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:

- 5 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-
- 10 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)	
20		Referee:
		"The difference between covariant and Backward Lyapunov vectors is already known but the au- thors treat this subtle point in a very precise way and this is surely a merit for the paper."
25		Response:
30		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:
35		"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."
40		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.

2 Responses to referee 2

5 2.1 Major comments

Comment(I) ______ Referee:

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"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 $\Psi(t_0, t_1) : \mathbb{R}^n \to \mathbb{R}^n$ be the flow map, generated from the Lorenz-96 equations

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

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

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

while the mean trajectory of the "model" state is given by the deterministic evolution, $\mathbf{x}_{k+1}^b = \Psi_{\delta}(\mathbf{x}_k^b)$. 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 $\nabla \Psi_{\delta}|_{\mathbf{x}_k^b}$. 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

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

where L is defined in Eq. (1), 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.

25 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) _

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10 **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 30 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 35 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 40 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 45

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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

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10	Comment (I)	
	~ /	Referee:
		"How was the inflation factor α obtained? What is its value?"
		Response:
15		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."
20		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:
25		"Additive inflation should be also studied. It is a simple extension which will, however, bring new insights."
		Response:
30		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
35		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.
40		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.

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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 $i \in 1, \dots, 39$.

5	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.
10	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)
15	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.

20 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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Chaotic dynamics and the role of covariance inflation for reduced rank Kalman filters with model error

Colin Grudzien¹, Alberto Carrassi¹, and Marc Bocquet² ¹Nansen Environmental and Remote Sensing Center, Bergen, Norway ²CEREA, joint laboratory École des Ponts ParisTech and EDF R&D, Université Paris-Est, Champs-sur-Marne, France *Correspondence to:* Colin Grudzien, Colin.Grudzien@nersc.no

Abstract. The ensemble Kalman filter and its variants have shown to be robust for data assimilation in high dimensional geophysical models, with localization, using ensembles of extremely small size relative to the model dimension. A reduced rank representation of the estimated covariance, however, leaves a large dimensional complementary subspace unfiltered. Utilizing the dynamical properties of the filtration for the backward Lyapunov vectors, this paper explores a previously unexplained

5 mechanism, describing the intrinsic role of covariance inflation in reduced rank, ensemble based ensemble-based Kalman filters. Our derivation of the forecast error evolution describes the dynamic upwelling of the unfiltered error from outside of the span of the anomalies into the filtered subspace. Analytical results for linear systems explicitly describe the mechanism for the upwelling, and the associated recursive Riccati equation for the forecast error, while nonlinear approximations are explored numerically.

10 1 Introduction

It is well understood that in chaotic physical systems, dynamical instability is among the leading drivers of forecast uncertainty (Trevisan and Palatella, 2011a; Vannitsem, 2017) (Toth and Kalnay, 1997; Trevisan and Palatella, 2011a; Vannitsem, 2017). Recent mathematical and numerical results have, furthermore, established a rigorous framework for understanding the relationship between dynamical instability, in terms of the non-negative Lyapunov exponents, and the asymptotic properties of the uncer-

- 15 tainty in ensemble based ensemble-based data assimilation techniques: in perfect models, with weakly-nonlinear error growth, it was shown that the ensemble of anomalies projects the anomalies of ensemble Kalman filters project strongly on the span of the unstable-neutral backward Lyapunov vectors (Carrassi et al., 2009; Ng et al., 2011; González-Tokman and Hunt, 2013; Bocquet and Carrassi, 2017), and that the divergence of the ensemble Kalman filter depends significantly upon whether error in this space is sufficiently observed and corrected.
- Inspired by the Assimilation in the Unstable Subspace (AUS) (AUS) methodology of Anna Trevisan and her collaborators (Trevisan and Uboldi, 2004; Carrassi et al., 2007, 2008; Trevisan et al., 2010; Trevisan and Palatella, 2011b; Palatella et al., 2013; Palatella and Trevisan, 2015), recent mathematical results have rigorously validated the underlying hypothesis of AUS: for perfect, linear models, the uncertainty of the Kalman filter asymptotically collapses to the span of the backward Lyapunov vectors with non-negative exponents (Gurumoorthy et al., 2017). Furthermore, if a sub-optimal-reduced rank filter has an

estimated covariance initialized only in these modes, and the unstable-neutral subspace is uniformly, completely observed, the sub-optimal-reduced rank filter becomes asymptotically equivalent to the optimal Kalman filter (Bocquet et al., 2017). This phenomenon has, furthermore, been generalized as a criterion for the exponential stability of continuous time filters, in perfect models, in terms of the *detectability* detectability of the unstable-neutral subspace (Frank and Zhuk, 2017).

- 5 The above mathematical results demonstrate how the stable dynamics in perfect models dissipate forecast errors, in sequential filters, such that a reduced rank representation of the error covariance <u>matrix</u>, in the unstable-neutral subspace alone, suffices to control error growth. This behavior, similarly understood in the smoothing problem (Pires et al., 1996; Trevisan et al., 2010), is now also mathematically verified for the linear Kalman smoother, and its nonlinear ensemble formulation is shown numerically to exhibit the same behavior, in a weakly-nonlinear regime for error dynamics (Bocquet and Carrassi,
- 10 2017).

The work of Grudzien et al. (2017) extends the mathematical framework for AUS, so far established for perfect models, to the presence of additive model errors with additional qualifications. This work introduces novel bounds on the Kalman filter's asymptotic forecast uncertainty, and a necessary criterion for filter stability, as an inverse relationship between the model's dynamical instabilities and the precision of observations. Particularly, in the absence of observations, corrections to forecast

- 15 errors in the stable modes, this work demonstrates that the model dynamics alone are still once again sufficient to uniformly bound the errors in the span of the stable backward Lyapunov vectors. However, the uniform bound may be impractically large due to the excitation of model errors by the transient instabilities in stable directions. While uncertainty is *asymptotically* asymptotically dissipated by the stable dynamics, the reintroduction of uncertainty from model error significantly differentiates imperfect models. Newly injected errors are subject to the growth rates of the local (in time) Lyapunov exponents, and stable
- 20 Lyapunov exponents of sufficiently high variance may experience transient periods of growth. Therefore, strategies for representing the forecast error with a reduced low rank ensemble must be adapted for imperfect models to account for a residual error in the span of the stable, backward Lyapunov vectors which never vanishes and, moreover, may go through transient periods of growth. As a consequence, confining the error description within a reduced rank Kalman filter to only the unstableneutral subspace does not suffice when model error is present and suggests that one must include additional, asymptotically
- 25 stable, modes.

In this work we show, furthermore, that such an increase of the ensemble span does not automatically render the filter optimal: one may also need to account for the injection of error from unfiltered directions into the ensemble span. In particular, when a reduced rank, ensemble based an ensemble-based Kalman gain is used to correct the forecast errors, the dynamics induce error propagation which transmits uncertainty from the uncorrected, complementary subspace into the ensemble span.

- 30 In this study, the propagation of error in the linear Kalman filter, written in a basis of backward Lyapunov vectors, will reveal the leading order evolution of the unfiltered uncertainty. Although the evolution is derived for linear models, the mechanism for error propagation can be considered a generic feature of reduced rank ensemble Kalman filters: under. Under the condition that error evolution is weakly-nonlinear, the ensemble span will align with the span of the leading backward Lyapunov vectors therefore the error decomposition in the basis of backward Lyapunov vectors will be valid for the ensemble Kalman filter.
- 35 Similar to how we view 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), this work 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 paper is structured as follows: section 2.1 concerns essential results from the theory of Lyapunov vectors which will be are used throughout; sections 2.2 and 2.3 describe the basic framework for the Kalman filter, and will motivate our subsequent results; section 3 contains our main analytical result, i.e., the derivation of the evolution of exact forecast error under a sub-optimal reduced rank filter in a basis of backward Lyapunov vectors; finally, section 4 will use numerics to qualitatively explore the ideal linear recursion for the forecast error of the sub-optimal reduced rank filter, and its approximation in nonlinear models. Conclusions Implications of the results in this work are discussed in section 5, with an emphasis on future directions
- 10 of research and their challenges. Final conclusions are drawn in section 6.

2 Preliminaries

We begin by introducing our notation and the problem formulation-

, with definitions in bold. There is inconsistent use of the terminology for Lyapunov vectors in the literature, and so we choose to use the nomenclature of Kuptsov and Parlitz (2012) for its generality and self-consistency.

15 2.1 Lyapunov vectors

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Throughout the entire text, the conventional notation k = 0, 1, 2, ... is adopted to indicate that the quantity is defined at time t_k . Let $\mathbf{z}_{k-1} \in \mathbb{R}^n$ be an arbitrary vector, the matrix propagator of the forward model from t_{k-1} to t_k is given by \mathbf{M}_k , such that $\mathbf{z}_k = \mathbf{M}_k \mathbf{z}_{k-1}$. We denote the operator taking the system state from an arbitrary time t_l to t_k as $\mathbf{M}_{k:l} \triangleq \mathbf{M}_k \mathbf{M}_{k-1} \dots \mathbf{M}_{l+1}$, with the symbol \triangleq used to signify that the expression is a definition. We will denote $\mathbf{M}_{k:k} \triangleq \mathbf{I}_n$, where \mathbf{I}_n is the identity matrix (of size $n \times n$ in this case). At all times we assume \mathbf{M}_k to be non-singular and to be uniformly bounded in k.

Although much of the derivations that follow are done for linear dynamics, we are ultimately concerned with nonlinear systems — therefore, we will assume that Oseledec's theorem holds, even for linear model propagators. In general, this is a non-trivial assumption, but one which can be considered generic for the tangent-linear model of nonlinear systems (Barreira and Pesin, 2002, see the Multiplicative Ergodic theorem, Theorem 2.1.2). The backward Lyapunov vectors can be

- 25 defined by a choice of an orthonormal eigenbasis for the far-past operator (Kuptsov and Parlitz, 2012). Define the matrix \mathbf{E}_k to be the orthogonal matrix whose *i*-th column is the *i*-th **backward Lyapunov vector (BLV)** at time *k*, corresponding to the Lyapunov exponent λ_i , a wide class of nonlinear systems, due to the Multiplicative Ergodic Theorem (MET): with probability one, Oseledec's theorem holds, the Lyapunov exponents are well defined and the values of the Lyapunov exponents are independent of the initial condition (Barreira and Pesin, 2002, see their Theorems 2.1.1 and 2.1.2 for a full statement and proof).
- 30 A more general version of the MET, and its interpretation for several physical systems, is provided by Froyland et al. (2013) in their Theorem 1.1 and example 1.2.

We order the Lyapunov exponents

$$\lambda_1 \ge \dots \ge \lambda_{n_0} \ge 0 > \lambda_{n_0+1} \ge \dots \ge \lambda_n,\tag{1}$$

such that the unstable-neutral subspace is defined to be of dimension n_0 and the model state dimension is n. Note $\frac{1}{2}$, that we do not assume that the Lyapunov exponents are distinct.

- 5 We will Oseledec's theorem decomposes the (tangent-linear) model space into a direct sum of time-varying, covariant Oseledec spaces, referred to as an Oseledec splitting or decomposition. At times, we will refer to the covariant Oseledec spaces, as well as to the covariant, and to the forward Lyapunov vectors. These discussions will provide a deeper interpretation of our results for those familiar with these technical points. However, these discussions are not crucial to the understanding of our results, and we therefore limit the use of formal definitions to the backward Lyapunov vectors. For a more formal
- 10 discussion of the Oseledec spaces, constructions for Lyapunov vectors and related results for the full rank Kalman filter, see Grudzien et al. (2017); for a survey on the mathematical and numerical construction of Lyapunov vectors, see Kuptsov and Parlitz (2012); for a discussion of general Oseledec splitting, and a comparison of methods for its computation, see Froyland et al. (2013). The backward Lyapunov vectors can be defined by a choice of an orthonormal eigenbasis for the far-past operator, and/or by recursive OR factorizations of the (tangent-linear) model propagator (Kuptsov and Parlitz, 2012). Throughout the text, we
- 15 utilize the invariance of the BLVs backward Lyapunov vectors under the recursive QR algorithmof Benettin et al. (1980) and Shimada and Nagashima (1979).

Definition 1. Define the matrix \mathbf{E}_k to be the orthogonal matrix whose *i*-th column is the *i*-th backward Lyapunov vector (BLV) at time k, corresponding to the Lyapunov exponent λ_i .

