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Degenerate Kalman Filter Error Covariances and Their Convergence onto the Unstable Subspace*

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Abstract. The characteristics of the model dynamics are critical in the performance of (ensemble) Kalman filters. In particular, as emphasized in the seminal work of Anna Trevisan and coauthors, the error covariance matrix is asymptotically supported by the unstable-neutral subspace only, i.e., it is spanned by the backward Lyapunov vectors with nonnegative exponents. This behavior is at the core of algorithms known as assimilation in the unstable subspace, although a formal proof was still missing. This paper provides the analytical proof of the convergence of the Kalman filter covariance matrix onto the unstable-neutral subspace when the dynamics and the observation operator are linear and when the dynamical model is error free, for any, possibly rank-deficient, initial error covariance matrix. The rate of convergence is provided as well. The derivation is based on an expression that explicitly relates the error covariances at an arbitrary time to the initial ones. It is also shown that if the unstable and neutral directions of the model are sufficiently observed and if the column space of the initial covariance matrix has a nonzero projection onto all of the forward Lyapunov vectors associated with the unstable and neutral directions of the dynamics, the covariance matrix of the Kalman filter collapses onto an asymptotic sequence which is independent of the initial covariances. Numerical results are also shown to illustrate and support the theoretical findings.

Key words. Kalman filter, data assimilation, linear dynamics, Lyapunov vectors, control theory, covariance matrix

AMS subject classifications. 93E11, 93C05, 93B07, 60G35, 15A03

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1. Introduction.

1.1. Context and objectives.

Filtering methods are the techniques of estimation theory that process measurements sequentially as they become available. In a probabilistic Bayesian

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framework, the output of a filter is a probability density function (pdf), the conditional posterior pdf $p(\mathbf{x}|\mathbf{y})$ of the process $\mathbf{x}$, given the data $\mathbf{y}$ and a prior distribution $p(\mathbf{x})$. The posterior pdf fully characterizes the state's estimation and quantifies the uncertainty of the estimate. However, its exact calculation is extremely difficult in practice, and most often computationally intractable in high-dimensional, complex systems, such as numerical climate and weather models.

For linear dynamics, measurements with a linear dependence on the state variables, and Gaussian errors, the Kalman filter (KF) is the optimal filtering solution [15]. The Gaussian hypothesis implies an enormous simplification: the pdfs are all completely characterized by their first and second moments. In this case, the error covariance matrix quantifies the uncertainty of the state's estimate represented by the mean. The KF has been extremely successful for decades in numerous fields including navigation, economy, robotics, tracking objects, adaptive optics, and many computer vision applications.

A Monte Carlo formulation of the KF leads to the introduction of a class of *Gaussian* algorithms referred to as ensemble Kalman filters (EnKFs) [10]. They have been widely applied in atmospheric and oceanic contexts, where all methods designed for filtering or smoothing are referred to as data assimilation (DA). In the EnKF the transition probability of the process, as well as all the error covariances entering the assimilation of observations, are approximated using an ensemble of realizations (members in the EnKF jargon) of the model dynamics. The EnKF and its variants are currently among the most popular approaches for DA in high-dimensional systems. Evidence has emerged that a small number of members, typically 100, is sufficient in many applications, especially when using localization techniques [25, and references therein], hence making the EnKF feasible in situations where the forward step of DA is computationally expensive. The choice of the ensemble members is critical and a key aspect in the EnKF setup. While a large ensemble is generally desirable to explain and represent the actual uncertainty in the most realistic manner, their number is limited by the computational resources at disposal. In the absence of localization, the EnKF error covariances are thus degenerate (or rank deficient) by construction and it is then relevant to adequately choose these few (much fewer than the system's dimension) members so as to maximize the representation of the actual uncertainty.

For nonlinear chaotic dynamics, the assimilation in the unstable subspace (AUS), introduced by Anna Trevisan and collaborators [30, 7, 27, 28, 21], has shed light on an efficient way to operate the assimilation of observations by using the unstable subspace to describe the uncertainty in the estimate. AUS is based on two key properties of deterministic, typically dissipative, chaotic systems: (i) the perturbations tend to project on the unstable manifold of the dynamics, and (ii) the dimension of the unstable manifold is typically much smaller than the full phase-space dimension. Applications to atmospheric, oceanic, and traffic models [8, 31, 22] showed that even in high-dimensional systems, an efficient error control is achieved by monitoring only the unstable directions, and sometimes even a subset of them, making AUS a computationally efficient alternative to standard procedures.

