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1 Assessing the Performance of Data Assimilation Algorithms which employ Linear
2 Error Feedback

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Data assimilation means to find an (approximate) trajectory of a dynamical model that (approximately) matches a given set of observations. A direct evaluation of the trajectory against the available observations is likely to yield a too optimistic view of performance, since the observations were already used to find the solution. A possible remedy is presented which simply consists of estimating that optimism, thereby giving a more realistic picture of the ‘out of sample’ performance. Our approach is inspired by methods from statistical learning employed for model selection and assessment purposes in statistics. Applying similar ideas to data assimilation algorithms yields an operationally viable means of assessment. The approach can be used to improve the performance of models or the data assimilation itself. This is illustrated by optimising the feedback gain for data assimilation employing linear feedback.

8 Data assimilation means to find an (approximate) trajectory of a dynamical
9 model that (approximately) matches a given set of observations. A fundamental
10 problem of data assimilation experiments in atmospheric contexts is that there
11 is no possibility of replication, that is, truly “out of sample” observations from
12 the same underlying flow pattern but with independent observational errors are
13 typically not available. A direct evaluation against the available observations
14 is likely to yield unrealistic results though, since the observations were already
15 used to find the solution. A possible remedy is presented which simply consists
16 of estimating that optimism, thereby giving a more realistic picture of the ‘out of
17 sample’ performance. The approach is particularly simple when applied to data
18 assimilation algorithms employing linear error feedback. A realistic performance
19 assessment is obtained by comparing with the true trajectory. In addition this
20 method provides a simple and efficient means to determine the optimal feedback
21 gain operationally since it only requires known quantities to be calculated. The
22 optimality of this gain is verified numerically. Further, we illustrate theoretical
23 results which demonstrate that in linear systems with gaussian perturbations,
24 the feedback thus determined will approach the optimal (Kalman) gain in the
25 limit of large observational windows (the proof will be given elsewhere).

26 I. INTRODUCTION

27 Data Assimilation involves the incorporation of observational data into a numerical model
28 to produce a model state that accurately describes the observed reality. This procedure
29 uses an explicit dynamical model for the time evolution of the observed reality. The results
30 produced by data assimilation must satisfy two requirements. Firstly they must be close to
31 the observations up to a certain degree of accuracy and secondly they should be consistent
32 with the dynamical model to a certain degree of accuracy. In other words, the trajectory
33 produced by data assimilation must be close to the observations and it must be close to
34 being an orbit of the model.

35 Once the observations have been used to estimate these trajectories, they should not be
36 used to evaluate the performance of the model (at least not without precaution) as this

might give unrealistic results. Simply comparing the observations with the output of the data assimilation scheme will provide an overly optimistic picture of performance. Moreover, assessing the performance using this tracking error could easily be cheated. An example is taking the output to be the observations themselves.

As we will see in Section II, a more realistic evaluation of the performance needs to take into account that the output and the observation errors are correlated. To this end, we investigate the concept of out-of-sample error from statistics and adapt it to the problem of data assimilation. In statistics, estimates of the out-of-sample error are used to measure how well a statistical model, after fitting it to observations, generalises to unseen data^{1,2}. Although the concept of the out-of-sample error is a very general one, actual implementations differ considerably depending on the structure of the estimation problem. Further, a fundamental assumption often made in statistics is that the observations (conditionally on the explanatory variables) are independent and identically distributed. In the case of linear regression models, a popular statistic for model selection in statistical learning is the Cp statistic^{3,4}. Other examples are Akaike's Information Criterion (AIC) or the Bayesian Information Criterion (BIC). These concepts differ in terms of precise interpretation and range of applicability.

The aim of this paper is to provide similar tools in the context of data assimilation. The underlying problem is essentially the same as in statistics. Suppose a time series of observations has been assimilated into a dynamical model. Then the output should be close to hypothetical observations from the same flow patterns but with independent errors. If the results are not close to these hypothetical observations, then this can only mean that the model is in fact not able to explain the dynamics underlying the observations. The out-of-sample error should be a measure of how close the output will be to such hypothetical observations. Although observations from the same flow pattern but with independent errors are typically not available in practice, we show that the out-of-sample error can be estimated using terms that are operationally available. Specifically we show that the out-of-sample error is the sum of the tracking error and a term which we call the optimism. This optimism gives us a representation of how the model and observations depend on each other and it quantifies how much the tracking error misestimates the out-of-sample error. The derived expression is reminiscent of the Cp statistic used in model selection in statistical learning^{3,4}. We show that the optimism takes a very simple form if we assume that the model employs a linear error feedback. There are many data assimilation algorithms that implement such a

69 feedback⁵. More details and references concerning such algorithms can be found in section II.

70 Wahba *et al.*⁶ apply the ideas of out-of-sample performance to data assimilation for linear
71 systems. In this publication they use generalised cross validation to get an estimate of the
72 true performance. The key equation in this paper is equation (2.11) which is similar to
73 equation (7.46) in Hastie, Tibshirani, and Friedman³ with the new aspect being the stochastic
74 approximation to the denominator. The results presented in Wahba *et al.*⁶ however, apply
75 only in a linear context. As it will be shown, the analysis presented in our paper does not
76 require linear models but merely linear error feedback.

77 We stress that although in terms of the problem we are addressing there is a strong
78 similarity between statistics and data assimilation, our analysis will be different. For instance,
79 although the data assimilation uses linear error feedback, the dependence of the output
80 on the observations as a whole is nonlinear, due to the nonlinearity of the dynamic model.
81 Further, the observations are not independent. The derivation of the Cp statistic, AIC,
82 BIC and many other related concepts used in statistics however assumes either linearity,
83 independence or both (see Hastie, Tibshirani, and Friedman³, Sec 7.4).

84 We demonstrate the usefulness of our approach with three numerical examples. In all
85 three cases, we consider a simple data assimilation scheme by means of filtering with a
86 linear error feedback. A persistent problem in practice is to find a suitable feedback. The
87 feedback acts as a coupling between the true dynamics and the model. If the coupling is too
88 weak the stability of the system cannot be guaranteed while if the coupling is too strong,
89 results deteriorate because the noise will be overly attenuated. Striking the right balance
90 requires a reliable assessment of the performance which is provided by our estimate of the
91 out-of-sample performance. Note that this is relevant even in the case of linear systems
92 with gaussian perturbations as computing the theoretically optimal Kalman Gain requires
93 knowledge of the dynamical noise which is usually not available in practice. Our experiments
94 demonstrate that the technique can be used in situations where the feedback gain matrix is
95 completely unspecified and also in situations where it has a pre-determined structure but
96 contains unknown parameters.

97 In section II we define the tracking error, out-of-sample error and the optimism. These
98 considerations are valid for any data assimilation algorithm in the case of additive observa-
99 tional noise. We also consider general data assimilation algorithms which employ linear error
100 feedback and determine an analytical expression for the optimism. Section III contains several

numerical experiments. In Section III A we apply the methodology to a linear system with gaussian perturbations. We minimise an estimate of the out-of-sample error to determine a feedback gain. We then compare this with the asymptotic Kalman Gain which is known to be optimal in this situation. Our experiments suggest that the gain determined numerically agrees with the optimal Kalman Gain in the limit of large observation windows. We discuss a theoretical result which confirms this finding. Next we consider a situation in which the data assimilation algorithm is constrained to have poles in certain locations which determines the gain up to a single parameter. This parameter is determined by minimising an estimate of the out-of-sample error.

The remaining experiments consider non linear systems. In Section III B we consider a system in Lur'e form. These systems are special in that, despite being non linear, they permit observers with linear error dynamics. Again a linear feedback is used and we show how an estimate of the out-of-sample error can be used to determine the feedback. The performance of this feedback is assessed numerically by considering the error between the reconstructed and the true orbit. Our results indicate that this strategy of choosing the feedback gives close to optimal performance. Repeating the experiment with the Lorenz '96 system in Section III C confirm the results.