Lemma 1. There is an $n \times n$ upper triangular matrix \mathbf{U}_k , such that the (tangent-linear) model propagator satisfies The 20 diagonal elements of \mathbf{U}_k , denoted U_k^i , define the

$$\mathbf{M}_k = \mathbf{E}_k \mathbf{U}_k \mathbf{E}_{k-1}^{\mathrm{T}}.$$

(3)

Define the product of matrices,

$$\mathbf{U}_{k:l} riangleq \mathbf{U}_k \cdots \mathbf{U}_l,$$

the i-th Lyapunov exponent is equal to the limit

25
$$\lambda_i = \lim_{l \to -\infty} \frac{1}{k-l} \log\left(|U_{k:l}^{ii}| \right), \tag{4}$$

where $U_{k,l}^{ii}$ is the *i*-th diagonal element of the matrix $\mathbf{U}_{k,l}$. The local Lyapunov exponents are defined by $\log (|U_k^{ii}|)$.

Proof. Equation (2) follows from Eq. (31) of Kuptsov and Parlitz (2012) and is a simple-consequence of the invariance of the BLVs under the recursive QR decomposition (Grudzien et al., 2017). Computing Lyapunov exponents via recursive QR factorizations as in Eq. (4) is the standard method, described by e.g., Shimada and Nagashima (1979) and Benettin et al. (1980).

The decomposition in Eq. (2) represents a change of basis of the model space into the upper triangular dynamics of the moving frame of BLVs, defining a basis for the backward Lyapunov filtration (Legras and Vautard, 1996). In particular, \mathbf{E}_{k-1}^{T} takes the model state into the orthogonal projection coefficients in the basis of the BLVs at time k-1. We will denote the projection coefficients of an arbitrary vector \mathbf{z}_k into a basis of BLVs with a "hat", i.e. $\mathbf{E}_k^{\mathrm{T}} \mathbf{z}_k \triangleq \widehat{\mathbf{z}}_k$. Using the orthogonality of the matrix \mathbf{E}_k , the invariant dynamics in the BLVs is written

$$\widehat{\mathbf{z}}_{k} = \mathbf{U}_{k} \widehat{\mathbf{z}}_{k-1} \quad \Leftrightarrow \quad \mathbf{z}_{k} = \mathbf{M}_{k} \mathbf{z}_{k-1}. \tag{5}$$

The operator \mathbf{U}_k thus describes the invariant, upper triangular dynamics, transferring the model state into its forward representation in the BLVs at time k.

2.2 The Kalman filter

5

We seek to estimate the distribution of a Gaussian random variable-vector $\mathbf{x}_k \in \mathbb{R}^n$ evolved via a linear Markov model with 10 additive white noise,

$$\mathbf{x}_k = \mathbf{M}_k \mathbf{x}_{k-1} + \mathbf{w}_k,\tag{6}$$

and with observations $\mathbf{y}_k \in \mathbb{R}^d$ given in the form

$$\mathbf{y}_k = \mathbf{H}_k \mathbf{x}_k + \mathbf{v}_k. \tag{7}$$

The forecast mean, \mathbf{x}_{k}^{b} , is propagated from the last posterior mean, \mathbf{x}_{k-1}^{a} by the deterministic component of Eq. 6, i.e., 15

$$\mathbf{x}_{k}^{\mathsf{b}} = \mathbf{M}_{k} \mathbf{x}_{k-1}^{\mathsf{a}}.$$
(8)

The model variables $\mathbf{x}_k \in \mathbb{R}^n$ and observational variables $\mathbf{y}_k \in \mathbb{R}^d$, and observation vectors are related via the linear observation operator $\mathbf{H}_k : \mathbb{R}^n \mapsto \mathbb{R}^d$. Model and observation noise, \mathbf{w}_k and \mathbf{v}_k , are assumed mutually independent, unbiased, Gaussian white sequences such that

20
$$\mathbb{E}[\mathbf{v}_k \mathbf{v}_l^{\mathrm{T}}] = \delta_{k,l} \mathbf{R}_k$$
 and $\mathbb{E}[\mathbf{w}_k \mathbf{w}_l^{\mathrm{T}}] = \delta_{k,l} \mathbf{Q}_k$, (9)

where \mathbb{E} is the expectation, $\mathbf{R}_k \in \mathbb{R}^{d \times d}$ is the observation error covariance matrix at time t_k , and $\mathbf{Q}_k \in \mathbb{R}^{n \times n}$ stands for the model error covariance matrix. The error covariance matrix \mathbf{R}_k can be assumed invertible without losing generality. To avoid pathologies, we assume that the model error and the observational and the observation error covariance matrices are uniformly bounded. For $1 \le t < s \le n$, and given a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, we define $\mathbf{A}^{t:s} \in \mathbb{R}^{n \times s-t+1} \mathbf{A}^{t:s} \in \mathbb{R}^{n \times (s-t+1)}$ to be the matrix composed (inclusively) of columns s through t of A.

25

Definition 2. The forecast error is defined as the difference of the mean state estimated by the filter and the unknown random state, i.e.,

$$\boldsymbol{\epsilon}_k \stackrel{\Delta}{=} \mathbf{x}_k^{\mathrm{b}} - \mathbf{x}_k. \tag{10}$$

The innovation is the measured difference between the forecast and in the observation space and the observation,

$$\boldsymbol{\delta}_k \triangleq \mathbf{y}_k - \mathbf{H}_k \mathbf{x}_k = \mathbf{H}_k \boldsymbol{\epsilon}_k - \mathbf{v}_k. \tag{11}$$

We define the true exact forecast error covariance at time k to be

$$\mathbf{B}_{k} \triangleq \mathbb{E}\left[\boldsymbol{\epsilon}_{k} \boldsymbol{\epsilon}_{k}^{\mathrm{T}}\right].$$
(12)

5 On the other hand, suppose some filter, yet to be identified, is used to estimate the forecast mean and error covariance — the estimated forecast error covariance will be denoted \mathbf{P}_k , defined according to the chosen estimation algorithm.

Suppose that $\mathbf{K}_k \in \mathbb{R}^{n \times d}$ is some estimator which takes the forecast state to the analysis state. In the case of the *ideal* theoretical Kalman filter, where the true exact forecast error covariances are computed exactly, $\mathbf{P}_k \equiv \mathbf{B}_k$, the gain \mathbf{K}_k will be defined

10
$$\mathbf{K}_{k} \triangleq \mathbf{P}_{k} \mathbf{H}_{k}^{\mathrm{T}} \left(\mathbf{H}_{k} \mathbf{P}_{k} \mathbf{H}_{k}^{\mathrm{T}} + \mathbf{R}_{k} \right)^{-1}$$
$$= \mathbf{B}_{k} \mathbf{H}_{k}^{\mathrm{T}} \left(\mathbf{H}_{k} \mathbf{B}_{k} \mathbf{H}_{k}^{\mathrm{T}} + \mathbf{R}_{k} \right)^{-1}.$$
(13)

In this text, we will vary the choice of the analysis update operator \mathbf{K}_k , but the functional form of the recursion for the analysis update of the mean will be unchanged and defined as

$$\mathbf{x}_{k}^{\mathrm{a}} riangleq \mathbf{x}_{k}^{\mathrm{b}} + \mathbf{K}_{k} \left(\mathbf{y}_{k} - \mathbf{H}_{k} \mathbf{x}_{k}^{\mathrm{b}}
ight)$$

$$15 \qquad = \mathbf{x}_k^{\mathsf{b}} - \mathbf{K}_k \mathbf{H}_k \boldsymbol{\epsilon}_k + \mathbf{K}_k \mathbf{v}_k. \tag{14}$$

Therefore, for any estimator, the forecast mean can be derived recursively from Eq. (8) and Eq. (14) as

$$\mathbf{x}_{k+1}^{\mathsf{b}} \triangleq \mathbf{M}_{k+1} \left(\mathbf{x}_{k}^{\mathsf{b}} - \mathbf{K}_{k} \mathbf{H}_{k} \boldsymbol{\epsilon}_{k} + \mathbf{K}_{k} \mathbf{v}_{k} \right)$$
(15)

where \mathbf{K}_k is some choice for the gain. The recursion on the forecast error can be derived equal to

$$\boldsymbol{\epsilon}_{k+1} \triangleq \mathbf{M}_{k+1} \left[\left(\mathbf{I}_n - \mathbf{K}_k \mathbf{H}_k \right) \boldsymbol{\epsilon}_k + \mathbf{K}_k \mathbf{v}_k \right] - \mathbf{w}_{k+1}, \tag{16}$$

20 though ϵ_k , \mathbf{v}_k and \mathbf{w}_{k+1} are assumed to be unknown.

2.3 Rank deficiency in the Kalman filter

In an ideal a linear model, with known, Gaussian observational Gaussian observation and model error distributions, the estimated and true error covariances of the KF are equalexact: the posterior error distribution for the state is Gaussian, and the KF completely describes the Bayesian posterior through its recursive equations for the estimated mean and covariance.

However, it is often the case that the recursion for the posterior error distribution is approximated with a reduced rank surrogate in which the estimated covariance, \mathbf{P}_k , and resulting true exact error covariance, \mathbf{B}_k , may not be equal (Chandrasekar et al., 2008). This mis-match between the approximated and true forecast error covariance, and the resultant sub-optimal analysis update, can lead to systematic underestimation of the true-forecast error and filter divergence.

Nonetheless, it is possible in an ideal setting to analytically describe the error statistics of a reduced rank Bayesian Kalman filter — to illustrate this, assume we have a linear model with known Gaussian error distributions. Suppose we apply the
analysis update in a reduced rank set of BLVs, as has been done in EKF-AUS (Trevisan and Palatella, 2011b). Suppose, furthermore, the true exact error covariance, B_k, is known. Then the gain

$$\mathbf{K}_{k} \triangleq \mathbf{E}_{k}^{1:n_{0}} \left(\mathbf{E}_{k}^{1:n_{0}}\right)^{\mathrm{T}} \mathbf{B}_{k} \mathbf{E}_{k}^{1:n_{0}} \left(\mathbf{E}_{k}^{1:n_{0}}\right)^{\mathrm{T}} \mathbf{H}_{k}^{\mathrm{T}} \times \left[\mathbf{H}_{k} \mathbf{E}_{k}^{1:n_{0}} \left(\mathbf{E}_{k}^{1:n_{0}}\right)^{\mathrm{T}} \mathbf{B}_{k} \mathbf{E}_{k}^{1:n_{0}} \left(\mathbf{E}_{k}^{1:n_{0}}\right)^{\mathrm{T}} \mathbf{H}_{k}^{\mathrm{T}} + \mathbf{R}_{k}\right]^{-1}$$

$$(17)$$

yields the exact Bayesian update Kalman estimator with respect to a subset of the anomaly variables, defined by the span of

- 10 the leading n_0 BLVs. We may use Eq. (16) to derive the analytical recursion for the covariance of the true forecast error under the sub-optimal analysis operator forecast error covariance, \mathbf{B}_{k+1} , under the reduced rank gain in Eq. (17). As in the ideal KF, this will describe the ideal forecast error recursion with respect to a rank deficient estimator — the **rank deficiency (or reduced rank**) is defined by The **rank deficiency (or reduced rank**) is defined by the restriction of the Kalman estimator to a low dimensional subspace. Note that, although the estimator is restricted to the span of $\mathbf{E}_k^{1:n_0}$, the observation operator
- 15 is still applied to the full state vector, and thus the analysis does not equal the restriction of the Bayesian update to a low dimensional subspace the leading n_0 BLVs. We recover the restricted Bayesian update using the estimator in Eq. (17) precisely when $\mathbf{H}_k \mathbf{E}_k^{n_0+1:n} \equiv \mathbf{0}_{d \times (n=n_0)}$.

The significance of deriving an analytical recursion for the forecast error under the sub-optimal reduced rank estimator in Eq. (17) is as follows. The analysis operator in Eq. (17) is characteristic of the generic typical gain for the ensemble Kalman

- 20 filter (EnKF) in large, geophysical models: the ensemble based ensemble-based gain applies its update with respect to the subspace defined by the span of the ensemble of anomalies, which is typically of low usually of reduced rank and aligns with the span of the leading BLVs (Bocquet and Carrassi, 2017). The EnKF is(Ng et al., 2011; Bocquet and Carrassi, 2017). The standard EnKF can, therefore, be considered a Monte Carlo estimate of the true error statistics resulting from a rank deficient analysis update Kalman estimator as in Eq. (17). The *ideal error distribution* that the EnKF samples is thus characterized by
- 25 the recursion derived for the error under the rank deficient Bayesian estimator. This is the motivation of section 3, where we will define a sub-optimal analysis gain, reduced rank gain which operates within the span of an arbitrary number of the leading BLVs, and derive the resulting true exact forecast error covariance.