The AUS approach has recently motivated a research effort toward a proper mathematical formulation and assessment of its driving idea, i.e., the span of the estimation error covariance matrices asymptotically (in time) tends to the subspace spanned by the unstable and neutral backward Lyapunov vectors (BLVs). A proper statement of this latter property in precise mathematical terms is of vast importance for the design of efficient reduced-order uncertainty quantification and DA methods.

The first recent result along this line is given in [13]. It is proved that for linear, discrete, autonomous and nonautonomous, deterministic systems (perfect model) with noisy observations, the covariance equations in the KF asymptotically bound the rank of the forecast and the analysis error covariance matrices to be less than or equal to the number of nonnegative Lyapunov exponents of the system. Further, the support of these error covariance matrices is shown to be confined to the space spanned by the unstable and neutral BLVs. The results in [13] were obtained assuming a full-rank covariance matrix at initial time. The conditions that imply the convergence, for possibly degenerate (low-rank) initial matrices remained unresolved, yet they are fundamental to link these mathematical findings with concrete reduced-rank DA methods, particularly the EnKF.

This is the subject of the present work, which studies the convergence in the general setting of degenerate covariance matrices. A pivotal result is the analytic proof of the KF covariance collapse, for any initial error covariance (of arbitrary rank), onto the unstable-neutral subspace. We also provide rigorous mathematical results for the rate of convergence on the stable subspace and for the asymptotic rank of the error covariance matrix. Finally, we derive an expression for the asymptotic error covariance matrix as a function of the initial one. This in turn allows us to prove, under certain observability conditions, the existence of an asymptotic sequence of error covariance matrices, which is independent of the initial condition.

In the following, we set up the notations and discuss the organization of the paper.

1.2. Problem formulation. The purpose of this paper is the estimation of the unknown state of a system based on partial and noisy observations. The dynamical and observational models are both assumed to be linear, and expressible as

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

$$\mathbf{y}_k = \mathbf{H}_k \mathbf{x}_k + \mathbf{v}_k, \tag{2}$$

with $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{y} \in \mathbb{R}^d$ being the system's state and observation, respectively, related via the linear observation operator $\mathbf{H}_k : \mathbb{R}^n \mapsto \mathbb{R}^d$. Throughout the entire text the conventional notation $k = 0, 1, 2, \ldots$ is adopted to indicate that the quantity is defined at time t_k. The matrix $\mathbf{M}_{k:l}$ is taken to represent the resolvent of the linear forward model from time t_l to time t_k, and is assumed to be nonsingular throughout this paper. In particular $\mathbf{M}_{k:k} = \mathbf{I}_n$, where $\mathbf{I}_n$ is the identity matrix (of size $n \times n$ in this case). We designate $\mathbf{M}_k$ as the one-step matrix resolvent of the forward model from t_{k-1} to t_k: $\mathbf{M}_k \triangleq \mathbf{M}_{k:k-1}$ and, consequently, $\mathbf{M}_{k:l} = \mathbf{M}_k \mathbf{M}_{k-1} \ldots \mathbf{M}_{l+1}$, with the symbol $\triangleq$ used to signify that the expression is a definition. We will assume that the Lyapunov spectrum of the dynamics defined by $\mathbf{M}_{k:0}$ is nondegenerate, i.e., the Lyapunov exponents are all distinct. This assumption substantially simplifies the derivations that follow. Nonetheless, most of the results in this paper can be generalized to the degenerate case.

The model and observation noise, $\mathbf{w}_k$ and $\mathbf{v}_k$, are assumed mutually independent, unbiased Gaussian white sequences with statistics

$$\mathrm{E}[\mathbf{v}_k \mathbf{v}_l^{\mathrm{T}}] = \delta_{k,l} \mathbf{R}_k, \quad \mathrm{E}[\mathbf{w}_k \mathbf{w}_l^{\mathrm{T}}] = \delta_{k,l} \mathbf{Q}_k, \quad \mathrm{E}[\mathbf{v}_k \mathbf{w}_l^{\mathrm{T}}] = \mathbf{0}, \tag{3}$$

where $\mathbf{R}_k \in \mathbb{R}^{d\times d}$ 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.

