyapunov exponents for an SDE system as in the case of the discrete map perturbed by noise.

We elaborate on the above points in the following, where we will describe the configuration of our SDE simulations and the derived results.

Let

$$\mathrm{d}\mathbf{x} = \mathbf{L}(\mathbf{x})\mathrm{d}t + \sigma \mathrm{d}\mathbf{W}(t) \quad (3)$$

where $\mathbf{L}$ is defined in Eq. (1), $\mathbf{W}(t)$ is an n-dimensional, standard normal Weiner process, and $\sigma > 0$ is a diffusion coefficient, representing uniform variances of the noise in space and time. We note that for SDEs with additive noise (the above configuration being a special case), there is no difference between the Itô and Stratonovich integral of the SDE (Kloeden and Platen, 2013, see page 109), which simplifies our discussion. We utilize the differential operators defined on page 339, and the approximations for the multiple Stratonovich integrals on pages 202 - 203, to derive the integration rule for the order 2.0 strong Taylor scheme on page 359 of Kloeden and Platen (2013). The order 2.0 strong Taylor scheme reduces to the usual order 2.0 Taylor scheme in a deterministic setting, and the mean trajectory of the "model" state is propagated with the deterministic, order 2.0 Taylor scheme. The time step for both the true and model trajectory is fixed at $h = 0.0025$. The tangent-linear equations of the "model" trajectory is integrated with an order 4.0 Runge-Kutta scheme, with time step 0.005. The interval between observations is kept fixed as $\delta = 0.1$, maintaining the weakly-nonlinear error growth.

We choose the diffusion coefficient $\sigma = 0.25$, plotting the analysis RMSE of EKF, EKF-AUS and EKF-AUSE over 100,000 forecast cycles. In the case of $\sigma = 0.25$, the results are almost identical to Fig. 2 of our original manuscript. We find that diffusion coefficients of $\sigma = 0.1$ and 0.5 are qualitatively the same and are not pictured here.

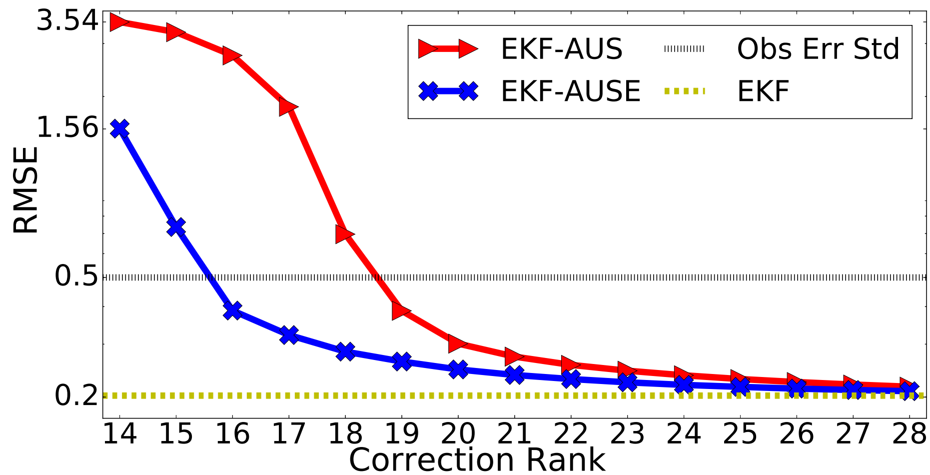

Figure 1. SDE diffusion $\sigma = 0.25$. Analysis RMSE of EKF-AUS plotted with triangles and EKF-AUSE plotted with X's, varying over the rank of the sub-optimal gain. Horizontal lines are the observational error standard deviation and EKF analysis RMSE. Note the log scale of the y-axis.

Given the similarity of the SDE simulation with diffusion coefficient of $\sigma = 0.25$ (Fig. 1 above) to our earlier simulation with discrete nonlinear maps, we choose this parameter configuration to evaluate the impact of multiplicative inflation on the reduced rank EKF-AUS. We, once again, choose a filtered subspace of dimension 17 and vary the inflation parameter α on the x-axis in Fig. 2 below.