3 Filtering in the backward Lyapunov basis vectors

Consider the forecast error recursion for the linear KF in Eq. (16). As we are motivated by reduced rank ensemble covariances,

30 suppose \mathbf{K}_k is defined as a sub-optimal reduced rank gain which corrects only the leading *r* BLVs, with r < n. The subspace defined by the span of the anomalies defines a subspace of "filtered variables" where we perform our analysis. The "unfiltered

subspace" is uniquely defined (up to the inner product) as the orthogonal complement to the filtered space, i.e., the subspace in which the reduced rank Kalman estimator makes no correction.

Definition 3. We denote the filtered subspace filtered subspace by the column span of the vectors $\mathbf{E}_{k}^{f} \triangleq \mathbf{E}_{k}^{1:r}$ and the unfiltered subspace unfiltered subspace $\mathbf{E}_{k}^{u} \triangleq \mathbf{E}_{k}^{r+1:n}$ for all k. The projection coefficients of a vector $\mathbf{z} \in \mathbb{R}^{n}$ into the filtered and unfiltered subspace will be denoted $\mathbf{\hat{z}}^{f} \triangleq \left(\mathbf{E}_{k}^{f}\right)^{\mathrm{T}} \mathbf{z}$ and $\mathbf{\hat{z}}^{u} \triangleq \left(\mathbf{E}_{k}^{u}\right)^{\mathrm{T}} \mathbf{z}$, respectively. We can-

We thus decompose the forecast error into its orthogonal projections in the filtered and unfiltered subspaces as

$$\boldsymbol{\epsilon}_{k} \stackrel{\Delta}{=} \mathbf{E}_{k}^{\mathrm{f}} \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{f}} + \mathbf{E}_{k}^{\mathrm{u}} \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{u}}. \tag{18}$$

For r = n, define $\mathbf{E}_{k}^{f} \triangleq \mathbf{E}_{k}$ and $\mathbf{E}_{k}^{u} \triangleq \mathbf{0}_{n}$ such that $\hat{\boldsymbol{\epsilon}}_{k}^{f}$ is the full error written in an orthogonal change of basis — this case will only be referred to for comparison.

10 For $i, j \in \{f, u\}$, we write the sub-covariances in the basis defined by \mathbf{E}_k as

$$\widehat{\mathbf{B}}_{k}^{ij} \triangleq \mathbb{E}\left[\widehat{\boldsymbol{\epsilon}}_{k}^{i}\left(\widehat{\boldsymbol{\epsilon}}_{k}^{j}\right)^{\mathrm{T}}\right].$$
(19)

such that the true exact forecast error covariance is given

5

$$\mathbf{B}_{k} \equiv \mathbf{E}_{k} \begin{pmatrix} \widehat{\mathbf{B}}_{k}^{\text{ff}} & \widehat{\mathbf{B}}_{k}^{\text{fu}} \\ \widehat{\mathbf{B}}_{k}^{\text{uf}} & \widehat{\mathbf{B}}_{k}^{\text{uu}} \end{pmatrix} \mathbf{E}_{k}^{\text{T}}, \tag{20}$$

where $\widehat{\mathbf{B}}_{k}^{\text{ff}}$ and $\widehat{\mathbf{B}}_{k}^{\text{uu}}$ are symmetric . We will write matrices, and $\widehat{\mathbf{B}}_{k}^{\text{fu}} = \left(\widehat{\mathbf{B}}_{k}^{\text{uf}}\right)^{\text{T}}$. We similarly express \mathbf{U}_{k} as a block matrix as ,

15
$$\mathbf{U}_{k} \triangleq \begin{pmatrix} \mathbf{U}_{k}^{\mathrm{ff}} & \mathbf{U}_{k}^{\mathrm{fu}} \\ \mathbf{0}_{(n-r) \times r} & \mathbf{U}_{k}^{\mathrm{uu}} \end{pmatrix}$$
. (21)

For an arbitrary rank filtered subspace, the sub-optimal reduced rank gain \mathbf{K}_k , which corrects only correcting the span of $\mathbf{E}_k^{\mathrm{f}}$, is defined by

$$\mathbf{K}_{k} \triangleq \mathbf{E}_{k}^{\mathrm{f}} \widehat{\mathbf{K}}_{k}, \\ \widehat{\mathbf{K}}_{k} \triangleq \mathbf{B}_{k}^{\mathrm{ff}} \left(\mathbf{E}_{k}^{\mathrm{f}}\right)^{\mathrm{T}} \mathbf{H}_{k}^{\mathrm{T}} \left[\mathbf{H}_{k} \mathbf{E}_{k}^{\mathrm{f}} \mathbf{B}_{k}^{\mathrm{ff}} \left(\mathbf{E}_{k}^{\mathrm{f}}\right)^{\mathrm{T}} \mathbf{H}_{k}^{\mathrm{T}} + \mathbf{R}_{k}\right]^{-1},$$
(22)

20 Where where $\hat{\mathbf{K}}_k$ represents the projection coefficients of the sub-optimal reduced rank gain into the filtered variables.

For every $k \ge 1$, we decompose the model error covariance into the basis of filtered and unfiltered BLVs as

$$\mathbf{Q}_{k} \triangleq \mathbf{E}_{k} \begin{pmatrix} \widehat{\mathbf{Q}}_{k}^{\text{ff}} & \widehat{\mathbf{Q}}_{k}^{\text{fu}} \\ \widehat{\mathbf{Q}}_{k}^{\text{uf}} & \widehat{\mathbf{Q}}_{k}^{\text{uu}} \end{pmatrix} \mathbf{E}_{k}^{\text{T}}$$
(23)

where $\widehat{\mathbf{Q}}_{k}^{\text{ff}}$ and $\widehat{\mathbf{Q}}_{k}^{\text{uu}}$ are symmetric matrices, and $\widehat{\mathbf{Q}}_{k}^{\text{fu}} = \left(\widehat{\mathbf{Q}}_{k}^{\text{uf}}\right)^{\text{T}}$.

With the above notation, and using Eq. (2), the evolution of the true forecast error under the sub-optimal reduced rank gain is derived from Eq. (16) as

$$\boldsymbol{\epsilon}_{k+1} = \mathbf{M}_{k+1} \left(\mathbf{I}_n - \mathbf{E}_k^{\mathrm{f}} \widehat{\mathbf{K}}_k \mathbf{H}_k \right) \boldsymbol{\epsilon}_k + \mathbf{M}_{k+1} \mathbf{E}_k^{\mathrm{f}} \widehat{\mathbf{K}}_k \mathbf{v}_k - \mathbf{w}_{k+1} = \left(\mathbf{E}_{k+1} \mathbf{U}_{k+1} \mathbf{E}_k^{\mathrm{T}} - \mathbf{E}_{k+1} \mathbf{U}_{k+1} \mathbf{I}_{n \times r} \widehat{\mathbf{K}}_k \mathbf{H}_k \right) \boldsymbol{\epsilon}_k + \mathbf{E}_{k+1} \mathbf{U}_{k+1} \mathbf{I}_{n \times r} \widehat{\mathbf{K}}_k \mathbf{v}_k - \mathbf{w}_{k+1}.$$
(24)

5 Equation (24) describes the evolution of the true forecast error in forecast error with respect to the sub-optimal filter, and suggests, as in Eq. (5), how we may write the error evolution into the invariant upper triangular dynamics of the BLVs. Specifically, we consider the projections of the forecast error into the filtered and unfiltered subspaces in the moving frame of BLVs. Computing the evolution of $\hat{\epsilon}_{\mu}^{f}$ and $\hat{\epsilon}_{\nu}^{u}$ under the forecast-analysis update cycle in Eq. (24). Computing the evolution of $\hat{\boldsymbol{\epsilon}}_{k}^{f}$ and $\hat{\boldsymbol{\epsilon}}_{k}^{u}$, we may, we will derive the exact recursion for $\hat{\mathbf{B}}_{k}^{ff}$, i.e., the exact. This will describe the exact forecast uncertainty in the filtered subspace - under a gain which operates in the span of the leading r BLVs.

10

Evolution of unfiltered error 3.1

Here we will derive We begin by deriving the evolution of error in the unfiltered subspace, and verify by verifying that it evolves according to the free evolution. Notice first the following relation,

$$\left(\mathbf{E}_{k+1}^{\mathsf{u}}\right)^{\mathrm{T}}\mathbf{E}_{k+1}\mathbf{U}_{k+1}\mathbf{I}_{n\times r} = \mathbf{0}_{(n-r)\times r},\tag{25}$$

due to the fact that \mathbf{E}_{k+1} is an orthogonal matrix and, therefore, that the above product is equal to the lower left block of \mathbf{U}_{k+1} , 15 which is upper triangular. With substitution of Eq. (18) into in Eq. (24) for ϵ_k , multiplying on the left by $(\mathbf{E}_k^{\mathbf{u}})^{\mathrm{T}}$ to move into the unfiltered subspace, and by utilizing Eq. (25) to cancel the error in the filtered space, we find

$$\widehat{\boldsymbol{\epsilon}}_{k+1}^{\mathrm{u}} = \left(\mathbf{E}_{k+1}^{\mathrm{u}}\right)^{\mathrm{T}} \mathbf{E}_{k+1} \mathbf{U}_{k+1} \mathbf{E}_{k}^{\mathrm{T}} \left(\mathbf{E}_{k}^{\mathrm{f}} \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{f}} + \mathbf{E}_{k}^{\mathrm{u}} \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{u}}\right) - \left(\mathbf{E}_{k+1}^{\mathrm{u}}\right)^{\mathrm{T}} \mathbf{w}_{k+1}$$
(26)

$$= \mathbf{U}_{k+1}^{\mathrm{uu}} \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{u}} - \widehat{\mathbf{w}}_{k+1}^{\mathrm{u}}.$$
(27)

Equation (27) demonstrates that the evolution of the error in the unfiltered subspace follows exactly the free forecast evolution. The unfiltered error can be induced as mean zero, with covariance covariance of unfiltered error at time k equal to can be computed from Eq. (27) as

$$\widehat{\mathbf{B}}_{k}^{\mathrm{uu}} = \mathbf{U}_{k:0}^{\mathrm{uu}} \widehat{\mathbf{B}}_{0}^{\mathrm{uu}} \left(\mathbf{U}_{k:0}^{\mathrm{uu}}\right)^{\mathrm{T}} + \sum_{l=1}^{k} \mathbf{U}_{k:l}^{\mathrm{uu}} \widehat{\mathbf{Q}}_{l}^{\mathrm{uu}} \left(\mathbf{U}_{k:l}^{\mathrm{uu}}\right)^{\mathrm{T}}.$$
(28)

The initial uncertainty in the unfiltered subspace evolves as $\mathbf{U}_{k:0}^{uu} \widehat{\mathbf{B}}_{0}^{uu} (\mathbf{U}_{k:0}^{uu})^{\mathrm{T}}$ and thus, when $r > n_0$, vanishes exponentially. 25 This implies that asymptotic unfiltered error is independent of the initialization, similar to the results of Bocquet et al. (2017). The remaining sum in Eq. (28) represents the contribution to the current forecast uncertainty from the model error at all subsequent times times after initialization, propagated under the upper triangular evolution in the BLVs. Therefore, while the initial error is forgotten, the asymptotic error in the reduced rank filter here explicitly depends on the dimension of the unfiltered subspace and the local variability of the stable BLVs therein.

The error in the *i*-th BLV in Eq. (28) is given by the invariant evolution of perturbations, formerly studied by Grudzien et al. (2017): when the filtered subspace dimension is of dimension $r \ge n_0$, we can recursively, and stably, compute the unfiltered uncertainty via

$$\widehat{\mathbf{B}}_{k+1}^{uu} = \widehat{\mathbf{Q}}_{k+1}^{uu} + \mathbf{U}_{k+1}^{uu} \widehat{\mathbf{B}}_{k}^{uu} \left(\mathbf{U}_{k+1}^{uu}\right)^{\mathrm{T}}.$$
(29)

When $r < n_0$, we see explicitly that the filter will diverge as a consequence of leaving an unstable direction unfiltered.