The forecast error covariance matrix $\mathbf{P}_k$ of the KF satisfies the following recurrence, the discrete-time dynamic Riccati equation [15, 13]

$$\mathbf{P}_{k+1} = \mathbf{M}_{k+1}\left(\mathbf{I}_n + \mathbf{P}_k\boldsymbol{\Omega}_k\right)^{-1}\mathbf{P}_k\mathbf{M}_{k+1}^{\mathrm{T}} + \mathbf{Q}_{k+1}, \tag{4}$$

where

$$\boldsymbol{\Omega}_k \triangleq \mathbf{H}_k^{\mathrm{T}}\mathbf{R}_k^{-1}\mathbf{H}_k \tag{5}$$

is the precision matrix of the observations transferred in state space. To avoid pathological behaviors, we will assume in this paper that the $\{\boldsymbol{\Omega}_k\}_{k=0,1,\ldots}$ are uniformly bounded from above, which is a very mild hypothesis.

Equation (4) highlights that the error covariance matrix, $\mathbf{P}_{k+1}$, is the result of a two-step process, consisting of the *update* or *analysis* step at time t_k leading to the analysis error covariance matrix $\mathbf{P}_k^{\mathrm{a}}$,

$$\mathbf{P}_k^{\mathrm{a}} = \left(\mathbf{I}_n + \mathbf{P}_k\boldsymbol{\Omega}_k\right)^{-1}\mathbf{P}_k, \tag{6}$$

and the *forecast* step which consists of the forward propagation of the analysis error covariance,

$$\mathbf{P}_{k+1} = \mathbf{M}_{k+1}\mathbf{P}_k^{\mathrm{a}}\mathbf{M}_{k+1}^{\mathrm{T}} + \mathbf{Q}_{k+1}. \tag{7}$$

It is worth mentioning that (4) still holds when $\mathbf{P}_k$ is degenerate, i.e., $\mathrm{rank}(\mathbf{P}_k) < n$. This is the typical circumstance encountered in the EnKF [10, and references therein]. In this case, assuming that the model is perfect ($\mathbf{Q}_k = \mathbf{0}$) and under the same hypotheses of linear observation and evolution operators as well as of Gaussian statistics for the initial condition and observational errors, (4) will apply to the EnKF too.

1.3. Outline of the paper. In the rest of the paper, we will refer to (4) as the recurrence equation for $\mathbf{P}_k$, although we will mostly study the *perfect dynamical model case*, in which $\mathbf{Q}_k = \mathbf{0}$. In section 2 we demonstrate a relation between $\mathbf{P}_k$ at any arbitrary time, $t_k > t_0$, and the initial error covariance matrix $\mathbf{P}_0$, in the general case with $\mathbf{P}_0$ possibly being degenerate. An alternative proof based on the linear symplectic representation of the KF is proposed in Appendix A. In the following section 3, we derive a useful bound that plays a central role in all results and derivations discussed in this study. Then in section 4 we study the asymptotic behavior of $\mathbf{P}_k$ (for $k \to \infty$) along with other relevant properties. Section 5 provides a proof, using a condition on the initial $\mathbf{P}_0$ and certain observability conditions, that the error covariances collapse onto an asymptotic sequence which is independent of the initial covariance matrix $\mathbf{P}_0$. Section 6 describes the numerical results corroborating and illustrating the theoretical findings while the conclusions are drawn in section 7.

2. Computation of the forecast error covariance matrix $\mathbf{P}_k$.

In this section we consider the perfect model case, i.e., $\mathbf{Q}_k = \mathbf{0}$ for all k. The stochastic model case, $\mathbf{Q}_k \neq \mathbf{0}$, is briefly considered in section 3.

The recurrence equation (4) is rational in $\mathbf{P}_k$. Furthermore if we assume that the $\mathbf{P}_k$ are invertible, we can take the inverse of both sides of the recurrence and obtain

$$\mathbf{P}_{k+1}^{-1} = \mathbf{M}_{k+1}^{-\mathrm{T}} \left(\mathbf{P}_k^{-1} + \mathbf{\Omega}_k\right) \mathbf{M}_{k+1}^{-1}, \tag{8}$$

which shows that $\mathbf{P}_{k+1}^{-1}$ is an affine function of $\mathbf{P}_k^{-1}$. This relation is usually called the *information filter* [26, section 3.2].