II. TRACKING ERROR, OUTPUT ERROR AND OPTIMISM IN DATA ASSIMILATION

Data assimilation is the procedure by which trajectories $\{z_n \in \mathbb{R}^D, n = 1, \dots, N\}$ (in some state space which we take to be $\mathbb{R}^D$) are computed with the help of a dynamical model and observations, $\{\eta_n, n = 1, \dots, N\}$. These trajectories should reproduce the observations up to some degree of accuracy for all $n = 1, \dots, N$. We express this latter part of the procedure formally as: The output $y_n = h(z_n)$ is close to the observations $\{\eta_n, n = 1, \dots, N\}$ up to some degree of accuracy, where $h : \mathbb{R}^D \rightarrow \mathbb{R}^d$ is a function which maps the model's state space into the observation space. This function is usually part of the problem specification. The exact structure of the model and of h is not important at this stage.

Suppose we have observations $\{\eta_n \in \mathbb{R}^d, n = 1, \dots, N\}$ from some real world dynamical phenomenon. We assume η_n can be written as

$$\eta_n = \zeta_n + \sigma r_n \tag{1}$$

where $\{\zeta_n, n = 1, \dots, N\}$ are unknown quantities representing the desired signal, and $\sigma \in \mathbb{R}^{d \times d}$ is the observational error standard deviation. We assume that $\{\zeta_n, n = 1, \dots, N\}$ can be modelled as some stochastic process. The observation errors or noise, $\{r_n, n = 1, \dots, N\}$ are assumed to be independent with mean $\mathbb{E}r_n = 0$ and variance $\mathbb{E}r_n r_n^T = \mathbb{1}$ and they are independent of $\{\zeta_n, n = 1, \dots, N\}$.

Deviation of the output from the observations can be quantified by means of the tracking error,

$$E_T = \mathbb{E}[y_n - \eta_n]^2. \quad (2)$$

The tracking error though is not a very useful performance measure of data assimilation approaches. It is not difficult to design algorithms which achieve zero tracking error by simply using the observations as output, that is any DA algorithm which satisfies $y_n = \eta_n$, $n = 1, \dots, N$ achieves optimal performance with respect to E_T as a performance measure.

A performance measure which is much harder to hedge is the output error

$$E_O = \mathbb{E}[y_n - \zeta_n]^2. \quad (3)$$

A useful relation between E_O and E_T can be established. Substituting the expression (1) for the observations into (2) and expanding, we get

$$E_T = \mathbb{E}[y_n - \eta_n]^2 = \mathbb{E}[y_n - \zeta_n]^2 + \text{tr}(\sigma^T \sigma) - 2\text{tr}(\sigma \mathbb{E}[r_n y_n^T]) \quad (4)$$

since ζ_n and r_n are independent. The notation 'tr' denotes the trace of the matrix.

We re-write this as

$$E_O + \text{tr}(\sigma^T \sigma) = \mathbb{E}[y_n - \eta_n]^2 + 2\text{tr}(\sigma \mathbb{E}[r_n y_n^T]). \quad (5)$$

The term $2\sigma \mathbb{E}[r_n y_n^T]$ is called the *optimism*. The optimism should be understood as a correlation between r_n and y_n , where y_n depends on $\{r_k, k = 1, \dots, N\}$. It is a measure of how much the tracking error misestimates the output error. We will argue that both the optimism and the tracking error (i.e the first term on the right hand side of (5)) can be estimated using operationally available quantities. This will give us a handle on the output error which is, as we have argued, directly related to the true performance of the data assimilation.

The quantity $E_O + \sigma^2$ can be interpreted as an "Out-of-sample error" as follows: Define hypothetical observations

$$\eta'_n = \zeta_n + r'_n, \quad n = 1, \dots, N \quad (6)$$

155 where $\{\zeta_n, n = 1, \dots, N\}$ is as before, $\{r'_n, n = 1, \dots, N\}$ is a process with the same
 156 distribution as $\{r_n, n = 1, \dots, N\}$ but independent from it. Then the out-of-sample error is
 157 the error between $\{y_n, n = 1 \dots, N\}$ and $\{\eta'_n, n = 1, \dots, N\}$, which can be written as

$$\mathbb{E}[y_n - \eta'_n]^2 = E_O + \sigma^2. \quad (7)$$

158 The key difference between the tracking error and the out-of-sample error is the absence of
 159 correlation between $\{y_n, n = 1 \dots, N\}$ and $\{r'_n, n = 1, \dots, N\}$ in the latter, which is precisely
 160 the optimism.

161 Equation (5) shows that the tracking error augmented with further terms, can be a useful
 162 measure of performance. Further the tracking error and optimism are relatively easy to
 163 estimate. In our experiments we will estimate the tracking error through an empirical average,
 164 namely

$$\hat{E}_T = \frac{1}{N} \sum_{k=1}^N (y_k - \eta_k)^2. \quad (8)$$

165 Estimates of the optimism will be discussed next.

166 We will first calculate a general expression for the optimism for data assimilation schemes
 167 which employ a linear error feedback. Most operational data assimilation schemes work in
 168 cycles over time. The *background field*, $\hat{z}_n$, is computed at the start of each cycle and usually
 169 it is based on information from previous cycles. Since any cycle uses observations available
 170 up to that point, the background field at time n only depends on $\eta_1, \dots, \eta_{n-1}$. Nonetheless,
 171 the background field $\hat{z}_n$ is supposed to be a first guess of the the state of the system at time
 172 n .

173 In this paper we consider data assimilation algorithms which combine the new observation
 174 and background through a relationship of the form

$$z_n = \hat{z}_n + \mathbf{K}_n(\eta_n - h(\hat{z}_n)) \quad (9)$$

175 where $\mathbf{K}_n$ is a $D \times d$ matrix and can depend on $\eta_1, \dots, \eta_{n-1}$ but not on η_n . As before, the
 176 mapping $h : \mathbb{R}^D \rightarrow \mathbb{R}^d$, maps points from model state space to observation space. The
 177 modified background, z_n , is referred to as the *analysis*.

178 The matrix $\mathbf{K}_n$ is the error feedback gain. Equation (9) tells us that the analysis has a
 179 linear dependence on the current observation, η_n and it depends on the previous observations
 180 through $\mathbf{K}_n$ and $\hat{z}_n$. Data assimilation schemes that fall into the presented approach include

Successive Correction Method (SCM)^{7,8}; Optimal Interpolation (OI)⁹; 3D-Var^{10,11}; Kalman
 Filter variants,¹² and certain Synchronisation approaches. Synchronisation between dynamical
 systems has been studied for some time, see for example Pikovsky, Rosenblum, and Kurths¹³;
 Huijberts, Nijmeijer, and Pogromsky¹⁴; Boccaletti *et al.*¹⁵. Synchronisation in the setting of
 data assimilation has also been studied, see Bröcker and Szendro¹⁶; Szendro, Rodríguez, and
 Lopez¹⁷; Yang, Baker, and Li¹⁸. These methods differ only on the approach they take to
 calculate the background $\hat{z}_n$ and the matrix $\mathbf{K}_n$ ⁵.