3.2 Evolution of filtered error

5

While the evolution of the unfiltered error in Eq. (28) is a simple extension of the results from Grudzien et al. (2017), that
10 work did not explicitly consider the evolution of error in a reduced rank filter — we

We now consider the evolution of the projection of the forecast error into the filtered space, with respect to the reduced rank gain. From Eq. (24) we derive

$$\widehat{\boldsymbol{\epsilon}}_{k+1}^{\mathrm{f}} = \left(\mathbf{E}_{k+1}^{\mathrm{f}}\right)^{\mathrm{T}} \mathbf{E}_{k+1} \mathbf{U}_{k+1} \mathbf{E}_{k}^{\mathrm{T}} \left(\mathbf{E}_{k}^{\mathrm{f}} \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{f}} + \mathbf{E}_{k}^{\mathrm{u}} \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{u}}\right) - \left(\mathbf{E}_{k+1}^{\mathrm{f}}\right)^{\mathrm{T}} \mathbf{E}_{k+1} \mathbf{U}_{k+1} \mathbf{I}_{n \times r} \widehat{\mathbf{K}}_{k} \mathbf{H}_{k} \left(\mathbf{E}_{k}^{\mathrm{f}} \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{f}} + \mathbf{E}_{k}^{\mathrm{u}} \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{u}}\right) + \left(\mathbf{E}_{k+1}^{\mathrm{f}}\right)^{\mathrm{T}} \left(\mathbf{E}_{k+1} \mathbf{U}_{k+1} \mathbf{I}_{n \times r} \widehat{\mathbf{K}}_{k} \mathbf{v}_{k} - \mathbf{w}_{k+1}\right).$$
(30)

15 Similar to Eq. (25), we see that the terms

$$\left(\mathbf{E}_{k+1}^{\mathrm{f}}\right)^{\mathrm{T}}\mathbf{E}_{k+1}\mathbf{U}_{k+1}\mathbf{E}_{k}^{\mathrm{T}}\mathbf{E}_{k}^{\mathrm{f}} = \mathbf{U}_{k+1}^{\mathrm{ff}},\tag{31}$$

$$\left(\mathbf{E}_{k+1}^{\mathrm{f}}\right)^{\mathrm{T}}\mathbf{E}_{k+1}\mathbf{U}_{k+1}\mathbf{E}_{k}^{\mathrm{T}}\mathbf{E}_{k}^{\mathrm{u}} = \mathbf{U}_{k+1}^{\mathrm{fu}},\tag{32}$$

using the orthogonality of the BLVs. Therefore, substitution into Eq. (24) yields

$$\widehat{\boldsymbol{\epsilon}}_{k+1}^{\mathrm{f}} = \left(\mathbf{U}_{k+1}^{\mathrm{ff}} - \mathbf{U}_{k+1}^{\mathrm{ff}} \widehat{\mathbf{K}}_{k} \mathbf{H}_{k} \mathbf{E}_{k}^{\mathrm{f}}\right) \widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{f}}$$
(33a)

20
$$+ \mathbf{U}_{k+1}^{\mathrm{ff}} \widehat{\mathbf{K}}_k \mathbf{v}_k - \widehat{\mathbf{w}}_{k+1}^{\mathrm{f}}$$
(33b)

$$+\left(\mathbf{U}_{k+1}^{\mathrm{fu}}-\mathbf{U}_{k+1}^{\mathrm{ff}}\widehat{\mathbf{K}}_{k}\mathbf{H}_{k}\mathbf{E}_{k}^{\mathrm{u}}\right)\widehat{\boldsymbol{\epsilon}}_{k}^{\mathrm{u}}.$$
(33c)

The terms (33a) and (33b) correspond to the standard recursion on the KF forecast error. When If the filtered subspace is the entire state space (i.e., $\mathbf{E}_k^{f} \triangleq \mathbf{E}_k$, it is) the term (33c) is identically zero, and the terms (33a) and (33b) are equivalent to a change of basis for the forecast error recursion in Eq. (16), written in the invariant dynamics for the moving frame of the BLVs.

25 The remaining term in the recursion on the filtered error For r < n, the remaining term (33c) is our primary object of interest. The term Term (33c) is fundamentally different from the relationship described by terms (33a) and (33b), which represents the usual stabilizing effect of the forecast-analysis cycle. Instead, Eq. term (33c) describes two different processes:

(i) $U_{k+1}^{f_u}$ represents the purely dynamical upwelling of the unfiltered error into the filtered variables; (ii) $U_{k+1}^{f_l} \hat{\mathbf{K}}_k \mathbf{H}_k \mathbf{E}_k^u$ is the correction in the filtered subspace, due to the sensitivity of these variables to observations in the unfiltered subspace, forward propagated to time t_{k+1} ; (ii) $U_{k+1}^{f_u}$ represents the purely dynamical upwelling of the unfiltered error into the filtered variables. Generically $U_{k+1}^{f_u} - U_{k+1}^{f_l} \hat{\mathbf{K}}_k \mathbf{H}_k \mathbf{E}_k^u \neq 0$. When \mathbf{K}_k yields the restricted Bayesian update, i.e., for $\mathbf{H}_k \mathbf{E}_k^u \equiv \mathbf{0}_{d \times (u-v)}$, term

5 (33c) represents dynamical upwelling alone. Generically $\mathbf{U}_{k+1}^{fu} - \mathbf{U}_{k+1}^{ft} \hat{\mathbf{K}}_k \mathbf{H}_k \mathbf{E}_k^u \neq \mathbf{0}_{r \times (u-r)}$ and $\hat{\boldsymbol{\epsilon}}_k^u$ is Gaussian distributed with covariance given by Eq. (28), and thus is almost surely non-zero. This demonstrates that the *forecast error in the filtered* subspace depends on the unfiltered error via the forward evolution, whereas the unfiltered error does not depend on the error in the *filtered space*.

This implies that the direct application of EKF-AUS from perfect dynamics (Trevisan and Palatella, 2011b) to a noisy,

- 10 linear system systematically underestimates the uncertainty linear system with model error systematically underestimates the uncertainty in the span of the leading r BLVs. Specifically, EKF-AUS neglects the injection of the errors from the *trailing* vectors trailing vectors, $\hat{\epsilon}_k^{u}$, into the forecast of the leading vectors $\hat{\epsilon}_{k+1}^{f}$, represented in Eq. 33e(33c). Even when the uncertainty in the stable BLVs is bounded uniformly (Grudzien et al., 2017), error in the trailing BLVs moves up the Lyapunov filtration, and may cause filter divergence. In perfect, linear models, where uncertainty in the stable BLVs van-
- 15 ishes exponentially, the injection of error from the stable BLVs into the unstable subspace results in temporary mis-estimation though does not pose an issue to the asymptotic stability (Bocquet et al., 2017). However, with model error, the term (33c) demonstrates that EKF-AUS reduced rank Kalman filters must be augmented to correct a persistent underestimation.

It is important to note that the error in the unfiltered subspace moves upward through the backward Lyapunov filtration precisely because the unfiltered subspace is defined by the span of the trailing BLVs, governed by the invariant upper triangular

20 dynamics. The span of the trailing BLVs is *not equal to* not equal to the direct sum of the trailing Oseledec spaces, which are themselves *covariant* covariant with the dynamics. This choice for the unfiltered subspace comes naturally, however, as the filtered subspace (the image space of \mathbf{K}_k) is given by the span of the leading BLVs, and is equivalent to the span of the leading covariant Lyapunov vectors (Kuptsov and Parlitz, 2012, see Eq. 43).

The unfiltered subspace is uniquely defined (up to the inner product) as the *orthogonal complement* to the filtered space, 25 i.e., the subspace in which the gain makes no correction in the analysis step. In ensemble data assimilation it has been demonstrated numerically for perfect models, with weakly-nonlinear error growth, that the ensemble span of the ensemble Kalman filter and smoother typically aligns with the span of the unstable-neutral backward and covariant Lyapunov vectors (Ng et al., 2011; Bocquet and Carrassi, 2017), and thus the upwelling of unfiltered error may be considered a generic phenomena. In particular, we may consider a rank deficient EnKF to *sample the error statistics of an estimator which applies a rank deficient*

30 *analysis update, confined to the span of the leading BLVs*(Kuptsov and Parlitz, 2012, see their Eq. (43)).

In principle, data assimilation could be designed to prevent dynamical upwelling of unfiltered error by defining the unfiltered space to be the direct sum of the trailing, stable Oseledec spaces — in. In this case, unfiltered error would be covariant with the dynamics and leave the filtered error unaffected, while the filtered space would be defined by the orthogonal complement to trailing Oseledec spaces. Nevertheless, this design is artificial and would lead to poor filter performance: the . The orthogonal

35 complement to the trailing Oseledec spaces , defining the filtered space, is equal to the span of the leading forward forward (or

adjoint-covariant) Lyapunov vectors (Kuptsov and Parlitz, 2012, see Eq. 43) (Kuptsov and Parlitz, 2012, see their Eq. (43)), which has been shown not to contain the largest mass of the uncertainty (Ng et al., 2011). Furthermore, the dynamics in the forward Lyapunov vectors are defined by the <u>recursive</u> QL factorization (Kuptsov and Parlitz, 2012), and the lower triangular propagator would transmit error from the filtered subspace dynamics for the forecast error would transmit filtered uncertainty to the un-

5 filtered subspace, creating a *dynamic downwelling* which cannot be accounted for in the ensemble subspace. Defining the unfiltered space as the direct product of the stable, covariant Oseledec spaces would thus be contrary to the covariant dynamics and the properties of ensemble based covariances.

With the recursive form of the filtered error in Eq. (33), we directly compute the covariance of the filtered error, and the cross covariance of the filtered and unfiltered error, in the basis of BLVs. We define the operators

10
$$\Phi_{k+1} \triangleq \mathbf{U}_{k+1}^{\mathrm{fu}} - \mathbf{U}_{k+1}^{\mathrm{ff}} \widehat{\mathbf{K}}_k \mathbf{H}_k \mathbf{E}_k^{\mathrm{u}}, \tag{34}$$

$$\boldsymbol{\Sigma}_{k} \triangleq \left[\mathbf{I}_{r} - \widehat{\mathbf{K}}_{k} \mathbf{H}_{k} \mathbf{E}_{k}^{\mathrm{f}} \right] \widehat{\mathbf{B}}_{k}^{\mathrm{ff}} \left[\mathbf{I}_{r} - \widehat{\mathbf{K}}_{k} \mathbf{H}_{k} \mathbf{E}_{k}^{\mathrm{f}} \right]^{\mathrm{T}} + \widehat{\mathbf{K}}_{k} \mathbf{R}_{k} \widehat{\mathbf{K}}_{k}^{\mathrm{T}},$$
(35)

where Φ_k is the operator which describes the propagation of unfiltered error into the filtered space and the operator Σ_k corresponds to the analysis error covariance for the standard KF, written in the basis of BLVs.