However, a relevant situation in applications is when the $\mathbf{P}_k$ are degenerate. In this case the inverse of both sides of (8) are undefined, and a suitable generalization of (8) is required. To that end, we introduce an analytic continuation of (4). A regularized $\mathbf{P}_0$ is defined as

$$\mathbf{P}_0(\varepsilon) \triangleq \mathbf{P}_0 + \varepsilon \mathbf{I}_n \tag{9}$$

with $\varepsilon > 0$ and we define the subsequent $\mathbf{P}_k(\varepsilon)$ via the recurrence

$$\mathbf{P}_{k+1}(\varepsilon) \triangleq \mathbf{M}_{k+1} \left(\mathbf{I}_n + \mathbf{P}_k(\varepsilon)\mathbf{\Omega}_k\right)^{-1} \mathbf{P}_k(\varepsilon)\mathbf{M}_{k+1}^{\mathrm{T}}. \tag{10}$$

From (9), (10), $\mathbf{P}_k(\varepsilon)$ is seen to be full rank. Moreover, taking the limit $\varepsilon \to 0^+$, leads $\mathbf{P}_0(\varepsilon)$ continuously back to $\mathbf{P}_0$ and (10) to (4), so that we have

$$\lim_{\varepsilon \to 0^+} \mathbf{P}_k(\varepsilon) = \mathbf{P}_k(0) = \mathbf{P}_k. \tag{11}$$

Then, we take the inverse of both sides of (10),

$$\begin{aligned} \mathbf{P}_{k+1}^{-1}(\varepsilon) &= \mathbf{M}_{k+1}^{-\mathrm{T}} \mathbf{P}_k^{-1}(\varepsilon) \left(\mathbf{I}_n + \mathbf{P}_k(\varepsilon)\mathbf{\Omega}_k\right) \mathbf{M}_{k+1}^{-1} \\ &= \mathbf{M}_{k+1}^{-\mathrm{T}} \mathbf{P}_k^{-1}(\varepsilon) \mathbf{M}_{k+1}^{-1} + \mathbf{M}_{k+1}^{-\mathrm{T}} \mathbf{\Omega}_k \mathbf{M}_{k+1}^{-1}. \end{aligned} \tag{12}$$

This recurrence can easily be solved and it yields

$$\mathbf{P}_k^{-1}(\varepsilon) = \mathbf{M}_{k:0}^{-\mathrm{T}} \mathbf{P}_0^{-1}(\varepsilon) \mathbf{M}_{k:0}^{-1} + \mathbf{\Gamma}_k, \tag{13}$$

where

$$\mathbf{\Gamma}_k \triangleq \sum_{l=0}^{k-1} \mathbf{M}_{k:l}^{-\mathrm{T}} \mathbf{\Omega}_l \mathbf{M}_{k:l}^{-1}. \tag{14}$$

This matrix, known as the information matrix [14], is a measure of the observability of the system since it propagates the precision matrices $\mathbf{\Omega}_l$ up to t_k, and (13) states that the precision in the state estimate is the sum of the forecast precision in the initial condition plus the precision of the observations transferred into the model space.

Let us now recall the partial order defined in the cone $\mathcal{C}^n$ of the symmetric positive semi-definite matrices of $\mathbb{R}^{n\times n}$, of which we will make great use in this study. Similarly the partial order acts in the cone $\mathcal{C}_+^n$ of the symmetric positive definite matrices of $\mathbb{R}^{n\times n}$. We will refer to this partial order using the standard comparison symbols. In Appendix B, its definition is provided along with some additional properties that we rely on in this study. From (13) and using this partial order, we have

$$\mathbf{P}_k^{-1}(\varepsilon) \geq \mathbf{\Gamma}_k. \tag{15}$$

Let us assume that the system is observable, a condition defined here as $\det(\mathbf{\Gamma}_k) \neq 0$ according to [14] and references therein. This yields $\mathbf{P}_k(\varepsilon) \leq \mathbf{\Gamma}_k^{-1}$ (see Appendix B, point 3), which implies

$$\mathbf{P}_k \leq \mathbf{\Gamma}_k^{-1}. \tag{16}$$

By taking the inverse of both sides of (13) we have

$$\begin{aligned}\mathbf{P}_k(\varepsilon) &= \left(\mathbf{M}_{k:0}^{-\mathrm{T}}\mathbf{P}_0^{-1}(\varepsilon)\mathbf{M}_{k:0}^{-1} + \mathbf{\Gamma}_k\right)^{-1} \\ &= \left[\left(\mathbf{I}_n + \mathbf{\Gamma}_k\mathbf{M}_{k:0}\mathbf{P}_0(\varepsilon)\mathbf{M}_{k:0}^{\mathrm{T}}\right)\mathbf{M}_{k:0}^{-\mathrm{T}}\mathbf{P}_0^{-1}(\varepsilon)\mathbf{M}_{k:0}^{-1}\right]^{-1} \\ &= \mathbf{M}_{k:0}\mathbf{P}_0(\varepsilon)\mathbf{M}_{k:0}^{\mathrm{T}}\left(\mathbf{I}_n + \mathbf{\Gamma}_k\mathbf{M}_{k:0}\mathbf{P}_0(\varepsilon)\mathbf{M}_{k:0}^{\mathrm{T}}\right)^{-1}.\end{aligned} \tag{17}$$