We now consider the optimism as in (5) in the context of DA scheme with linear feedback
 as in (9). We assume that the function $h(x_n)$ is linear so that $h(x_n) = \mathbf{H}x_n$, where $\mathbf{H}$ is a
 $d \times D$ matrix. Then,

$$\mathbb{E}[r_n y_n^T] = \mathbb{E}[r_n (\mathbf{H}z_n)^T] = \mathbb{E}[r_n z_n^T] \mathbf{H}^T \quad (10)$$

$$= \mathbb{E}[r_n \{(\mathbb{1} - \mathbf{K}_n \mathbf{H})\hat{z}_n + \mathbf{K}_n(\zeta_n + \sigma r_n)\}^T] \mathbf{H}^T \quad (11)$$

$$= \mathbb{E}[r_n ((\mathbb{1} - \mathbf{K}_n \mathbf{H})\hat{z}_n)^T] \mathbf{H}^T \\ + \mathbb{E}[r_n (\mathbf{K}_n \zeta_n)^T] \mathbf{H}^T + \mathbb{E}[r_n (\mathbf{H} \mathbf{K}_n \sigma r_n)^T] \quad (12)$$

$$= \mathbb{E}[r_n r_n^T \sigma^T \mathbf{K}_n^T] \mathbf{H}^T \quad (13)$$

$$= \text{tr}(\mathbb{E}[r_n r_n^T] \sigma^T \overline{\mathbf{K}}_n^T \mathbf{H}^T) \quad (14)$$

where $\overline{\mathbf{K}}_n = \mathbb{E}[\mathbf{K}_n]$. The first two equalities, (10) and (11), are obtained by substituting the
 relevant information while (12) is obtained by simply expanding the previous equation. The
 derivation from (12) to (13) requires some explanation. Notice first that only the third term
 of (12) survives. The first term is equal to zero because $\hat{z}_n$ and $\mathbf{K}_n$ are uncorrelated with
 r_n . The second term is also equal to zero because ζ_n is independent of r_n and because the
 coupling matrix $\mathbf{K}_n$ depends on the observations $(\eta_1 \dots \eta_{n-1})$ and thus is uncorrelated with
 r_n .

Therefore, we are only left with the third term of (12) in (13). Since $\mathbb{E}(r_n r_n^T) = \mathbb{1}$, (14)
 implies that

$$2\text{tr}(\sigma \mathbb{E}[r_n y_n^T]) = 2\text{tr}(\sigma \cdot \sigma^T \overline{\mathbf{K}}_n^T \mathbf{H}^T). \quad (15)$$

In the case when $d = 1$, which is the case we consider in the numerical experiments later,
 this reduces to

$$2\sigma \mathbb{E}[y_n r_n] = 2\mathbf{H} \overline{\mathbf{K}}_n \sigma^2. \quad (16)$$

199 We recall that the assumptions necessary to derive this formula are a linear observation
 200 operator, r_n is independent of $\{\eta_1, \dots, \eta_{n-1}\}$, $\mathbb{E}r_n = 0$, $\mathbb{E}r_n r_n^T = \mathbb{1}$ and $\mathbf{K}_n$ depends only on
 201 the observations $(\eta_1, \dots, \eta_{n-1})$.

202 In our numerical experiments we approximate the expected value of a random variable by
 203 the empirical mean. In particular E_T is replaced by its empirical average in (5), resulting in
 204 the following estimate for E_O for all subsequent numerical experiments (in which $\mathbf{K}_n$ is in
 205 fact constant):

$$\hat{E}_O = \hat{E}_T + \frac{1}{N} \sum_{n=1}^N 2\sigma^2 \text{tr}(\bar{\mathbf{K}}_n^T \mathbf{H}^T) - \sigma^2. \quad (17)$$

206 Let us briefly digress on how the background $\hat{z}_n$ and $\mathbf{K}_n$ might be calculated in the context
 207 of synchronisation, although this is in fact irrelevant for the optimism. Suppose that the
 208 reality is given by the non linear dynamical system

$$\begin{aligned} x_{n+1} &= \tilde{f}(x_n) \\ \zeta_n &= \tilde{h}(x_n) \\ \eta_n &= \zeta_n + \sigma r_n \end{aligned} \quad (18)$$

209 where $x_n \in \mathbb{R}^D$ is referred to as the state and $\zeta_n \in \mathbb{R}^d$ are the true observations. For this
 210 non linear dynamical system we construct a sequential scheme

$$\begin{aligned} \hat{z}_{n+1} &= f(z_n) \\ z_{n+1} &= \hat{z}_{n+1} - \mathbf{K}_n(h(\hat{z}_{n+1}) - \eta_{n+1}) \\ y_n &= h(z_n) \end{aligned} \quad (19)$$

211 where $\mathbf{K}_n$ is a $D \times d$ coupling matrix which depends on the observations $\eta_1, \dots, \eta_n$ but
 212 not on η_{n+1} ; and y_n is the model output where we hope that $y_n \cong \zeta_n$. Here f and h are
 213 approximations to the functions $\tilde{f}$ and $\tilde{h}$, respectively. The coupling introduced in this
 214 scheme creates a linear feedback, in the sense that the error between $y_n = h(\hat{z}_n)$ and the
 215 observations η_n is fed back into the model.

216 Synchronisation refers to a situation in which, due to coupling, the error $y_n - \eta_n$ becomes
 217 small asymptotically irrespective of the initial conditions for the model¹³. Often a control
 218 theoretic approach is taken to determine conditions which guarantee the model output,
 219 $y_n = h(z_n)$, converging to the observations, η_n or even z_n converging to x_n (strictly speaking,
 220 the difference converging to zero; note that this can only be expected in case of noise free
 221 observations).

It has been highlighted above that the tracking error is not an ideal measure of performance; however the output error is and moreover, it can be calculated using terms that are readily available. An important question that arises in operational practice is to how to choose the gain matrix $\mathbf{K}$. The numerical experiments detailed below consider different conditions under which to select the appropriate coupling matrix to use in the assimilation. For the first linear experiment we consider arbitrary candidates for the gain matrix, while for the second linear experiment we consider gains that guarantee a certain structure of the system matrix (or more specifically the poles thereof).

III. NUMERICAL EXPERIMENTS

We now demonstrate the usefulness of our approach with three numerical examples. In Section III A we present the methodology for a linear system with gaussian perturbations. We minimise an estimate of the out-of-sample error to determine a feedback gain and compare this with the asymptotic Kalman Gain which is known to be optimal in this situation.

The remaining two experiments concern nonlinear systems. In Section III B we present numerical results for the Hénon Map and in Section III C results are established for the Lorenz'96 System. Again a linear feedback is used and we show how an estimate of the out-of-sample error can be used to determine the feedback.

There is some repetition in the obtained results, however this repetition validates our approach across different experiments. The three systems we consider all use a data assimilation scheme that employs linear error feedback. However the underlying systems in each are different; one is linear, one is in Lur'e form and one is nonlinear. The similarities in the results confirm that our methodology applies to many different dynamical systems.

A. Numerical Experiment 1: Linear Map

In this first linear example the following experimental setup was used: The reality is given by

$$x_{n+1} = \underbrace{\begin{bmatrix} -1 & 10 \\ 0 & 0.5 \end{bmatrix}}_{\mathbf{A}} x_n + \rho q_{n+1} \quad (20)$$

247 with corresponding observations

$$\eta_n = \mathbf{H}x_n + \sigma r_n \quad (21)$$

248 where $\mathbf{H} = [1 \ 0]$, $\zeta_n = \mathbf{H}x_n$ and $\rho \in \mathbb{R}^{D \times D}$ is the model error standard deviation. We assume
 249 that the model and observations are corrupted by random noise. For these experiments we
 250 have $x_n \in \mathbb{R}^2$ and $\eta_n \in \mathbb{R}$. The model errors, q_n , are assumed to be serially independent
 251 errors with mean $\mathbb{E}q_n = 0$ and variance $\mathbb{E}q_n q_n^T = \mathbb{1}$.

252 We set up an observer analogous to our sequential scheme (19),

$$z_{n+1} = \hat{z}_{n+1} + \mathbf{K}_n(\eta_{n+1} - \mathbf{H}\hat{z}_{n+1}), \quad y_n = \mathbf{H}z_n \quad (22)$$

253 where

$$\hat{z}_{n+1} = \underbrace{\begin{bmatrix} -1 & 10 \\ 0 & 0.5 \end{bmatrix}}_{\mathbf{A}} z_n. \quad (23)$$

254 In this case the model is coupled to the observations through a linear coupling term which
 255 is dependent on the difference between the actual output and the expected output value
 256 based on the next estimate of the state. For these experiments we will take the coupling
 257 matrix $\mathbf{K}_n$ to be constant so from here on we write $\mathbf{K}_n = \mathbf{K}$.