We first consider the recursion for the cross covariance. In particular, by combining Eq. (33) and Eq. (27), we obtain

15
$$\widehat{\mathbf{B}}_{k+1}^{\text{fu}} = \Phi_{k+1} \widehat{\mathbf{B}}_{k}^{\text{uu}} \left(\mathbf{U}_{k+1}^{\text{uu}} \right)^{\text{T}} + \widehat{\mathbf{Q}}_{k+1}^{\text{fu}} + \mathbf{U}_{k+1}^{\text{ff}} \left(\mathbf{I}_{r} - \widehat{\mathbf{K}}_{k} \mathbf{H}_{k} \mathbf{E}_{k}^{\text{f}} \right) \widehat{\mathbf{B}}_{k}^{\text{fu}} \left(\mathbf{U}_{k+1}^{\text{uu}} \right)^{\text{T}}.$$
(36)

We now consider the covariance of the forecast error in the filtered variables. Using the identity in Eq. (35) we derive the recursion for the filtered error covariance $\widehat{\mathbf{B}}_{k+1}^{\text{ff}}$ as

$$\mathbf{B}_{k+1}^{\mathrm{ff}} = \mathbf{U}_{k+1}^{\mathrm{ff}} \boldsymbol{\Sigma}_{k} \left(\mathbf{U}_{k+1}^{\mathrm{ff}} \right)^{\mathrm{T}} + \widehat{\mathbf{Q}}_{k+1}^{\mathrm{ff}}$$
(37a)

$$+ \mathbf{\Phi}_{k+1} \widehat{\mathbf{B}}_{k}^{\mathrm{uu}} \mathbf{\Phi}_{k+1}^{\mathrm{T}}$$
(37b)

$$+ \mathbf{U}_{k+1}^{\mathrm{ff}} \left[\mathbf{I}_r - \widehat{\mathbf{K}}_k \mathbf{H}_k \mathbf{E}_k^{\mathrm{f}} \right] \widehat{\mathbf{B}}_k^{\mathrm{fu}} \boldsymbol{\Phi}_{k+1}^{\mathrm{T}}$$
(37c)

$$+ \boldsymbol{\Phi}_{k+1} \widehat{\mathbf{B}}_{k}^{\text{uf}} \left[\mathbf{I}_{r} - \widehat{\mathbf{K}}_{k} \mathbf{H}_{k} \mathbf{E}_{k}^{\text{f}} \right]^{\text{T}} \left(\mathbf{U}_{k+1}^{\text{ff}} \right)^{\text{T}}.$$
(37d)

When the filtered space is the whole space, i.e., $\mathbf{E}_{k}^{f} = \mathbf{E}_{k}$, the term (37a) entirely describes the evolution of the forecast error in the basis of BLVs — this is indeed just the forward propagation of the analysis error covariance for the KF. The term (37b) represents the contribution of uncertainty from the unfiltered subspace, propagated via the Φ_{k} operator, while terms (37c) and (37d) describe the forward evolution of the cross <u>covariance</u> covariances of the uncertainty, into the filtered space.

25

20

3.3 Assimilation in the unstable subspace exact (AUSE)

Having derived the exact error covariance associated to the linear, sub-optimal estimator, which applies an analysis update reduced rank Kalman estimator, characteristic of the EnKFensemble based Kalman gain in geophysical models, we will summarize the result.

Definition 4. For all k, let the matrix \mathbf{B}_k be decomposed as in Eq. (20). Then, define the recursive relationship

$$\widehat{\mathbf{B}}_{k}^{\mathrm{uu}} = \widehat{\mathbf{Q}}_{k}^{\mathrm{uu}} + \mathbf{U}_{k}^{\mathrm{uu}} \widehat{\mathbf{B}}_{k-1}^{\mathrm{uu}} (\mathbf{U}_{k}^{\mathrm{uu}})^{\mathrm{T}},$$
(38a)

$$\mathbf{\Phi}_{k+1} = \mathbf{U}_{k+1}^{\mathrm{fu}} - \mathbf{U}_{k+1}^{\mathrm{ff}} \widehat{\mathbf{K}}_k \mathbf{H}_k \mathbf{E}_k^{\mathrm{u}}, \tag{38b}$$

$$\widehat{\mathbf{B}}_{k+1}^{\text{fu}} = \Phi_{k+1} \widehat{\mathbf{B}}_{k}^{\text{uu}} \left(\mathbf{U}_{k+1}^{\text{uu}} \right)^{\text{T}} + \widehat{\mathbf{Q}}_{k+1}^{\text{fu}} + \mathbf{U}_{k+1}^{\text{ff}} \left(\mathbf{I}_{r} - \widehat{\mathbf{K}}_{k} \mathbf{H}_{k} \mathbf{E}_{k}^{\text{f}} \right) \widehat{\mathbf{B}}_{k}^{\text{fu}} \left(\mathbf{U}_{k+1}^{\text{uu}} \right)^{\text{T}},$$
(38c)

5
$$\boldsymbol{\Sigma}_{k} = \left[\mathbf{I}_{r} - \widehat{\mathbf{K}}_{k}\mathbf{H}_{k}\mathbf{E}_{k}^{\mathrm{f}}\right]\widehat{\mathbf{B}}_{k}^{\mathrm{ff}}\left[\mathbf{I}_{r} - \widehat{\mathbf{K}}_{k}\mathbf{H}_{k}\mathbf{E}_{k}^{\mathrm{f}}\right]^{\mathrm{T}} + \widehat{\mathbf{K}}_{k}\mathbf{R}_{k}\widehat{\mathbf{K}}_{k}^{\mathrm{T}}, \qquad (38d)$$

$$\widehat{\mathbf{B}}_{k+1}^{\mathrm{ff}} = \mathbf{U}_{k+1}^{\mathrm{ff}} \mathbf{\Sigma}_{k} \left(\mathbf{U}_{k+1}^{\mathrm{ff}}\right)^{\mathrm{T}} + \widehat{\mathbf{Q}}_{k+1}^{\mathrm{ff}} + \mathbf{\Phi}_{k+1} \widehat{\mathbf{B}}_{k}^{\mathrm{uu}} \mathbf{\Phi}_{k+1}^{\mathrm{T}} + \mathbf{U}_{k+1}^{\mathrm{ff}} \left[\mathbf{I}_{r} - \widehat{\mathbf{K}}_{k} \mathbf{H}_{k} \mathbf{E}_{k}^{\mathrm{f}}\right] \widehat{\mathbf{B}}_{k}^{\mathrm{fu}} \mathbf{\Phi}_{k}^{\mathrm{T}} + \mathbf{\Phi}_{k} \widehat{\mathbf{B}}_{k}^{\mathrm{uf}} \left[\mathbf{I}_{r} - \widehat{\mathbf{K}}_{k} \mathbf{H}_{k} \mathbf{E}_{k}^{\mathrm{f}}\right]^{\mathrm{T}} \left(\mathbf{U}_{k+1}^{\mathrm{ff}}\right)^{\mathrm{T}},$$
(38e)

to be the Kalman Filter, Assimilation in the Unstable Subspace Exact (KF-AUSE) Riccati equation, for a filtered subspace of dimension $1 \le r \le n$.

- 10 Proposition 1. Assume that the initial forecast errora Gaussian prior distribution is given for x₀, the state of the system defined by Eq. (6). Assume that the initial uncertainty, ε₀, has is of mean zero and covariance B₀, and suppose observations of the state are given as in Eq. (6). Let K_k be defined as in Eq. (22) for all k, such that K_k is the sub-optimal gain which makes corrections only in the Kalman estimator restricted to the span of E^f_k (rank 1 ≤ r < n). The forecast error, as in Eq. (22). Then, the forecast error defined by Eq. (16), has covariance B_k ≜ E_k B_k E^T_k, is Gaussian, mean zero, with covariance matrix
- 15 defined recursively by the KF-AUSE Riccati equation, Eq. (38).

Equation-

Proof. Proving the covariance is given by Eq. (38) is defined to be the Kalman Filter, Assimilation in the Unstable Subspace Exact (KF-AUSE) Riccati equation, for a filtered subspace of dimension r, the content of sections 3.1 and 3.2. That the error is mean zero and Gaussian is easily proven by induction.

It should be noted that the KF-AUSE Riccati equation is also valid for the true exact forecast error covariance in perfect models of a reduced rank Kalman filter in *perfect models*, where $\mathbf{Q}_k \triangleq \mathbf{0}_n$ for all k. Let $r = n_0$, $\mathbf{Q}_k \triangleq \mathbf{0}_n$ and $\mathbf{P}_k \triangleq \mathbf{E}_k^{\mathbf{f}} \mathbf{\Gamma}_k \left(\mathbf{E}_k^{\mathbf{f}}\right)^{\mathrm{T}}$ be defined as the *estimated* forecast error covariance for EKF-AUS (Trevisan and Palatella, 2011b), then the recursion is defined by

$$\boldsymbol{\Gamma}_{k+1} \triangleq \mathbf{U}_{k+1}^{\mathrm{ff}} \left[\mathbf{I}_r - \widehat{\mathbf{K}}_k \mathbf{H}_k \mathbf{E}_k^{\mathrm{f}} \right] \boldsymbol{\Gamma}_k \left[\mathbf{I}_r - \widehat{\mathbf{K}}_k \mathbf{H}_k \mathbf{E}_k^{\mathrm{f}} \right]^{\mathrm{T}} \left(\mathbf{U}_{k+1}^{\mathrm{ff}} \right)^{\mathrm{T}} + \mathbf{U}_{k+1}^{\mathrm{ff}} \widehat{\mathbf{K}}_k \mathbf{R}_k \widehat{\mathbf{K}}_k^{\mathrm{T}} \left(\mathbf{U}_{k+1}^{\mathrm{ff}} \right)^{\mathrm{T}},$$
(39)

- analogous to term (37a). Comparing Eq. (38) and Eq. (39), we see that even in perfect models the estimated error covariance of EKF-AUS in the filtered subspace and the true exact error covariance do not agree, i.e., $\Gamma_{k+1} \neq \widehat{B}_{k+1}^{\text{ff}}$. This is because the estimated AUS error in Eq. (39) neglects the upwelling of the *initial error* initial error in the unfiltered subspace, described by terms (37b), (37c) and (37d). However, in this case, the unfiltered initial the unfiltered error decays exponentially and the mis-estimation in the filtered space doesn't does not threaten filter stability: the AUS estimated error covariance converges to
- 30 the true exact error in its asymptotic limit, though possibly arithmetically (Bocquet et al., 2017).

3.4 Discussion: dynamical upwelling and covariance inflation

In ideal, linear models, the KF-AUSE Riccati equation (38) describes the exact evolution of the forecast error decomposed into a basis of BLVs, where a sub-optimal gain applies the Bayesian update with respect to an arbitrary number, r, of the leading basis vectors. Although the analysis update in Eq. (22) is sub-optimal, and defined via a rank deficient filtered subspace, the

- 5 recursion in Eq. (38) has no mis-estimation of its error statistics. We emphasize, however, We emphasize that the KF-AUSE Riccati equation (38) is not intended to provide a computational advantage — its computation requires knowledge of error in the unfiltered subspace and, in nonlinear models, a *full rank representation* full rank representation of the tangent linear dynamics. Nonetheless, this recursion is demonstrative of an important concept: in-for a reduced rank Kalman estimator that applies its analysis update in the span of the leading BLVs, the true exact error in the same span will always depend on the
- unfiltered error always depend on the unfiltered error in the trailing vectors. 10

The upwelling of uncertainty from the unfiltered subspace to the filtered (filtered) ensemble span thus explains one of the dynamical mechanisms determining the intrinsic role of covariance inflation in a reduced rank the EnKF, providing a theoretical motivation for its use to prevent filter divergence. If one wishes to correct the error in the span of the leading BLVs exactly, it requires calculating

- Generally, the reasons for using covariance inflation in the EnKF are wide, including treatment of model error, sampling 15 error, intrinsic bias, and non-Gaussianity of error distributions (Raanes et al., 2018, see section 2.2 for a survey). However, Eq. (38) demonstrates that even when excluding nonlinearity, non-Gaussianity, and intrinsic deficiencies of the EnKF, the exact correction to the error in the ensemble span requires the covariance of the unfiltered error as well as the cross covariance of the error in the filtered and unfiltered subspaces, as in Eq. (38). In practical applications practice, one must find a suitable
- 20 approximation of the upwelling phenomenon to prevent the systematic underestimation of the forecast error, and/or, extend the rank of the ensemble-based correction to control the transient growth of errors in the stable modes.

Reduced rank Kalman filters have previously corrected for the upwelling of model errors with both multiplicative and additive covariance inflation methods. For instance, although Although it was not explicitly formulated as such, the SEEK filter of Pham et al. (1998) can been seen to compensate for model errors originating in the unfiltered, stable subspace: while

- components of the model error covariance which are orthogonal to the filtered subspace are left neglected, there is an implicit 25 treatment by utilizing its forgetting factor to inflate the variance of the estimated error in the filtered subspace (Nerger et al., 2005). The contribution of the unfiltered error to the estimated error was also studied in ensemble methods by Raanes et al. (2015), in which the authors explored sampling methodology to compensate for the unresolved model errors, residing outside of the ensemble span. Our work adds to this discussion, now highlighting the *explicit mechanism* explicit mechanism which necessitates these covariance inflation techniques under a rank deficient gain.
- 30

The dynamical upwelling of model error differs from the sampling errors misrepresentation of the covariance due to truncation error or sampling error induced by nonlinear dynamics in perfect models, treated in the modified EKF-AUS-NL (Palatella and Trevisan, 2015) and in the finite size ensemble Kalman filter, (EnKF-N) (Bocquet, 2011; Bocquet et al., 2015). Rather, we We have shown that the upwelling of the unfiltered error through the Lyapunov filtration acts as a linear effect and is acute in the presence of additive model errors which are excited by transient instabilities. While the effect of the dynamical upwelling could be neglected in perfect models (Bocquet et al., 2017), the work of Grudzien et al. (2017) has demonstrated that transient instability in the span of the stable BLVs can drive the unfiltered error to become impractically large — furthermore, this error is transmitted into the filtered subspace, driving filter divergence if it is left uncorrected. However, the significance of

5 results with AUS in perfect models is not lost: if the dimension of the filtered space is sufficiently large, such that dynamical stability in the unfiltered subspace is strong enough to rapidly dissipate rapidly dissipates unfiltered errors, the effect of the upwelling may become negligible.