The limit $\varepsilon \to 0^+$ finally leads to

$$\mathbf{P}_k = \mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^{\mathrm{T}}\left(\mathbf{I}_n + \mathbf{\Gamma}_k\mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^{\mathrm{T}}\right)^{-1}. \tag{18}$$

Equation (18) is extremely important as it directly relates $\mathbf{P}_k$ to $\mathbf{P}_0$. In particular it shows that $\mathbf{P}_k$ depends on two concurring factors, the matrix $\mathbf{\Gamma}_k$ encoding all information about the observability of the system, and the matrix $\mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^{\mathrm{T}}$ representing the free forecast of the initial covariances. The latter exemplifies the uncertainty propagation under the model dynamics, the former the ability of the observations to counteract the error growth.

We now use the matrix shift lemma that asserts that for any matrices $\mathbf{A} \in \mathbb{R}^{l\times m}$ and $\mathbf{B} \in \mathbb{R}^{m\times l}$, we have $\mathbf{A}f(\mathbf{BA}) = f(\mathbf{AB})\mathbf{A}$, with $x \mapsto f(x)$ being any function that can be expressed as a formal power series. A derivation is recalled in Appendix C. Here, we choose $f(x) = (1+x)^{-1}$, $\mathbf{A} = \mathbf{M}_{k:0}^{\mathrm{T}}$, and $\mathbf{B} = \mathbf{\Gamma}_k\mathbf{M}_{k:0}\mathbf{P}_0$, to obtain an alternative formulation of (18)

$$\mathbf{P}_k = \mathbf{M}_{k:0}\mathbf{P}_0\left[\mathbf{I}_n + \mathbf{M}_{k:0}^{\mathrm{T}}\mathbf{\Gamma}_k\mathbf{M}_{k:0}\mathbf{P}_0\right]^{-1}\mathbf{M}_{k:0}^{\mathrm{T}} \tag{19}$$

or, in a more condensed form,

$$\mathbf{P}_k = \mathbf{M}_{k:0}\mathbf{P}_0\left[\mathbf{I}_n + \mathbf{\Theta}_k\mathbf{P}_0\right]^{-1}\mathbf{M}_{k:0}^{\mathrm{T}}, \tag{20}$$

where

$$\mathbf{\Theta}_k \triangleq \mathbf{M}_{k:0}^{\mathrm{T}}\mathbf{\Gamma}_k\mathbf{M}_{k:0} = \sum_{l=0}^{k-1}\mathbf{M}_{l:0}^{\mathrm{T}}\mathbf{\Omega}_l\mathbf{M}_{l:0}. \tag{21}$$

This matrix is also related to the observability of the system but pulled back at the initial time t_0.

A more general, albeit less straightforward, proof of the expressions for $\mathbf{P}_k$ as a function of $\mathbf{P}_0$ can be obtained using the underlying symplectic structure of the KF and is described in Appendix A.

3. Free forecast of P_0 as an upper bound. In this section we demonstrate that an upper bound for $\mathbf{P}_k$ is given by the *free* forecast of $\mathbf{P}_0$; the term free is used in this study to mean without the observational forcing applied at analysis times. It is worth mentioning already that, although the existence of this bound is indeed very intuitive, its formal proof is provided here because it plays a pivotal role in all the convergence results that follow. The bound can be derived directly from the general expression for $\mathbf{P}_k$, (20), but we opted for showing a different approach, independent of (20), that better highlights the relevance of the bound for the results that follow.