258 The error dynamics in this linear example are given by

$$\begin{aligned} e_{n+1} &= x_{n+1} - z_{n+1} \\ &= (\mathbf{A} - \mathbf{KHA})e_n + \mathbf{K}r_{n+1} - (\mathbb{1} - \mathbf{KH})q_{n+1}. \end{aligned} \quad (24)$$

259 Since the noisy part of the error dynamics (Eq. 24) is stationary, synchronisation can
 260 be guaranteed if the eigenvalues of the matrix $(\mathbf{A} - \mathbf{KHA})$ all lie within the unit circle.
 261 Synchronisation here means that the error dynamics is asymptotically stationary with finite
 262 covariance. To achieve this, we use a result from control theory, for which we need a few
 263 definitions. Let $\mathbf{HA} = \mathbf{C}$ so that the error dynamics are described by the system matrix
 264 $(\mathbf{A} - \mathbf{KC})$. A pair of matrices $(\mathbf{A}, \mathbf{C})$ is called *observable* if the observability matrix

$$\mathcal{O} = [\mathbf{C} \ \mathbf{CA} \ \mathbf{CA}^2 \ \dots \ \mathbf{CA}^{D-1}]^T \quad (25)$$

265 has full rank. If this condition holds then the poles of the matrix $(\mathbf{A} - \mathbf{KC})$ can be placed
 266 anywhere in the complex plane by proper selection of $\mathbf{K}$. In particular they can be placed
 267 within the unit circle¹⁹.

268 In our example, $x_n \in \mathbb{R}^2$ so our observability matrix is

$$\mathcal{O} = [\mathbf{H}\mathbf{A} \quad \mathbf{H}\mathbf{A}^2]^T. \quad (26)$$

269 It is straightforward to check that the linear system we are working with here is observable
270 even though $\mathbf{A}$ is not stable.

271 It is well known in Kalman Filter theory (see for example Anderson and Moore²⁰) that
272 the optimal gain matrix $\boldsymbol{\kappa}_n$ for a linear filter (in the sense of giving least error covariance) is
273 the Kalman Gain which is defined by

$$\boldsymbol{\kappa}_n = \Sigma_n \mathbf{H}^T (\mathbf{H} \Sigma_n \mathbf{H}^T + \sigma^2)^{-1} \quad (27)$$

274 where Σ_n is the error covariance matrix defined by $\Sigma_n = \mathbb{E}[(\hat{z}_n - x_n)(\hat{z}_n - x_n)^T]$ and expressed
275 by the following recursive equation,

$$\Sigma_n = \mathbf{A}(\Sigma_n - \Sigma_n \mathbf{H}^T (\mathbf{H} \Sigma_n \mathbf{H}^T + \sigma^2)^{-1} \mathbf{H} \Sigma_n) \mathbf{A}^T + \rho^2 \cdot \mathbb{1}. \quad (28)$$

276 Kalman Filter theory states that for n large, the error covariance Σ_n converges to Σ_∞ which
277 is the solution to

$$\Sigma_\infty = \mathbf{A}[\Sigma_\infty - \Sigma_\infty \mathbf{H}^T (\mathbf{H} \Sigma_\infty \mathbf{H}^T + \sigma^2)^{-1} \mathbf{H} \Sigma_\infty] \mathbf{A}^T + \rho^2 \cdot \mathbb{1}. \quad (29)$$

278 This in turn implies that the Kalman Gain (27) converges to the asymptotic gain which is
279 defined by

$$\boldsymbol{\kappa}_\infty = \Sigma_\infty \mathbf{H}^T (\mathbf{H} \Sigma_\infty \mathbf{H}^T + \mathbf{R})^{-1} \quad (30)$$

280 The asymptotic gain, $\boldsymbol{\kappa}_\infty$, is obtained by solving the Discrete Algebraic Riccati Equation
281 (DARE) given by (29) and using the solution to calculate (30). Using Maple's inbuilt DARE
282 solver we were able to find the solution to this equation for the experimental setup described
283 above. The Algebraic Riccati Equation is solved using the method described in Arnold III
284 and Laub²¹.

285 The aim of this experiment is to estimate the optimal gain matrix, $\boldsymbol{\kappa}_\infty$ without referring
286 to the DARE, in particular without knowledge of ρ . We do this by minimising the empirical
287 out-of-sample error with respect to $\mathbf{K}$. In other words, our estimate of $\boldsymbol{\kappa}_\infty$ is the minimiser of
288 $\hat{E}_O$ for a large (but finite) set of observations (paragraph a. below). This strategy is motivated
289 by our previous discussion about the out-of-sample error being an adequate measure of
290 performance. In fact, in the context of linear systems, we can prove (see Appendix A for

291 details) that the out-of-sample error is equivalent (in a certain sense) to the asymptotic
 292 covariance of e_n as a measure of performance. We also stress that estimating the optimism
 293 only requires knowledge of $\mathbf{A}, \mathbf{H}, \sigma$ but not ρ , the model noise. This is the term that is
 294 difficult to determine operationally, so estimating the optimism in an operational situation is
 295 possible as all the required terms are readily available. In paragraph b. we discuss a variant
 296 of this experiment where the gain matrix is supposed to be optimal under the constraint
 297 that the characteristic polynomial has a certain shape.

298 *a. Estimating optimal gain matrix* The results obtained in this first experiment are
 299 shown in Figure 1. The model noise is iid with $\mathbb{E}q_n = 0$, $\mathbb{E}q_n q_n^T = 1$ and $\rho = 0.01$ while
 300 for the observational noise, which was also iid with mean zero and variance one, we used
 301 $\sigma = 0.1$. We let n vary between zero and 3.5×10^5 . For each n the empirical out-of-sample
 302 error was minimised and the minimiser was recorded as an estimate of κ_∞ . The experiment
 303 was repeated for 100 realisations of the observational noise, r_n so that the estimates were
 304 different every time. As a measure of accuracy, 90% confidence intervals were constructed.
 305 We expect that the estimates converge to the asymptotic gain κ_∞ given by the solution of
 306 (29,30).

307 The results obtained are shown in Figure 1. Figure 1(a) shows a plot in blue squares
 308 of the quantity $\|\mathbf{K} - \kappa_\infty\| / \|\kappa_\infty\|$ against n . The figure shows that the gain matrix that
 309 minimises the out-of-sample error converges exponentially to the asymptotic gain. Moreover,
 310 it is illustrated in Figure 1(c) that the eigenvalues of the matrix $(\mathbf{A} - \mathbf{KHA})$ for each gain
 311 minimising the out-of-sample error, converge to the eigenvalues of the matrix $(\mathbf{A} - \kappa_\infty \mathbf{H}\mathbf{A})$.
 312 Figure 1(c) shows the quantity $\|\lambda - \lambda_\infty\| / \|\lambda_\infty\|$ against n in blue diamonds, where λ
 313 represents the eigenvalues of the matrix $(\mathbf{A} - \mathbf{KHA})$. The convergence of the eigenvalues is
 314 also exponential. The values of these eigenvalues confirm that the minimising gains stabilise
 315 the system since all of them are within the unit circle.

316 The remaining two figures in Figure 1 show a log plot of the same information outlined
 317 above. Figure 1(b) represents the convergence of the gain matrices while Figure 1(d) shows
 318 the same information for the eigenvalues. Both plots are almost straight lines as expected
 319 since the convergence has already been noted to be exponential. The addition to these plots
 320 are the 90% confidence intervals. As previously stated, the experiment was repeated for 100
 321 realisations of the observational noise and the plotted confidence intervals represents the
 322 uncertainty in the numerical experiment. The lower limit of the error bars was taken at the

FIG. 1. Figure 1(a) shows the convergence of the gain minimising the out-of-sample error to the asymptotic gain for increasing n . We plot the quantity $\|\mathbf{K} - \kappa_\infty\| / \|\kappa_\infty\|$ against n in blue squares. Figure 1(b) shows a log plot of the same information with 90% confidence intervals. Figure 1(c) shows the quantity $\|\lambda - \lambda_\infty\| / \|\lambda_\infty\|$ against n in blue diamonds, where $\lambda = (\lambda_1, \lambda_2)$ represents the eigenvalues of the matrix $(\mathbf{A} - \mathbf{KHA})$. It is evident that the eigenvalues of the matrix $(\mathbf{A} - \mathbf{KHA})$ for each gain minimising the out-of-sample error, converge to the eigenvalues of the matrix $(\mathbf{A} - \kappa_\infty \mathbf{HA})$, with n increasing. Figure 1(d) shows a log plot of the same information with 90% confidence intervals.