Uncorrected forecast errors leading to filter divergence has been previously studied in the context of perfect, nonlinear models, with an important connection to our above discussion: if an EnKF applies a correction of rank less than the number

- 10 of unstable and neutral Lyapunov exponents, it has been found the filter's estimated error can become small while the filter permanently loses track of the true trajectory (Ng et al., 2011). This behavior is easily understood in terms of the filter's failure to correct the error growth in the span of at least one of the unstable-neutral BLVs. For large geophysical models, where ensemble based covariances may be extremely rank deficient, hybridized gains have been shown to account for the failure of ensemble based gain to correct the error in the span of all the unstable-neutral BLVs (Penny, 2017). In hybridization
- 15 the Without augmenting the ensemble-based estimated error covariance is augmented by a static, climatological estimate using the climatological covariance, the rank of the estimator used for the analysis update is increased, and has the effect of applying a correction to additional modes outside of the ensemble span (Hamill and Snyder, 2000). The need to rectify the rank deficiency of the ensemble based Kalman gain takes on a new significance given our understanding of the dynamical upwelling of uncertainty. In the presence of model error, even when the ensemble rankis greater than the number of unstable-neutral
- 20 Lyapunov exponents, a hybridized gain or additive inflation (Whitaker and Hamill, 2012) may improve filter performance by keeping the errors in the span of the weakly stable BLVs small, diminishing the effect of their transient growth and upwelling.

Multiplicative inflation, acting only within the ensemble span, can rectify the under-estimation of uncertainty in the filtered subspace, due to neglecting Kalman gain, the effect of the upwelling of error. For example, the linear form of EKF-AUS does not include the upwelling of unfiltered error in its estimated covariance — inclusion of multiplicative inflation to the estimated

- 25 error covariance compensates for the upwelling of unfiltered errors which is not represented in the recursion for EKF-AUS, and simulates the terms (37b), (37c) and (37d) in the KF-AUSE recursion. Multiplicative inflation may also be used to account for mis-estimation of forecast errors resultant from nonlinear evolution, but this mis-estimation may also be accounted for using less ad hoc approaches including parameterizing this error with hyperpriors (Bocquet et al., 2015). We argue that the hyperprior in EnKF-N can, in principle, also upwelling of uncertainty into the filtered space can be selected to take into account
- 30 the structure of the ideal posterior for the reduced rank estimator, in the presence of model error, described by KF-AUSE (see also the discussion at the end of section 4.2).

Whitaker and Hamill (2012) hypothesized that additive inflation could better compensate for the effects of unresolved model error, while multiplicative inflation is best suited to account for sampling error, consistent with what was noted by Bocquet (2011) and Bocquet and Sakov (2012). This hypothesis is supported by our results and the above discussion: the combination of rank

35 deficiency of the analysis and the presence of additive model error determines an intrinsic role for covariance inflation

in ensemble based Kalman filters in chaotic, dynamical systems, due to the upwelling of unfiltered errors . However, our above discussion also highlights how the need for inflation can be mitigated by: (i) sufficiently increasing the ensemble size (Grudzien et al., 2017); (ii) rectifying the rank deficiency of the analysis update via hybridization (Penny, 2017); (iii) utilizing a hyperprior which takes into account the dynamical upwelling and mis-estimation of error (Bocquet et al., 2015); or (iv) some

5 combination of the above. In emulated with multiplicative inflation. In the following section, we numerically explore the effects of stability, transient instability, and the strength therein, on filter divergence and the need for covariance inflation with reduced rank estimators. following section, we numerically explore the interaction of the filtered subspace rank, the stability in the unfiltered directions, and multiplicative covariance inflation in relation to the effect of dynamical upwelling in reduced rank Kalman filters.

10 4 Numerical results

4.1 Experimental setup

Numerically studying the KF, we construct a discrete, linear model from the

We will explore two different discrete model configurations in which we vary the effect of nonlinearity. In the continuous model configuration with stochastic differential equations, we also achieve qualitatively similar results which will not be

15 included. It is important to remark that the analytic form for the forecast error in Eq. (38) is only a useful representation for weakly-nonlinear evolution of error, corresponding to the error evolution of the EnKF on short time scales. As the effect of nonlinearity is increased, the linear approximations utilized in our work will no longer be adequate, leading to truncation errors as discussed by, e.g., Palatella and Trevisan (2015).

In the following, we use two different formulations of the standard Lorenz 96 equations (L96) (Lorenz and Emanuel, 1998). 20 For each $m \in \{1, \dots, n\}$, the (L96) equations read $\frac{d\mathbf{x}}{dt} \triangleq \mathbf{L}(\mathbf{x})$,

$$L^{m}(\mathbf{x}) = -x^{m-2}x^{m-1} + x^{m-1}x^{m+1} - x^{m} + F$$
(40)

such that the components of the vector x are given by the variables x^m with periodic boundary conditions, $x^0 = x^n$, $x^{-1} = x^{n-1}$ and $x^{n+1} = x^1$. The term F in L96 is the forcing parameter. The tangent linear model (Kalnay, 2003) is governed by the equations of the Jacobian $\nabla_x \mathbf{L}(\mathbf{x})$, In *linear experiments*, we fix matrix, $\nabla \mathbf{L}(\mathbf{x})$.

25
$$\nabla L^m(\mathbf{x}) = (0, \cdots, -x^{m-1}, x^{m+1} - x^{m-2}, -1, x^{m-1}, 0, \cdots, 0).$$
 (41)

4.1.1 Discrete linear experiments

30

In linear experiments, we construct a discrete, linear model from the L96 system. Fixing the system dimension $n \triangleq 10$, and the linear propagator in our model \mathbf{M}_k is generated by computing the discrete, tangent linear model from the resolvent of the Jacobian equation, Eq. (41):-. This linear model satisfies Oseledec's theorem by construction (Barreira and Pesin, 2002). In generating the discrete, tangent linear model, the discretization time between observations is fixed at $\delta_k \triangleq 0.1$, $\delta_k \triangleq \delta = 0.1$ for all k. We numerically integrate the Jacobian equation with a fourth order Runge-Kutta scheme with a fixed time step of $h \triangleq 0.01$. The observational For the forcing value of F = 8, with 10 dimensions, there are three unstable, one neutral, and six stable Lyapunov exponents, i.e. $n_0 = 4$. The observation error covariance \mathbf{R}_k , model error covariance \mathbf{Q}_k and observation operator \mathbf{H}_k are all fixed as the identity \mathbf{I}_{10} , for simplicity, in this setup for simplicity.

5 In our *nonlinear experiments* with the

4.1.2 Discrete nonlinear experiments

In our experiments with the discrete extended Kalman filter (EKF) (Jazwinski, 1970) for nonlinear systems, we use Eq. (40) directly for our model state evolution, and fix the state dimension to $n \triangleq 40$. For the 40 dimensional L96, with standard forcing F = 8, the unstable neutral subspace is of dimension $n_0 = 14$, with one neutral Lyapunov exponent. The nonlinear trajectory is

10 integrated with a fourth order Runge-Kutta scheme, with a fixed step size of $h \triangleq 0.05$, with and an interval between observation times of $\delta_k \triangleq 0.1 \delta_k \triangleq \delta = 0.1$. At each observation time, before observations are given, the true trajectory is perturbed (in model space) by additive Gaussian noise with a proscribed prescribed covariance Q, fixed in time.

Let us define the nonlinear map $\Psi(t_0, t_1) : \mathbb{R}^n \to \mathbb{R}^n$ to be the flow map, generated from Eq. (40), that takes the model state from time t_0 to t_1 . Then, noting that $\Psi(t, t + \delta) = \Psi(s, s + \delta)$ for all t and s, we will define $\Psi_{\delta} \triangleq \Psi(0, \delta)$. In our experiments, the "truth" is thus evolved via the equation,

$$\mathbf{x}_{k+1} = \mathbf{\Psi}_{\delta}(\mathbf{x}_k) + \mathbf{w}_{k+1},\tag{42}$$

 $\mathbf{w}_{k+1} \sim N(\mathbf{0}, \mathbf{Q})$, while the mean trajectory of the "model" state is given by the deterministic evolution, $\mathbf{x}_{k+1}^{b} = \Psi_{\delta}(\mathbf{x}_{k}^{b})$. In our experimental design, the extended Kalman filter estimates the state of the nonlinear "true" state, perturbed by the noise \mathbf{w}_{k} , Eq. (42), and \mathbf{M}_{k+1} (the linear propagator for the covariance forward evolution) is defined by the map $\mathbf{M}_{k+1} \triangleq \nabla \Psi_{\delta}|_{\mathbf{x}_{k}^{b}}$.

The matrix Q is defined by the circulant matrix with $c_0 = 0.5, c_1 = 0.25, c_2 = 0.125, c_{39} = 0.25, c_{38} = 0.125$ and all other entries zero,

	$\left(c_{0} \right)$	c_{39}		c_2	c_1
	c_1	c_0	c_{39}		c_2
$\mathbf{Q} \triangleq$	÷	c_1	c_0	·	÷
	c_{38}		·	·	c_{39}
	(c_{39})	c_{38}		c_1	c_0 ,

The choice of the circulant matrix reflects the stationary statistics and periodic nature of the L96 model, and the fact that we wish to highlight the effect of analytically resolving complex model error. The observational observation error covariance matrix is fixed as $0.25 * \mathbf{I}_{40}$, the scalar matrix with eigenvalue 0.25. The observation operator is fixed in time as $\mathbf{H}_k \triangleq \mathbf{I}_{40}$.

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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. with the configuration using the circulant covariance matrix, **Q**, drawn specifically from Raanes et al. (2015). The interval

4.2 Linear Kalman filter

In a linear setting, we compute the exact forecast error covariance of KF-AUSE via the recursive Riccati equation, Eq. (38),

- 5 and compare it with that of the KF, for which the filtered space is the entire model space. This illustrates the ideal performance of a rank deficient , sub-optimal filter without estimation errors; we compare this relative to a full rank correction, where the sub-optimal filter applies corrections only to the leading r BLVs and the filter where the forecast error is treated analytically, without mis-estimation of the error covariances. We compute the average eigenvalues of the forecast covariance matrix for each the KF and KF-AUSE over 100,000 parallel forecast cycles and examine the stratification of the uncertainty in a basis of
- 10 BLVs, i.e., how strongly the covariance projects into each direction. Specifically, for both the KF and KF-AUSE we compute the average projection coefficient of the forecast error covariance into the *i*-th BLV at each forecast time, $(\mathbf{E}_k^i)^T \mathbf{B}_k \mathbf{E}_k^i$, and average this coefficient over *k*.

In order to visualize the full spectrum of the forecast error covariance, we use the 10 dimensional discrete, tangent-linear model of L96 as the linear model for our KF-AUSE experiments. For the standard forcing value of F = 8, there are three

15 unstable, one neutral, and six stable Lyapunov exponents, i.e, $n_0 = 4$. In Fig. 1, the averaged eigenvalues of the KF and KF-AUSE forecast error covariance are plotted, with triangle markers, differentiated by color. In each subplot, the KF remains the same but we vary the dimension of the filtered subspace, r, for KF-AUSE.