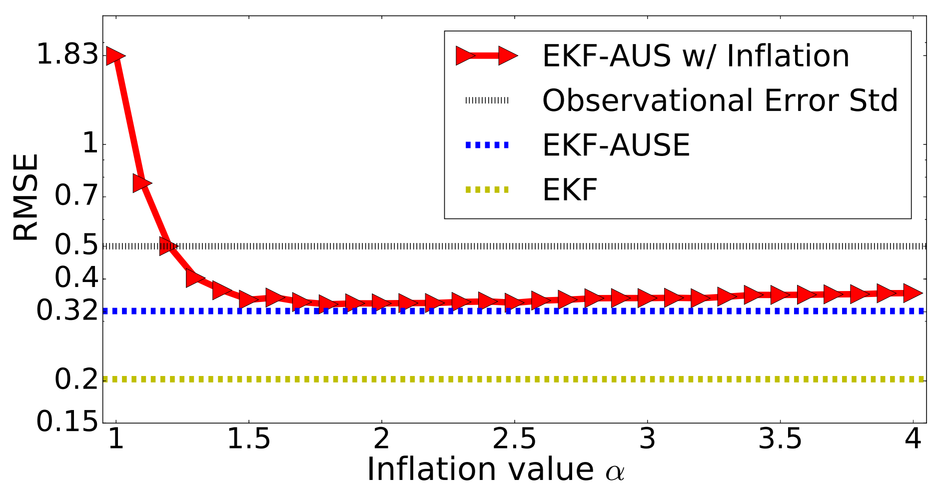

Figure 2. SDE diffusion $\sigma = 0.25$. Analysis RMSE of EKF-AUS (y-axis), correction rank 17, with multiplicative inflation plotted versus the inflation value α (x-axis). Horizontal lines are the observational error standard deviation, EKF-AUSE and EKF analysis RMSE. Note the log scale of the y-axis.

For the diffusion coefficient of $\sigma = 0.25$, the results for the SDE experiment are almost identical to those of our earlier experiments with discrete nonlinear maps.

Due to the similarity of the results, and the required addition explanation of the experimental configuration for SDEs, we do not believe that it is justified to include both the discrete map and SDE experimental configurations. Given a choice between the two designs, we prefer to use the discrete nonlinear map configuration, as in this case, there is an easy to interpret role of the local Lyapunov exponents which is more difficult to define in the case of an SDE, and goes beyond the scope of this work. We will, however, remark that: (i) the results are qualitatively the same in the SDE configuration; (ii) however, the full extension of AUS techniques to the presence of stochastic differential equations goes beyond the scope of this work and will be the subject of future research.

Comment(II)

Referee:

"The authors should compare their results with the ensemble Kalman filter with hyperpriors by Bocquet et al. 2015, as the goal of the latter paper was to remove the intrinsic need for inflation."

Response:

In discussing a comparison between the EnKF-N and the ideal recursion represented in EKF-AUSE, please note the following: the original EnKF-N (Bocquet, 2011; Bocquet et al., 2015) was designed to be used in the absence of model errors, in order to treat the misrepresentation of the statistics of the EnKF due to sampling errors. The construction for the EnKF-N, moreover, utilizes the hypothesis that the effective uncertainty lies within the span of a reduced rank ensemble. In the case of a perfect model with weakly nonlinear error evolution, this is a well posed hypothesis as evidenced by the results of Gurumoorthy et al. (2017); Bocquet et al. (2017). In this case, we can consider the forecast error evolution of an ideal, reduced rank Kalman filter to be asymptotically equivalent to the forecast error evolution of the true Kalman filter. Specifically, it is demonstrated that errors in the span of the trailing, stable BLVs vanish exponentially, and the EnKF-N does not need to treat the persistent upwelling of uncertainty that is present in the case of model errors. The EnKF-N of (Bocquet, 2011; Bocquet et al., 2015), rather seeks to address the sampling errors in ensemble based Kalman filters, especially in the presence of nonlinearity, which constitutes a wholly different source of error and reason for inflation.