FIG. 2. Figure 2(a) shows a plot of the tracking error in blue squares and the out-of-sample error in black diamonds. The errors are plotted against the inverse of α for $\sigma = 0.1$ and $\rho = 0.01$. Figure 2(b) shows a plot of the out-of-sample error in black diamonds for 100 realisations of the noise r_n with $\sigma = 0.1$ as well as the state error in blue circles. They are displayed for the range of α where the minimum occurs. The error bars in both curves represent 90% confidence intervals. The black vertical line draws attention to the minimum of the out-of-sample error which coincides with the minimum of the state error.

323 fifth percentile while the upper limit was taken at the 95th percentile thus creating the 90%
 324 confidence intervals.

325 *b. Gain Matrix with Symmetric Poles* In this part of the linear numerical experiment,
 326 we want $(\mathbf{A} - \mathbf{KHA})$ to have a certain characteristic polynomial. Suppose that the desired
 327 characteristic equation is given by

$$q(\lambda) = (\lambda + \alpha)(\lambda - \alpha) \quad (31)$$

328 so that $\lambda_1 = -\lambda_2$ and $|\lambda_1| = |\lambda_2| = \alpha$. The appropriate $\mathbf{K}$ for a desired characteristic
 329 polynomial, $q(\lambda)$ of the matrix $(\mathbf{A} - \mathbf{KHA})$ follows from Ackermann's Formula¹⁹ which is
 330 given by

$$\mathbf{K} = q(A)\mathcal{O}^{-1}[0 \dots 1]^T \quad (32)$$

331 where $\mathcal{O}$ is the observability matrix defined in (26).

332 The results obtained from our numerical experiment to test the validity of (16) are shown
 333 in Figure 2. Figure 2(a) shows a plot of the tracking error in blue squares and the out-of-
 334 sample error in black diamonds. The out-of-sample error calculated via (16) is equivalent to
 335 calculating the out-of-sample error explicitly using the output error. We can see that the
 336 tracking error tends to zero with decreasing α . This is what we expected and is confirmed
 337 by using our analytical expression for the optimism.

338 It is clear from Figure 2(a) that while the tracking error tends to zero, the out-of-sample
 339 error initially decreases and then increases resulting in a well-defined minimum. This is
 340 because as the coupling strength increases, the observations are tracked too closely and thus
 341 the output adapts too closely to the observations resulting in an increase of the out-of-sample
 342 error. On the other hand when α is large and the coupling strength is weak, the observations
 343 are tracked poorly resulting in large tracking and out-of-sample errors. In these experiments
 344 α was varied between 0 and 1 with the assimilation window taken to be $N = 10000$.

345 The well defined minimum of the out-of-sample error is also shown in Figure 2(b).
 346 Figure 2(b) shows the out-of-sample error in black diamonds for the range of α where
 347 the minimum occurs. The figure shows the out-of-sample error for 100 realisations of the
 348 observation noise r_n with $\sigma = 0.1$ so that the sample estimate is different each time. The
 349 error bars in the plot represent 90% confidence intervals for each value of α . The lower
 350 limit of the error bars is taken at the fifth percentile, while the upper limit is taken at the
 351 95th percentile, hence obtained 90% confidence intervals as a measure of accuracy. Some
 352 further experiments using different values of σ were carried out however the results are
 353 not included here. The results produced were the same as the ones presented in this paper;
 354 the only difference was the size of the error bars produced. A smaller value of σ resulted in
 355 smaller error bars.

356 To quantify the variation of the parameter α in this experiment, we considered the
 357 following calculation. The mean value of the optimal α plus/minus one standard deviation
 358 in this case is

$$\bar{\alpha}^* \pm \sqrt{(\alpha^* - \bar{\alpha}^*)^2} = 0.3698 \pm 0.028. \quad (33)$$

359 The second plot in Figure 2(b) illustrates the state error. This estimate of the state error
 360 is defined by

$$\hat{E}_S = \frac{1}{N} \sum_{n=1}^N (z_n - x_n)^2. \quad (34)$$

361 This is the error that ultimately wants to be analysed and minimised in data assimilation
 362 experiments. However, because the model noise (ρq_n) is difficult to determine, we cannot
 363 explicitly analyse the state error which is why we consider errors we can calculate, namely
 364 the tracking, output or out-of-sample errors. We can plot the state error $\hat{E}_S$ in this example
 365 because we have access to it, however in general this is not possible. The vertical line in
 366 Figure 2(b) draws attention to the minimum of the out-of-sample error. It is evident that the
 367 state error also has a minimum and the plot suggests that the minima of the out-of-sample
 368 and the state error are the same. Again, we ran the experiment for 100 realisations and
 369 plotted the error bars with 90% confidence intervals.

370 B. Numerical Experiment 2: Hénon Map

371 In this experiment, the reality is given by

$$x_{n+1} = \underbrace{\begin{bmatrix} a & b \\ 1 & 0 \end{bmatrix}}_A x_n + c \begin{bmatrix} (\mathbf{H}x_n)^2 \\ 0 \end{bmatrix} + d \quad (35)$$

372 which for the values $a = 0$, $b = 0.3$, $c = -1.4$, $d = [1 \ 0]^T$ is the chaotic Hénon Map with
 373 corresponding observations

$$\eta_n = \mathbf{H}x_n + \sigma r_n \quad (36)$$

374 where $\mathbf{H} = [1 \ 0]$, and $\zeta_n = \mathbf{H}x_n$. The model describing the reality is completely deterministic
 375 and we assume that the observations are corrupted by random noise. Notice that we now
 376 have a non linear term in the dynamical system. Such systems are said to be in Lur'e form.

377 Once again we consider data assimilation by means of synchronisation so we set up an
 378 observer roughly analogous to our sequential scheme (19) with certain differences,

$$z_{n+1} = \hat{z}_{n+1} + \mathbf{K}_n(\eta_{n+1} - \mathbf{H}\hat{z}_{n+1}), \quad y_n = \mathbf{H}z_n \quad (37)$$

379 where

$$\hat{z}_{n+1} = \underbrace{\begin{bmatrix} a & b \\ 1 & 0 \end{bmatrix}}_A z_n + c \begin{bmatrix} \eta_n^2 \\ 0 \end{bmatrix} + d \quad (38)$$

380 where a, b, c, d are the same as for the reality. In this case as in the first example, the
 381 model is coupled to the observations through a linear coupling term which is dependent on

the difference between the actual output and the output value expected based on the next estimate of the state. However there is also a non linear coupling introduced here by the presence of η_n^2 in the background term. Note that (16) is still valid nonetheless because $\hat{z}_{n+1}$ is still uncorrelated with r_{n+1} . For these experiments we will take the coupling matrix $\mathbf{K}_n$ to be constant so from here on in we write $\mathbf{K}_n = \mathbf{K}$.