In the top left panel of Fig. 1 the number of corrected modes is equal to n_0 , corresponding to correcting the error in the unstable-neutral subspace. Here, the leading eigenvalue of the forecast uncertainty of KF-AUSE is orders of magnitude above

- 20 the forecast uncertainty in the KF. This should be contrasted with perfect models where, asymptotically, there can only be four non-zero eigenvalues, and under generic conditions, the KF and EKF-AUS will coincide (Bocquet et al., 2017). In accordance with the results of Grudzien et al. (2017), correcting <u>error in</u> the first stable mode (r = 5) brings a substantial reduction in forecast uncertainty (see top right Fig. 1). We see the forecast uncertainty likewise diminishes as each additional mode is corrected, as the KF-AUSE covariance converges to that of the KF.
- It is of special interest how the projection coefficients of the forecast error covariance relates to the dimension of the filtered subspace, r. In the KF, the projection coefficients are closely aligned with the eigenvalue profile, descending in the order of the Lyapunov exponents, and this line is not pictured due to the redundancy. However, in the forecast error covariance of KF-AUSE, the leading *uncorrected stable mode* is the dominant direction for the uncertainty among the BLVs, systematically across $n_0 \le r < n$, with projection coefficient on the order of the leading eigenvalue. This distinguishes the setting of additive
- 30 model error from perfect models where the projection coefficients of the forecast error covariance in the stable BLVs will be zero asymptotically (Gurumoorthy et al., 2017). In a straightforward implementation of KF-AUS in the presence of model error, which neglects corrections to the weakly stable modes and the upwelling of the unfiltered error on the order of the uncertainty in $\mathbf{B}_{k}^{n_{0}+1}$, this unfiltered error will furthermore transmit into the filtered subspace, driving filter divergence.



Figure 1. Eigenvalues of the KF and KF-AUSE forecast error covariance plotted with triangles. Projection coefficients of the KF-AUSE forecast error covariance plotted with X's. Dimension of the KF-AUSE filtered subspace is r. Note the log scale of the y-axis.

The structure of the forecast error covariance of KF-AUSE, revealed in the basis of BLVs, has special significance for the rank deficient EnKF. Particularly, we may understand the covariance of KF-AUSE to express the ideal forecast error of the rank deficient EnKF, and should guide any independent, identically distributed (**iid**) sampling scheme which represents this error distribution. The hyperprior in EnKF-N (Bocquet et al., 2015), used to describe the mis-estimation of the true error statistics

- 5 from a finite iid draw of samples, may also incorporate the structure of the ideal posterior under a rank deficient gain. Similarly to how the hyperprior for the covariance in EnKF-N is restricted to the cone of positive semi-definite symmetric matrices in perfect models, its extension to additive model error may incorporate a restriction to the covariance matrices which share the stratification of uncertainty expressed in KF-AUSE. Likewise, when unfiltered error is known to be large, the structure of the KF-AUSE covariance demonstrates the benefit of hybridization to rectify the rank deficiency: even if the hybrid gain induces
- 10 sampling error by corrupting the recursion for the estimated error, controlling the unfiltered error by some means can diminish the leading order source of uncertainty.

4.3 Extended Discrete extended Kalman filterwith nonlinear model dynamics

In our nonlinear experiments experiments with the discrete extended Kalman filter, we compute the analysis root mean square error (**RMSE**) of each the: (i) full rank extended Kalman filter (**EKF**), (ii) EKF-AUS and (iii) EKF-AUSE, for which Eq. (38)

15 is used to compute the estimated covariance and rank r gain. We will study the effect of analytically resolving the unfiltered error as compared with the straightforward implementation of EKF-AUS, which will make no correction to account for the unfiltered error complementary to the anomaly subspace in the trailing BLVs, or its upwelling into the leading BLVs.

Recall that EKF-AUS so far has historically only been studied in the perfect model scenario without additive model errors — we implement EKF-AUS in the presence of model error by computing a rank r estimated error covariance, which

includes the projection of the model error covariance, \mathbf{Q}_k into the span of the leading BLVs in the forecast Riccati equation, i.e. $(\mathbf{E}_k^{\rm f})^{\rm T} \mathbf{Q}_k \mathbf{E}_k^{\rm f} = \widehat{\mathbf{Q}}_k^{\rm ff}$. This corresponds to utilizing only the first line of the recursion for $\widehat{\mathbf{B}}_k^{\rm ff}$, Eq. (37a), to compute the estimated forecast error covariance of EKF-AUS. The implementation of EKF-AUSE thus differs by utilizing a *full rank* full rank ensemble of anomalies to compute the complete Riccati equation, Eq. (38). We utilize this *n* dimensional covariance

5 equation to compare the effect of the additional inflation, by including the terms in Eq. (37b), Eq. (37c) and Eq. (37d) in the correction to the filtered space, on the performance of filter RMSE.

We study the performance of EKF-AUS/E when the dimension of the filtered subspace is *greater than* greater than, or equal to, the dimension of the unstable-neutral subspace; the case $r < n_0$ will trivially lead to divergence (Bocquet et al., 2017). For the 40 dimensional L96, with standard forcing F = 8, $n_0 = 14$, with one neutral Lyapunov exponent. In Fig. 2, we plot the

10 analysis RMSE of EKF-AUS and EKF-AUSE with triangles and X's respectively, while we vary over the dimension of the filtered subspace, with the RMSE computed over 100,000 analysis cycles.

To benchmark the performance of EKF-AUS/E, we plot the observational observation error standard deviation and the analysis RMSE of the standard, full rank EKF in horizontal lines — the algorithms for EKF-AUS/E are tantamount to a change of basis for the EKF when the filtered subspace is equal to the full space, and thus this is the logical point of comparison. We are

15 interested in finding the necessary dimension of the filtered subspace such that EKF-AUS/E has an RMSE which: (i) performs better than the observational observation error standard deviation and (ii) performs comparably to filtering the entire space. When the RMSE of EKF-AUS/E falls below the observational observation error standard deviation, the filter has a forecast performance superior to initializing observations directly in the model; when it performs closely to the EKF, the filter can be considered close to optimal performance, while utilizing a sub-optimal correction based on only r < n directions.



Figure 2. 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 observation error standard deviation and EKF analysis RMSE. Note the log scale of the *y*-axis.

In Fig. 2, when the the dimension of the filtered subspace for both AUS/E reaches 28 the difference between both EKF-AUS/E and the full-rank EKF becomes negligible. The RMSE of the: (i) EKF is approximately 0.198; (ii) EKF-AUS, r = 28, is approximately 0.205. The fact that EKF-AUS obtains near optimal performance, representing the uncertainty in the leading r = 28 BLVs while neglecting the remaining, corroborates the claim of

- 5 Grudzien et al. (2017): in the presence of model noise, the filter correction should also incorporate weakly stable directions that can be instantaneously unstable. It is of particular interest, however, that the convergence of EKF-AUSE to the skill of the full rank EKF is substantially faster: EKF-AUSE obtains adequate filter performance (RMSE lower than observational observation error standard deviation) by correcting the error in only 16 BLVs while EKF-AUS requires a correction of rank 19. For other scalings of the matrix **Q**, multiplying **Q** by 0.1, 0.2, 1.5, 2, changing the observation dimension, e.g. d = 20 or
- 10 d = 30, and by varying the time between observations, e.g. $\delta_k = 0.01$ or 0.5 we obtain, we obtain qualitatively similar results, that are not pictured here. The profiles of the curves in Fig. 2 are similar across these experimental configurations: the RMSE of EKF-AUSE is improved over EKF-AUS by including the analyticalinflation factor analytically resolving the effect of the analytical, and the RMSE approaches an adequate/optimal level with a smaller dimension for the filtered space. This pattern demonstrates that including the inflation factor to the filtered subspace, resolving the upwelling of the unfiltered error, reduces
- 15 the necessary ensemble rank to obtain a stable filter. We emphasize again that EKF-AUSE does not represent a computational advantage as a *full-rank* full rank set of perturbations is used to describe the analytic form for the upwelling of the error.

To explain the convergence of EKF-AUS, which doesn't account for the unfiltered subspace, to the full rank EKF, we We look at the behavior of the local Lyapunov exponents for the L96 model to explain the convergence of EKF-AUS to the full rank EKF. In Fig. 3 we show the box plot statistics of the local Lyapunov exponents for exponents 14 through 28 of the L96 model. Exponent $\lambda_{14} = 0$, and the remaining pictured exponents correspond to the leading, stable BLVs. We emphasize that the local Lyapunov exponents of λ_{15} through λ_{18} , though having negative mean, are sufficiently unstable locally such that

EKF-AUS diverges when it disregards the upwelling of the error from these asymptotically stable modes.

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When the filtered subspace for EKF-AUS is of dimension 19, such that the leading *unfiltered* unfiltered BLV corresponds to λ₂₀, all unfiltered Lyapunov exponents have over 75% of local realizations strictly stable; this corresponds to the rank
25 when EKF-AUS has adequate performance. Likewise, the difference between EKF-AUS/E and the EKF is negligible when the leading unfiltered BLV corresponds to λ₂₉, with only 1.51% of its local realizations being non-negative. These findings are consistent with the results in Grudzien et al. (2017): in the presence of model error, unconstrained forecast error is strongly forced by the error in BLVs, which are asymptotically stable but, that experience strong and frequent local instability instabilities.

Finally, we are interested in how analytically computing the upwelling of error from the unfiltered subspace, as in EKF-30 AUSE, compares with a homogeneous, multiplicative inflation applied to the EKF-AUS algorithm. Multiplicative scalar inflation is among the most common approaches to mitigate for sampling and model error in Kalman filtering methods, and it is widely used in operational environmental forecasts utilizing the EnKF(Whitaker and Hamill, 2012). In our experiments, if $\mathbf{P}_k \triangleq (\mathbf{E}_k^{\text{ff}})^T (\Psi_k + \widehat{\mathbf{Q}}_k^{\text{ff}}) \mathbf{E}_k^{\text{ff}}$ is . We define $\mathbf{P}_k \triangleq (\mathbf{E}_k^{\text{ff}})^T (\Gamma_k + \widehat{\mathbf{Q}}_k^{\text{ff}}) \mathbf{E}_k^{\text{ff}}$ to be the estimated forecast error of EKF-AUS, we define the where Γ_k is defined in Eq. (39). The inflated covariance \mathbf{P}_k^I as $\mathbf{P}_k^I = (\mathbf{E}_k^{\text{ff}})^T (\alpha \Psi_k + \widehat{\mathbf{Q}}_k^{\text{ff}}) \mathbf{E}_k^{\text{ff}}$ is defined as 35 $\mathbf{P}_k^I = (\mathbf{E}_k^{\text{ff}})^T (\alpha \Gamma_k + \widehat{\mathbf{Q}}_k^{\text{ff}}) \mathbf{E}_k^{\text{ff}}$ for some chosen scalar α . The inflated covariance \mathbf{P}_k^I is used to compute the sub-optimal



Figure 3. Box plot statistics of the local Lyapunov exponents, for Lyapunov exponents 14 through 24, over 100,000 realizations for the 40 dimensional L96 model. The mean (*i*-th Lyapunov exponent) is plotted as a triangle with median the horizontal line. Box contains inner two quartiles of realizations, with whiskers extending to 1.5 the inner quartile width from the third and first quartile. Outliers are realizations outside of this range, plotted individually.

reduced rank gain, as a simple way to compensate for the underestimation of the forecast error when using the recursion in Eq. (37a). Furthermore, the inflated covariance is subsequently used in the recursion for the subsequent analysis and forecast error covariances.

From the results in Fig. 2, we select the dimension of the filtered subspace to be 17, such that EKF-AUSE has RMSE below the observational observation error standard deviation while EKF-AUS (without inflation) has diverged. In Fig. 4, we plot the analysis RMSE of EKF-AUSE, with filtered subspace dimension 17, the observational observation error standard deviation and the full-rank EKF analysis RMSE as in Fig. 2 as horizontal lines. Additionally, we plot the analysis RMSE (y-axis) of EKF-AUS as a function of the inflation value (the x-axis) applied to the forecast error covariance, with the inflation valuesplotted as . The inflation values, α , are defined as the evenly spaced points in [1,4] at increments of 0.1, denoted by triangles. The RMSE

10 of all the above is again computed over 100,000 forecast cycles.

Figure 4 highlights distinctly the impact of including multiplicative inflation to EKF-AUS: the performance of EKF-AUS with inflation quickly becomes comparable to the analytically resolved EKF-AUSE, which in this case, represents the lowermost bound for the RMSE of EKF-AUS with homogeneous inflation. The lowest RMSE for EKF-AUS with inflation, realized in Fig. 4, is approximately 0.322 compared to the RMSE of EKF-AUSE, approximately 0.304. Figure 4 confirms the role

15 of multiplicative inflation as compensating for the upwelling of unfiltered error under weakly-nonlinear error growth, and explains the underlying dynamical mechanism: multiplicative inflation brings the estimated forecast error covariance of EKF-AUS closer to the ideal covariance given by EKF-AUSE.