Therefore, comparing the EnKF-N of (Bocquet, 2011; Bocquet et al., 2015) with EKF-AUSE would not provide any meaningful conclusions, and would conflate the disparate sources of uncertainty, as we already discussed throughout section 3.4, and lines 1 - 7, page 20, of our manuscript. Indeed, the recent work of Raanes et al. (2018), providing an extension of the EnKF-N to the presence of model errors, utilizes an additional, adaptive inflation factor to account for the underestimation of uncertainty due to model errors. However, in our manuscript we have emphasized that although the EnKF-N does not currently take into account dynamical upwelling in its formulation to treat the presence of model errors, an eventual goal would be to incorporate the ideal recursion for a reduced rank filter into the hyperprior. This is discussed specifically in: lines 21 - 23, page 13; lines 28 - 31, page 13; lines 8 - 15, page 16; lines 7 - 11, page 21. Formerly, the hyperprior of the EnKF-N has been uninformative in the sense that the hyperprior on the covariance is with respect to all positive semi-definite matrices, thus constituting a Jefferys prior. However, as demonstrated in Fig. 1 of our manuscript, for a reduced rank filter in the presence of model error, there is additional structure which gives a refinement to this set of matrices. Specifically, if the EnKF-N has a reduced rank filtered subspace, then we may view the EnKF-N as a Monte Carlo estimate of the ideal recursion of KF-AUSE, with an error covariance that is stratified across the unfiltered and filtered subspaces — this is discussed in the manuscript in lines 14 - 18 page 6, and lines 5 - 7, page 21. This work goes beyond the scope of the manuscript and is the subject of future research.

In response to your suggestion, we will expand on our earlier discussions, including reference specifically to the recent submission of Raanes et al. (2018), and further clarify the differences between the two treated sources of uncertainty.

2.2 Minor comments

Comment(I)

Referee:

"How was the inflation factor α obtained? What is its value?"

Response:

In our submission, page 19, lines 11-12 we state,

> "Additionally, we plot the analysis RMSE of EKF-AUS as a function of the inflation value applied to the forecast error covariance, with the inflation values plotted as triangles."

We apologize that this sentence was not totally clear. We meant to indicate that the selected inflation is equal to the x-value at each point marked with a triangle in the graph, with the corresponding y-value equal to the RMSE. In our revisions we will indicate that the values of inflation, α, are given as the x-values in the graph, for evenly spaced points in $[1, 4]$ at increments of 0.1.

Comment(II)

Referee:

"Additive inflation should be also studied. It is a simple extension which will, however, bring new insights."

Response:

We believe that it is interesting, and highly relevant, to study the effect of covariance and/or gain augmentation to reduce the effect of the dynamical upwelling and the presence of residual error in the unfiltered directions. We earlier summarized our thoughts on additive inflation in our original submission in lines 1 - 34, page 13, and lines 15 - 18, page 16. In these sections, we emphasized that augmenting a reduced rank gain by additive inflation or hybridization may reduce the effect of dynamical upwelling by keeping errors in the trailing BLVs small. However, we also state that this will generally induce sampling errors by corrupting the error estimates in the standard KF recursion. This will likewise induce mis-estimation of the error in KF-AUSE, which is simply the analytically derived forecast error in the case of a reduced rank gain.

The logical extension of our work studying additive inflation would thus include deriving the ideal recursion on the forecast error covariance with respect to an ensemble based gain, augmented with a sub-optimal correction in the trailing BLVs. By deriving the recursion, one can analytically study the effects of the sub-optimal correction on the propagation of errors, and how various computationally efficient approximations of this error evolution affects the RMSE. This would be the exact analogue of the work that we have completed, where we have studied the forecast error evolution with respect to a reduced rank gain, and the approximation of the dynamical upwelling in the ideal recursion with the computationally efficient alternative of multiplicative inflation. However, the mathematical complexity in obtaining an ideal recursion for additive inflation, as described above, is such that it cannot be included in this manuscript.