We need to choose the matrix $\mathbf{K}$ appropriately so that we can vary the coupling strength. For illustration purposes consider the error dynamics for the noise-free situation so that $\eta_n = \mathbf{H}x_n$. The error dynamics in this case are given by

$$\begin{aligned}
e_{n+1} &= x_{n+1} - z_{n+1} \\
&= x_{n+1} - \hat{z}_{n+1} - \mathbf{KH}(x_{n+1} - \hat{z}_{n+1}) \\
&= (\mathbb{I} - \mathbf{KH})(x_{n+1} - \hat{z}_{n+1}) \\
&= (\mathbf{A} - \mathbf{KHA})(x_n - z_n) \\
&= (\mathbf{A} - \mathbf{KHA})e_n.
\end{aligned} \tag{39}$$

The matrix $(\mathbf{A} - \mathbf{KHA})$ is stable even if $\mathbf{K} = \mathbf{0}$. This means that synchronisation occurs even if there is no linear coupling between the model output and observations because of the non linear coupling introduced in the model (38). The eigenvalues for such a case are $\lambda_{1,2} = \pm\sqrt{b}$, where b is as in the matrix $\mathbf{A}$. However, it might be that with noise, the out-of-sample error is not optimal for this coupling and can be improved by some additional linear coupling.

It is straightforward to check that the system we are working with here is observable provided that $b \neq 0$. The appropriate $\mathbf{K}$ for a desired characteristic polynomial, $q(\lambda)$ of the matrix $(\mathbf{A} - \mathbf{KHA})$ again follows from Ackermann's Formula (32). Suppose that the desired characteristic equation is given by

$$q(\lambda) = (\lambda + \alpha)(\lambda - \alpha) \tag{40}$$

so that $\lambda_1 = -\lambda_2$ and $|\lambda_1| = |\lambda_2| = \alpha$. Then by Ackermann's formula we get

$$\mathbf{K} = \begin{bmatrix} 1 - \alpha^2/b \\ a\alpha^2/b^2 \end{bmatrix} \Rightarrow \mathbf{HK} = 1 - \frac{\alpha^2}{b} \tag{41}$$

401 where $a = 0$ and $b = 0.3$ as in the matrix $\mathbf{A}$. From (41) we see that $\mathbf{H}\mathbf{K} = 1$ if $\alpha = 0$. Thus,

$$y_n = \mathbf{H}z_n = (\mathbb{1} - \mathbf{H}\mathbf{K})\mathbf{H}\hat{z}_n + \mathbf{H}\mathbf{K}\eta_n \rightarrow \eta_n, \quad (42)$$

402 meaning that our data assimilation scheme simply replaces y_n with η_n , implying that the
 403 tracking error is zero. In other words, in this example, it is possible to render the eigenvalues
 404 of the error dynamics exactly zero and also to obtain zero tracking error. However, the data
 405 assimilation is not perfect and the out-of-sample and state errors will not necessarily be
 406 small.

407 Therefore, from (16) we know that

$$\hat{E}_O = \hat{E}_T - 2\sigma^2 \left(1 - \frac{\alpha^2}{b}\right) - \sigma^2. \quad (43)$$

408 Recall that the aim of this work is to find a way to estimate the out-of-sample error to get a
 409 more realistic picture of model performance. We have already determined that when there
 410 is no linear coupling (i.e. $\mathbf{K} = \mathbf{0}$) the system is stable and synchronisation occurs. We can
 411 see from (43) that this happens when $\alpha = \pm\sqrt{b}$. There are two further cases to consider.
 412 When $\alpha^2 > b$ the feedback, due to the linear coupling, is negative. Therefore, in this case
 413 we will not be able to improve the out-of-sample error. However as α tends to zero the
 414 optimism will increase and be bounded by $2\sigma^2$. Therefore when $\alpha^2 < b$ it may be possible to
 415 improve the out-of-sample error and determine a coupling matrix $\mathbf{K} \neq \mathbf{0}$, that minimises the
 416 out-of-sample error, to be used in the model. We calculate the errors as we did for the linear
 417 numerical example in Section III A.

418 The results obtained from our numerical experiment to test the validity of (16) are shown
 419 in Figure 3. Figure 3(a) shows the tracking error in blue squares and the out-of-sample error
 420 in black diamonds. We can see that the tracking error tends to zero with decreasing α . This
 421 is what we expected and is confirmed by using our analytical expression for the optimism.
 422 In these experiments α was varied between 0 and 1 with the assimilation window taken to
 423 be $N = 10000$.

424 By analysing the expression for the optimism in this case, we see that there is a point
 425 where the tracking and out-of-sample errors meet. This happens when $\alpha^2 = b$. To the left of
 426 this, when $\alpha^2 > b$, the tracking error is greater than the out-of-sample error. To the right,
 427 when $\alpha^2 < b$, the tracking error is smaller than the out-of-sample error. In fact the tracking
 428 error tends to zero while the out-of-sample error decreases and then starts to increase again
 429 resulting in a well defined minimum.

FIG. 3. Figure 3(a) shows a plot of the tracking error in blue squares and the out-of-sample error in black diamonds. The errors are plotted against the inverse of α for $\sigma = 0.01$. Figure 3(b) shows a plot of the out-of-sample error in black diamonds for 100 realisations of the noise r_n with $\sigma = 0.01$. It is displayed for the range of α where the minimum occurs. The error bars represent 90% confidence intervals. The state error is show in blue circles also for 100 realisations of the observation noise with 90% confidence intervals. The vertical line draws attention to the minimum of both curves.

430 The well defined minimum of the out-of-sample error is shown more clearly in Figure 3(b).
 431 Figure 3(b) shows the out-of-sample error in black diamonds for the range of α where the
 432 minimum occurs. The figure shows the out-of-sample error for 100 realisations of the noise
 433 r_n for $\sigma = 0.01$. The error bars represent 90% confidence intervals for each α . Once again we
 434 would like to quantify the variation of the parameter α . The mean value of the optimal α
 435 plus/minus one standard deviation in this case is

$$\bar{\alpha}^* \pm \sqrt{(\alpha^* - \bar{\alpha}^*)^2} = 0.2238 \pm 0.0079. \quad (44)$$

436 Figure 3(b) also shows a plot of the state error in blue circles for 100 realisations. The
 437 black, vertical line draws attention to the minimum of both curves. We can see that the
 438 minimising gain is the same for both errors. When running data assimilation schemes, the
 439 state error is the error we are interested in minimising, however we only have access to the
 440 error in observation space. Even though this is the case, we have shown numerically that the

441 minimising gain is the same for both errors, even in this non linear situation.

442 As with the linear numerical experiment presented in Section III A, further experiments
 443 using different values of σ where carried out. The results produced were the same as the
 444 ones presented here; the only difference was the size of the error bars produced. A smaller
 445 value of σ resulted in smaller error bars much like it did for the linear numerical example.

446 What is particularly of interest here is that even though the dynamical system included
 447 a non linear term, the methodology still applies, provided that the matrix $(\mathbf{A} - \mathbf{KHA})$ is
 448 stable. As an aside, the experiment suggests that the eigenvalues of the linear part of the
 449 error dynamics have to be $< 1 - \epsilon$ with some small but non-zero ϵ in order to stabilise the
 450 error dynamics.

451 C. Numerical Experiment 3: Lorenz '96

452 For this third numerical experiment, the reality is given by the Lorenz'96 model which is
 453 governed by the following equations

$$\dot{x}_i = -x_{i-1}(x_{i-2} - x_{i+1}) - x_i + F \quad (45)$$

454 and exhibits chaotic behaviour for $F = 8$. By integrating the above differential equation with
 455 a time step $\delta = 1.5 \times 10^{-2}$, we obtain a discrete model for our reality which we denote by

$$x_{n+1} = \Phi(x_n). \quad (46)$$

456 We take corresponding observations of the form

$$\eta_n = \mathbf{H}x_n + \sigma r_n \quad (47)$$

457 where $\mathbf{H}$ is the observation operator and r_n is iid noise. We shall take the state dimension to
 458 be $D = 12$, the observation space to be $d = 4$ and we define the observation operator so that
 459 we observe every third element of the state; that is (x_1, x_4, x_7, x_{10}) . The system we construct
 460 here is fully non-linear with linear observations.