Figure 4. Analysis RMSE of EKF-AUS (<u>y-axis</u>), correction rank 17, with multiplicative inflation plotted versus the inflation value α (<u>x-axis</u>). Horizontal lines are the observational observation error standard deviation, EKF-AUSE and EKF analysis RMSE. Note the log scale of the *y*-axis.

It is important to remark that the analytic form for the inflation in Eq. (38) is only a useful representation for the weakly-nonlinear evolution of

5 Discussion: the reduced rank KF covariance and gain augmentation

- Whitaker and Hamill (2012) found evidence that additive inflation could better compensate for the effects of unresolved model
 error, while multiplicative inflation is best suited to account for sampling error; for more nonlinear error evolution, multiplicative inflation will also compensate for the sampling erroras described by Palatella and Trevisan (2015), and the performance of EKF-AUSE is not expected to provide a bound in this regime. The ways that multiplicative inflation can mitigate the nonlinear sources of error are discussed by, e. g., Bocquet (2011); Bocquet et al. (2015) consistent with what was noted by Bocquet (2011) and Bocquet and Sakov (2012). This hypothesis is supported by our results as follows. The combination of
- 10 rank deficiency of the analysis and the presence of additive model error determines an intrinsic role for covariance inflation in ensemble-based Kalman filters due to the persistent, residual unfiltered model error and its resultant upwelling into the ensemble span. The dynamical upwelling forms the basis for a systematic underestimation of the uncertainty in the ensemble space, as demonstrated in Fig. 2. This can be compensated for with multiplicative inflation in the ensemble span, which emulates the additional uncertainty that is neglected in the standard, reduced rank Kalman filter recursion — this effect is
- 15 <u>exhibited in Fig. 4</u>. Figure 5 gives a conceptual diagram of the number of samples (<u>ensemble members</u>) needed to prevent divergence of the EnKF in different dynamical regimes, and the effect of multiplicative inflation on this requirement.



Figure 5. Conceptual representation of the number of samples necessary to prevent divergence of the EnKF in different filtering regimes. Dark green represents near-optimal filter performance and dark red represents filter divergence. In perfect-linear models, only n_0 samples are needed for an asymptotically optimal performance. Without inflation, in noisy linear and perfect, weakly-nonlinear regimes, near optimal performance can be obtained by correcting error in all modes up to the moderately stable BLVs — here n_{WS} corresponds to the number of unstable/ neutra/ weakly-stable modes, while n_{mS} furthermore includes moderately-stable modes. Additional samples may be necessary to control error growth with noisy, weakly-nonlinear evolution. Multiplicative inflation corrects for the upwelling from the uncorrected stable modes so that near optimal performance can be obtained when the error growth in unstable/ neutral/ weakly-stable modes are corrected.

However, multiplicative inflation (in the ensemble span) neglects the fundamental issue that the unfiltered error lying outside of the ensemble span can be the major driver of the uncertainty in a reduced rank filter with model error. Figure 1 shows that when the upwelling is analytically resolved, the largest uncertainty typically lies in the leading unfiltered BLV, even when this is an asymptotically stable mode. We provide a conceptual, two-dimensional visualization of the difference between the

- 5 standard (full rank) Kalman filter forecast error covariance and the reduced rank Kalman filter forecast error covariance in Fig. 6. Unless local Lyapunov exponents in the unfiltered space are strongly stable, thereby rapidly dissipating the unfiltered perturbations of model error, transient instabilities can make the unfiltered errors large enough to prevent useful state estimates (Grudzien et al., 2017). This is evidenced in Fig. 4 where neither EKF-AUSE or EKF-AUS, with multiplicative inflation, achieve an RMSE comparable with the full rank EKF. For this reason, it is highly pertinent to explore the role of augmenting
- 10 the EnKF gain with a sub-optimal correction which provides some control on the transient error growth in the orthogonal



Figure 6. Conceptual digram of the shape of the exact forecast error covariance of the full rank Kalman filter and the exact reduced rank Kalman filter. The U axis represents the span of the unstable-neutral BLVs, where the forecast uncertainty projects most strongly in the standard (full rank) Kalman filter. The S axis represents the span of the stable BLVs, where the uncertainty is the largest (though bounded), for a reduced rank Kalman filter that neglects corrections to these modes. The comparison between the full rank and reduced rank Kalman filter covariance corresponds to the behavior exhibited in the curves in Fig. 1.

complement to the ensemble span. Ideally, some constraint on the unfiltered error, even if sub-optimal, would further close the gap between the RMSE of EKF-AUSE and EKF in Fig. 4.

This issue of instability forcing unfiltered error is even more acute in practice. For large geophysical models, computational limitations may prohibit the use of an ensemble of size sufficient to even span the unstable-neutral subspace, let alone the

- 5 weakly stable modes which exhibit transient instabilities. In this case, the unfiltered error in the unstable-neutral modes can grow, possibly exponentially, and the filter may experience catastrophic filter divergence, due to the failure of the ensemble-based gain to correct the error in the span of all the unstable-neutral BLVs (Penny, 2017). In hybridization, the ensemble-based Kalman estimator is augmented by a static, climatologically based estimator — using a background climatological covariance, the rank of the estimator used for the analysis update is increased, and has the effect of applying a correction to additional
- 10 modes outside of the ensemble span (Hamill and Snyder, 2000). Likewise, the use of additive, random perturbations to the ensemble-based covariance has been shown to prevent filter divergence by rectifying the rank deficiency of the covariance, and therefore the rank deficiency of the ensemble-based gain (Corazza et al., 2007).

However, there is considerable difficulty in mathematically analyzing the exact recursive form for a sub-optimal augmentation of the ensemble-based covariance and ensemble-based Kalman gain. Although the dynamical upwelling of errors is a generic

- 15 dynamical feature of these systems, the one-way dependence of the error in the leading BLVs on the trailing BLVs does not persist, due to the introduction of estimation errors into the trailing modes via the augmented gain. Moreover, the surrogate covariance used to constrain error in the trailing BLVs will not generally agree with the exact error covariance in the trailing BLVs, making a closed form more difficult to derive. In this setting, it may be more appropriate to derive heuristic methods which attempt to: (i) provide some corrections in the trailing BLVs, albeit sub-optimal; (ii) describe the dynamical upwelling
- 20 of the residual error from the trailing BLVs into the leading BLVs; and (iii) describe the cross covariances, between the leading and trailing BLVs, with respect to the corrections.

Multiplicative inflation may be used in this case to account for mis-estimation of forecast errors resulting from these approximations, but this mis-estimation can also be accounted for using less ad hoc approaches including parameterizing this error with hyperpriors (Bocquet et al., 2015). We argue that the hyperprior in the EnKF-N can, in principle, also be selected to take into account the dynamical upwelling exhibited by KF-AUSE. Recently, an extension of the EnKF-N to the presence

5 of model error has utilized an adaptive multiplicative inflation term to compensate for model errors (Raanes et al., 2018), but we suggest that an alternative approach including gain augmentation (Bocquet et al., 2015, suggested in section 7), and a hyperprior parametrizing the resulting error distribution, including dynamical upwelling, would be a logical extension for future research.

6 Conclusions

- 10 Assimilation in the Unstable Subspace (AUS) (AUS) has provided a useful conceptual framework for understanding the dynamical properties of data assimilation cycling in perfect models. Both numerical and mathematical results have confirmed the underlying hypothesis of Anna Trevisan: in the setting of perfect, chaotic models, the evolution of uncertainty is confined to a space characterized by non-negative Lyapunov exponents, typically of much lower dimension than the full model state space (Palatella et al., 2013). In ensemble data assimilation, we see that the asymptotic characteristics of the anomalies exhibit
- 15 these properties, which can be exploited to reduce the computational burden of the assimilation cycle (Bocquet and Carrassi, 2017). This phenomena has recently also been exploited_utilized to reduce the numerical cost of synchronization in dynamical shadowing based data assimilation methods (de Leeuw et al., 2017). The work of Palatella and Grasso (2018) has furthermore proposed an extension of the EKF-AUS-NL algorithm to account for parametric model errors.
- This paper <u>now</u> demonstrates that the framework of AUS can likewise be used to understand the underlying mechanisms for the evolution of uncertainty <u>in reduced rank filters applied to chaotic dynamics in the presence of additive model error</u> for <u>ensemble-based filters in chaotic models with additive errors</u>. Due to the high dimensional models, and unresolved physical processes, this circumstance is ubiquitous in high-dimensional geoscience applications where standard EnKFs are extremely rank deficient. Utilizing the Lyapunov filtration for the backward vectors, we have shown how unfiltered error, outside of the span of the anomalies, is transmitted by the dynamics into the filtered subspace. In perfect models, or when stability in the
- 25 unfiltered subspace is sufficiently strong, this effect can be neglected due to the rapid dissipation of unfiltered errors. However, Grudzien et al. (2017) demonstrate how weakly stable modes of high variance can go through periods of transient instability, exciting unfiltered error. The dynamic upwelling of unfiltered error, characterized by the term (33c), acts as a linear effect on filters with small ensemble sizes. Under weakly-nonlinear error growth, the span of the anomalies projects strongly onto the span of the leading BLVs therefore, the Riccati equation, Eq. (38), highlights an important, and previously unexplained,

mechanism driving the need for covariance inflation in reduced rank, ensemble based ensemble-based Kalman filters.

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The role of inflation we describe differs from previous studies, e.g., the work of Palatella and Trevisan (2015), which studied the nonlinear interactions of error in perfect models. The phenomena of dynamical upwelling is also independent of the misestimation of error due to a finite sample size representing the true error statistics (Bocquet et al., 2015). Rather, we exhibit an

effect which can contribute to filter divergence over short time scales in ensemble data assimilation, when the error dynamics are linear or weakly-nonlinear, if and uncertainty is forced by additive model errors. This persistent dynamical upwelling of errors from the unfiltered space into the ensemble subspace is a phenomena which we prove analytically in linear models, and demonstrate numerically to be a valid approximation of weakly-nonlinear error growth in nonlinear models for reduced

5 rank extended Kalman filters. The KF-AUSE Riceati equation, Eq. (38), therefore represents the ideal recursion for the error covariance of a reduced rank Kalman filter.

If we treat the standard EnKF as Monte Carlo estimate of the error statistics characteristic of the KF-AUSE covariance, the ideal uncertainty for a reduced rank Kalman filterEg. (38), the dynamical upwelling explains the intrinsic role for covariance inflation in the reduced rank EnKF. But in addition, our work also confirms that the role of our results also suggest that this

- 10 need for covariance inflation may potentially be mitigated by: (i) sufficiently increasing the ensemble size to include asymptotically stable modes that produce transient instabilities, such that unfiltered error is rapidly dissipated by stable dynamics; (ii) increasing the rank of the analysis update itself, with a hybridized gain; (iii) parameterizing the upwelling of error via a hyperprior which targets the ideal evolution true forecast errorevolution of forecast errors; or (iv) some combination of the above. Our new understanding of the dynamics of error propagation thus opens new opportunities in algorithm design, where
- 15 the above techniques may be used directly to ameliorate the effects of dynamical upwelling.

Where there is dynamical chaos, AUS will continue to be a robust framework for the theory of data assimilation in physical models. Understanding the dynamical mechanisms that govern the evolution of error in fully nonlinear data assimilation, e.g., the unstable-neutral manifolds of the (stochastic) chaotic attractor, will be the subject of future research and may be considered the logical extension of the framework put forward by Anna Trevisan — her insight to the underlying processes in assimilation will continue to provide inspiration to both developers and practitioners of data assimilation methods.

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Conceptual representation of the number of samples necessary to prevent divergence of the EnKF in different filtering regimes. Dark green represents near-optimal filter performance and dark red represents filter divergence. In perfect-linear models, only n₀ samples are needed for an asymptotically optimal performance. Without inflation, in noisy linear and perfect weakly-nonlinear regimes, near optimal performance can be obtained by correcting all modes up to the moderately stable

BLVs — here n_{ws} corresponds to the number of unstable/ neutral weakly-stable modes, while n_{ms} furthermore includes 15 moderately-stable modes. Additional samples may be necessary to control error growth with noisy, weakly-nonlinear evolution. Multiplicative inflation corrects for the upwelling from the uncorrected stable modes so that near optimal performance can be obtained when the error growth in unstable/ neutral/ weakly-stable modes are corrected.