On the other hand, we may treat the sources of uncertainty described in this work approximately. We have highlighted this possibility, proposing a combination of some form of gain augmentation, with a hyperprior to account for the corrupted error estimates, to target these sources of uncertainty — this is suggested in lines 28 - 32, page 13, lines 8 - 18, page 16, lines 7 - 11, page 21. However, the purpose of this manuscript is only to provide a rigorous proof of phenomenon, and introducing the above approximations goes beyond the scope of this work. In order to more fully explain the significance of these extensions to additive inflation, and its mathematical complexity, we will include an additional discussion section in our revised manuscript elaborating on the above points.

Comment(III)

"The authors use complete observations. A study of incomplete observations is again a simple extension which will bring more merit to the manuscript."

Response:

We agree that this is a simple extension, and as such we provide a numerical demonstration in this response. Specifically, using our original configuration of discrete, nonlinear maps with additive noise, we simulate the effect of reducing the dimension of the observational subspace while keeping all other parameters fixed. However, we do not believe that the results with reduced observations: (i) are qualitatively different from the results with a fully observed system, or (ii) add significant new information about the effect of the dynamical upwelling in a reduced rank Kalman filter. The major difference in the results with reduced observations lies only in the minimum rank of the filtered subspace to prevent filter divergence.

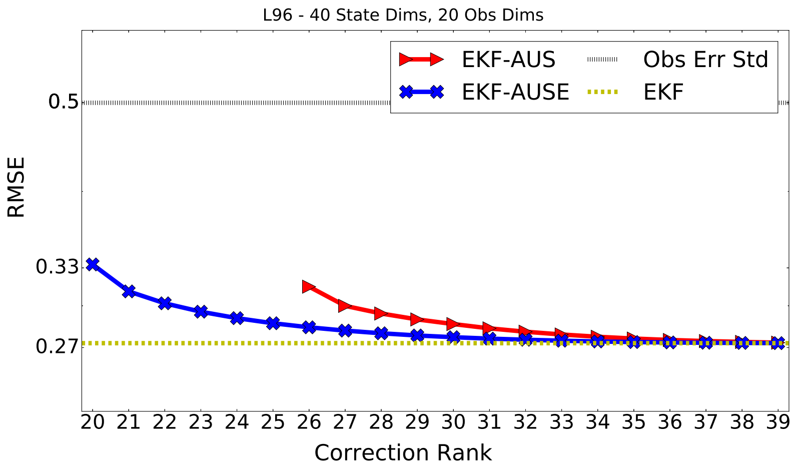

Figure 3. EKF-AUS and EKF-AUSE RMSE, plotted versus the rank of the filtered subspace. Observations are taken at all odd nodes $\mathbf{x}_k^i$ for $i \in 1, \cdots, 39$.

We see once again that EKF-AUSE has a lower minimum, and in general lower RMSE, than EKF-AUS. In the case of an observational subspace of dimension 20, Fig. 3, the minimum rank of the filtered subspace to prevent divergence is 20 for EKF-AUSE, while EKF-AUS has a minimum rank of 26. For all RMSE values not pictured in Figs. 3, the EKF-AUSE and EKF-AUS diverge due to numerical instability. We find qualitatively similar results when using an observational dimension of $d = 30$, and these results are not pictured here.

We decline from including these results in our revised manuscript, though, when we discuss the qualitative similarity of other experimental configurations, we will discuss that when reducing the observational dimension, the usual pattern persists. This will be added to the discussion in our original submission, in line 18, page 17, through line 3, page 18.

Comment(IV)

"Italics is used too often in the text to give an emphasis, it should be avoided."

Response:

We apologize for this distraction. We have removed most, but not all, of the italics. We have chosen to use the emphasis more selectively in a few key spots to emphasize important points — we hope that this is more satisfactory.

3 Response to short comments

Because the short comments are on relatively minor points, we will conclude here by saying that we appreciate the feedback and will implement the suggestions. Most importantly, we separate the definition of the KF-AUSE Riccati equation, and the related proposition, so that we can state the proposition in its fullest generality — this will be included in the revised text.

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