461 The assimilating model will use the Lorenz'96 model coupled to the observations through
 462 a simple linear coupling term, as done in the the previous numerical experiments. We set
 463 the coupling matrix $\mathbf{K}$, to be defined by

$$\mathbf{K} = \kappa \mathbf{H}^T \quad (48)$$

FIG. 4. Figure 4(a) presents the out-of-sample error (black diamonds) and the tracking error (blue squares). Figure 4(b) illustrates the out-of-sample error (black diamonds) and the state error (blue circles) with the error bars representing 90% confidence intervals. The black vertical line draws attention to the minimum of the out-of-sample error.

where κ is a coupling parameter taken to be between 0 and 1. With this information, the assimilating model is defined by the following equations

$$\hat{z}_{n+1} = \Phi(z_n); \quad z_{n+1} = \hat{z}_{n+1} + \kappa \mathbf{H}^T (\eta_{n+1} - \mathbf{H} \hat{z}_{n+1}). \quad (49)$$

Once again we will vary the coupling strength in the observer by adjusting the coupling parameter κ . If the coupling is too strong, the observations will be tracked too rigorously and so the observational noise will not be filtered out. If the coupling is too weak the observations are tracked poorly; so once again we expect the out-of-sample error to take a minimum at some non-trivial value of κ .

As always we are interested in the behaviour of the state error and, ultimately, this is the error we want to be minimal. We saw in Section III B that the minimiser for the out-of-sample error was the same as for the state error. We investigate this here too.

The results obtained are shown in Figure 4. Once again the observational noise is iid with $\mathbb{E}r_n = 0$, $\mathbb{E}r_n r_n^T = 1$ and $\sigma = 0.01$. Since the gain is given by equation (48), the optimism reduces to $8\sigma^2\kappa$. To see this note that the observation operator, $\mathbf{H}$, was defined so that every third element of the state was observed. It follows then that $\mathbf{H}\mathbf{H}^T = \mathbb{1}$, the identity

matrix. Since we are observing four states, the trace of $\mathbf{H}\mathbf{H}^T$ is equal to four. Thus, since the optimism is defined by $2\sigma^2\text{tr}(\mathbf{H}\mathbf{K})$ and $\mathbf{K}$ is given by equation (48), it follows that the optimism reduces to $8\sigma^2\kappa$.

To calculate the the errors, a transient time was ignored to give the system time to synchronise. In Figure 4(a) the out-of-sample error (black diamonds) is presented together with the tracking error (blue squares). The black vertical line draws the eye to the minimum of the out-of-sample error. As in the previous experiments, the tracking error reduces to zero while the out-of-sample error increases eventually with increasing coupling strength.

Figure 4(b) presents the out-of-sample error (black diamonds) and the state error (blue circles). The figure shows the errors for 100 realisations of the observational noise, r_n . The error bars represent 90% confidence intervals for each value of κ with the lower limit of the error bars taken at the fifth percentile and the upper limit taken at the 95th. The mean value of the optimal κ plus/minus one standard deviation in this case is

$$\bar{\kappa}^* \pm \sqrt{(\kappa^* - \bar{\kappa}^*)^2} = 0.3050 \pm 0.1184. \quad (50)$$

The black line draws attention to the minimum of the out-of-sample error and we once again see that the minima of the state and out-of-sample errors coincide. It is evident here that these results support the results determined previously in the numerical experiments. Further experiments using different values of σ where also carried out for this non linear system. The results produced were the same as the ones presented here; the only difference was the size of the error bars produced. Again, as with the results in the previous two experiments, a smaller value of σ resulted in smaller error bars.

The flatness of the curves and the uncertainty shown in the figures are rather deceptive in the plots presented in this paper. By looking at these figures, one might expect that the errors in the estimate of κ^* are in fact quite large. However this is not the case as it is the correlation between the errors in the plots that matters.

IV. CONCLUSIONS

A fundamental problem of data assimilation experiments in atmospheric contexts is that there is no possibility of replication, that is, truly “out of sample” observations from the same underlying flow pattern but with independent observational errors are typically not

506 available. A direct evaluation of assimilated trajectories against the available observations is
507 likely to yield optimistic results though, since the observations were already used to find the
508 solution.

509 A possible remedy was presented which simply consists of estimating that optimism,
510 thereby giving a more realistic picture of the ‘out of sample’ performance. The optimism
511 represents the correlation between the observations and the output of the data assimilation
512 scheme. This estimate depends on the observational noise, the observation operator and the
513 feedback gain matrix but not on the underlying dynamics or dynamical noise parameters.
514 The model noise is the term that is difficult to determine operationally, so estimating the
515 optimism in an operational situation is possible as all the required terms are readily available.
516 In this paper, this approach was applied to data assimilation algorithms employing linear error
517 feedback. Several numerical experiments concerning both linear and non-linear systems give
518 evidence to the success of this method as it provides more realistic assessment of performance.
519 This was demonstrated by comparing the out-of-sample performance with the true state
520 error of the algorithm which was available in these numerical simulations.

521 The approach outlined above also provides a simple and efficient means to determine the
522 optimal feedback gain by optimising the out-of-sample error with respect to the gain matrix.
523 Further, theoretical results demonstrate that in linear systems with gaussian perturbations,
524 the feedback thus determined will approach the optimal (Kalman) gain in the limit of large
525 observational windows. The numerical experiments presented in this paper support this
526 result for linear systems.

527 We cannot deduce the same thing for the non-linear systems since firstly, we do not have
528 a candidate for the asymptotic error or gain since the Kalman Filter equations do not hold
529 in these cases. Secondly, even if the existence of an optimal asymptotic gain could be proved,
530 the sequence of minimisers might not converge to it.

531 As an outlook for future work, it seems that the presence of dynamical noise in the
532 underlying system is important when considering the convergence of the optimal gain matrix
533 for non-linear systems. (Even in the linear case, the presence of nondegenerate dynamical
534 noise is essential for the proof to work). If there is no model noise present, then we cannot
535 expect the gain matrix to converge in a meaningful way as the optimal asymptotic gain may
536 not be well defined. For example it is possible that the dynamics of both the underlying
537 system and model enter a region of stability, resulting in a reduction of the error. In this

case it would make sense to reduce or completely eliminate the feedback gain matrix. This would need the gain matrix to be adaptive in some way; a concept not considered here.

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Appendix A

In this appendix, we want to clarify the relationship between the output error

$$E_{O,n} = \mathbb{E}[(\mathbf{H}(x_n - z_n))^2] \quad (\text{A1})$$

(which we give an index n here as it depends on n) and the error covariance matrix

$$\Gamma_n = \mathbb{E}[(x_n - z_n)(x_n - z_n)^T] \quad (\text{A2})$$

in the context of linear systems (Section III A). Re-writing the output error we obtain

$$\begin{aligned} E_{O,n} &= \mathbb{E}\{(\mathbf{H}(x_n - z_n))^T(\mathbf{H}(x_n - z_n))\} \\ &= \mathbb{E}\text{tr}\{(\mathbf{H}(x_n - z_n))^T\mathbf{H}(x_n - z_n)\} \\ &= \mathbb{E}\text{tr}\{\mathbf{H}(x_n - z_n)(x_n - z_n)^T\mathbf{H}^T\} \\ &= \text{tr}\{\mathbf{H}\Gamma_n\mathbf{H}^T\} \end{aligned} \quad (\text{A3})$$

and if we assume real values observations (i.e $d = 1$), we get $E_{O,n} = \mathbf{H}\Gamma_n\mathbf{H}^T$. This does not mean that $E_{O,n}$ carries the same information as Γ_n since $\mathbf{H}$ is not invertible.

To investigate this further, introduce the mappings $F : \mathbb{R}^D \times \mathbb{R}^{D \times D} \rightarrow \mathbb{R}^{D \times D}$, $(\mathbf{K}, \mathbf{M}) \rightarrow (\mathbf{A} - \mathbf{KHA})\mathbf{M}(\mathbf{A} - \mathbf{KHA})^T$ and $G : \mathbb{R}^D \rightarrow \mathbb{R}^{D \times D}$; $\mathbf{K} \rightarrow \sigma^2\mathbf{K}\mathbf{K}^T + \rho^2(\mathbb{1} - \mathbf{KH})(\mathbb{1} - \mathbf{KH})^T$ and $\Phi(\mathbf{K}, \mathbf{M}) = F(\mathbf{K}, \mathbf{M}) + G(\mathbf{K})$. Note that F is linear in $\mathbf{M}$, and we will write $F(\mathbf{K}) \cdot \mathbf{M}$ to emphasize this. It follows from linear filter theory that

$$\begin{aligned} \Gamma_{n+1} &= (\mathbf{A} - \mathbf{KHA})\Gamma_n(\mathbf{A} - \mathbf{KHA})^T + \sigma^2\mathbf{K}\mathbf{K}^T + \rho^2(\mathbb{1} - \mathbf{KH})(\mathbb{1} - \mathbf{KH})^T \\ &= F(\mathbf{K}) \cdot \Gamma_n + G(\mathbf{K}) = \Phi(\mathbf{K}, \Gamma_n). \end{aligned} \quad (\text{A4})$$

555 Suppose that $\mathbf{K}$ is stabilising, then $\Gamma_n \rightarrow \Gamma(\mathbf{K})$ which is a fixed point of (A4), i.e $\Gamma(\mathbf{K}) =$
 556 $F(\mathbf{K}) \cdot \Gamma(\mathbf{K}) + G(\mathbf{K})$. Note that $\Gamma(\mathbf{K})$ describes the asymptotic error performance of the
 557 feedback $\mathbf{K}$.

558 We will now show that the output error is able to distinguish (asymptotically) between
 559 better and worse feedbacks. For any two symmetric matrices $\mathbf{M}_1, \mathbf{M}_2$, we write $\mathbf{M}_1 \geq \mathbf{M}_2$ if
 560 $\mathbf{M}_1 - \mathbf{M}_2$ is positive semi-definite but not zero. Let $\mathbf{K}_1, \mathbf{K}_2$ be two stabilising feedbacks so that
 561 $\Gamma(\mathbf{K}_1) \geq \Gamma(\mathbf{K}_2)$; that is $\mathbf{K}_2$ performs better than $\mathbf{K}_1$. Further, assume $(\mathbb{1} - \mathbf{H}\mathbf{K}_1) \neq 0$ which
 562 implies that $(\mathbf{A} - \mathbf{K}_1\mathbf{H}\mathbf{A}, \mathbf{H})$ is observable. (This condition might seem artificial but we will
 563 see later that it is in fact rather natural). We will now show that $\mathbf{H}\Gamma(\mathbf{K}_1)\mathbf{H}^T > \mathbf{H}\Gamma(\mathbf{K}_2)\mathbf{H}^T$.
 564 Note that because $\Gamma(\mathbf{K}_1) \geq \Gamma(\mathbf{K}_2)$ we have

$$\mathbf{M}_n = F^n(\mathbf{K}_1)\{\Gamma(\mathbf{K}_1) - \Gamma(\mathbf{K}_2)\} \geq 0 \quad (\text{A5})$$

565 for any n since $F(\mathbf{K}_1)$ preserves positive and negative semi-definiteness. Further, the sequence
 566 $\mathbf{M}_n$ is decreasing. To see this, note that it must be monotone since

$$\mathbf{M}_{n+1} - \mathbf{M}_n = F(\mathbf{K}_1)\{\mathbf{M}_n - \mathbf{M}_{n-1}\} \quad (\text{A6})$$

567 and again $F(\mathbf{K}_1)$ preserves definiteness. It cannot be increasing though since $\mathbf{K}_1$ is stabilising
 568 and hence $\mathbf{M}_n \rightarrow 0$. Therefore $\mathbf{H}\mathbf{M}_n\mathbf{H}^T \geq 0$ and decreasing.

569 Assuming $\mathbf{H}\Gamma(\mathbf{K}_1)\mathbf{H}^T = \mathbf{H}\Gamma(\mathbf{K}_2)\mathbf{H}^T$ would then imply

$$\begin{aligned} 0 = \mathbf{H}\mathbf{M}_n\mathbf{H}^T &= \mathbf{H}F^n(\mathbf{K}_1)\{\Gamma(\mathbf{K}_1) - \Gamma(\mathbf{K}_2)\}\mathbf{H}^T \\ &= \mathbf{H}(\mathbf{A} - \mathbf{K}_1\mathbf{H}\mathbf{A})^n(\Gamma(\mathbf{K}_1) - \Gamma(\mathbf{K}_2))(\mathbf{A} - \mathbf{K}_1\mathbf{H}\mathbf{A})^{nT}\mathbf{H}^T \end{aligned} \quad (\text{A7})$$

570 for all n . Now using the spectral decomposition of $\mathbf{M}_0 = \Gamma(\mathbf{K}_1) - \Gamma(\mathbf{K}_2)$,

$$\mathbf{M}_0 = \sum_{i=1}^d \lambda_i v_i v_i^T \quad (\text{A8})$$

571 where λ_i are the eigenvalues of $\mathbf{M}_0$ and v_i are the corresponding eigenvectors, we see that

$$0 = \mathbf{H}\mathbf{M}\mathbf{H}^T = \sum_{i=1}^d \lambda_i (\mathbf{H}(\mathbf{A} - \mathbf{K}_1\mathbf{H}\mathbf{A})^n v_i)^2 \quad (\text{A9})$$

572 for all n . Since $\mathbf{M}_0 \neq 0$, there is a $\lambda_j > 0$ and hence

$$\mathbf{H}(\mathbf{A} - \mathbf{K}_1\mathbf{H}\mathbf{A})^n v_j = 0 \quad \forall n \quad (\text{A10})$$

573 which contradicts the observability of $(\mathbf{H}, \mathbf{A} - \mathbf{K}_1 \mathbf{H} \mathbf{A})$. This shows that $\mathbf{M}_0 = 0$ finishing
574 the proof.

575 From the preceding arguments, it follows that any minimiser of the output error must be
576 the asymptotic Kalman gain. To see this, assume $\mathbf{K}_2$ is the Kalman gain while $\mathbf{K}_1$ optimises
577 the output error $\mathbf{H} \Gamma(\mathbf{K}) \mathbf{H}^T$. By definition of the kalman gain, $\Gamma(\mathbf{K}_1) \geq \Gamma(\mathbf{K}_2)$, and the
578 preceding discussion shows that $\Gamma(\mathbf{K}_1) = \Gamma(\mathbf{K}_2)$ if $(\mathbb{1} - \mathbf{H} \mathbf{K}_1) \neq 0$.

579 To check that this is true, use that the asymptotic output error satisfies

$$\mathbf{H} \Gamma(\mathbf{K}) \mathbf{H}^T = (\mathbb{1} - \mathbf{H} \mathbf{K})^2 \{ \mathbf{H} \Gamma(\mathbf{K}) \mathbf{H}^T + \rho^2 \mathbf{H} \mathbf{H}^T \} + \sigma^2 (\mathbf{H} \mathbf{K})^2. \quad (\text{A11})$$

580 Taking the derivative with respect to $\mathbf{K}$ at $\mathbf{K}_1$ and using the optimality yields the condition

$$\mathbf{H} \mathbf{K}_1 = \frac{\mathbf{H} \Gamma(\mathbf{K}_1) \mathbf{H}^T + \mathbf{H} \mathbf{H}^T \rho^2}{\mathbf{H} \Gamma(\mathbf{K}_1) \mathbf{H}^T + \mathbf{H} \mathbf{H}^T \rho^2 + \sigma^2} \quad (\text{A12})$$

581 so $\mathbb{1} = \mathbf{H} \mathbf{K}_1 > 0$. As a final remark, $\mathbb{1} - \mathbf{H} \mathbf{K} = 0$ implies that $y_n = \eta_n$ (check example (22)
582 for constant $\mathbf{K}$), that is the data assimilation simply reports back the observations.

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