The error covariance matrix $\mathbf{P}_k$ is symmetric and our purpose is to make the recurrence equation look patently symmetric as well so that we can derive inequalities using the partial ordering in $\mathcal{C}^n$. As a positive semidefinite matrix, $\mathbf{P}_k$ can be decomposed into $\mathbf{P}_k = \mathbf{X}_k\mathbf{X}_k^\mathrm{T}$ using, for instance, a Choleski decomposition, with $\mathbf{X}_k \in \mathbb{R}^{n\times m}$ $(m \leq n)$. Here, as opposed to the rest of the paper and for the sake of generality, we consider the presence of model noise given that it only represents a minor complication. The recurrence equation can be written as

$$\mathbf{P}_{k+1} = \mathbf{M}_{k+1}\left(\mathbf{I}_n + \mathbf{X}_k\mathbf{X}_k^\mathrm{T}\mathbf{\Omega}_k\right)^{-1}\mathbf{X}_k\mathbf{X}_k^\mathrm{T}\mathbf{M}_{k+1}^\mathrm{T} + \mathbf{Q}_{k+1}. \tag{22}$$

We use again the matrix shift lemma but this time with $f(x) = (1+x)^{-1}$, $\mathbf{A} = \mathbf{X}_k$, and $\mathbf{B} = \mathbf{X}_k^\mathrm{T}\mathbf{\Omega}_k$ so that (4) becomes

$$\mathbf{P}_{k+1} = \mathbf{M}_{k+1}\mathbf{X}_k\left(\mathbf{I}_m + \mathbf{X}_k^\mathrm{T}\mathbf{\Omega}_k\mathbf{X}_k\right)^{-1}\mathbf{X}_k^\mathrm{T}\mathbf{M}_{k+1}^\mathrm{T} + \mathbf{Q}_{k+1}. \tag{23}$$

Using the partial order in $\mathcal{C}^m$, we have from

$$\left(\mathbf{I}_m + \mathbf{X}_k^\mathrm{T}\mathbf{\Omega}_k\mathbf{X}_k\right)^{-1} \leq \mathbf{I}_m \tag{24}$$

and from (23) that

$$\mathbf{Q}_{k+1} \leq \mathbf{P}_{k+1} \leq \mathbf{M}_{k+1}\mathbf{P}_k\mathbf{M}_{k+1}^\mathrm{T} + \mathbf{Q}_{k+1}. \tag{25}$$

Hence $\mathbf{P}_k$ is bounded from above by the free forecast $\widetilde{\mathbf{P}}_k$ that satisfies $\widetilde{\mathbf{P}}_0 = \mathbf{P}_0$ and the recurrence

$$\widetilde{\mathbf{P}}_{k+1} = \mathbf{M}_{k+1}\widetilde{\mathbf{P}}_k\mathbf{M}_{k+1}^\mathrm{T} + \mathbf{Q}_{k+1} \tag{26}$$

whose solution is, for $k \geq 0$,

$$\widetilde{\mathbf{P}}_k = \mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^\mathrm{T} + \mathbf{\Xi}_k, \tag{27}$$

where

$$\mathbf{\Xi}_0 \triangleq \mathbf{0} \quad \text{and, for } k \geq 1, \quad \mathbf{\Xi}_k \triangleq \sum_{l=1}^{k}\mathbf{M}_{k:l}\mathbf{Q}_l\mathbf{M}_{k:l}^\mathrm{T} \tag{28}$$

is known as the controllability matrix [14]. Therefore

$$\mathbf{Q}_k \leq \mathbf{P}_k \leq \mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^\mathrm{T} + \mathbf{\Xi}_k. \tag{29}$$

In particular, in the perfect model case, we obtain the pivotal inequality

$$\mathbf{P}_k \leq \mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^{\mathrm{T}}. \tag{30}$$

Under the aforementioned assumptions on linear dynamical and observational models and Gaussian error statistics, the inequalities (29) and (30) state that DA will always reduce and, in the worst case, leave unchanged, the state's estimate uncertainty with respect to the free run. This effect was already discussed in the context of nonlinear dynamics and in relation to the stability properties of DA systems in [7], although an analytic proof in the nonlinear case is not provided either in that work or in the present one.

4. Convergence of the error covariance matrix: Theoretical results. This section describes some of the implications of the recurrence equation and bounds described in the previous section that are relevant for the design of reduced-order formulations of the Kalman filter with unstable dynamics. We will assume here, again, to be in the perfect model scenario, $\mathbf{Q}_k = \mathbf{0}$.

4.1. Rank of $\mathbf{P}_k$. From the inequality (30), it is clear that the column space of $\mathbf{P}_k$, i.e., the subspace $\mathrm{Im}(\mathbf{P}_k) = \{\mathbf{P}_k\mathbf{x},\, \mathbf{x} \in \mathbb{R}^n\}$ satisfies

$$\mathrm{Im}(\mathbf{P}_k) \subseteq \mathbf{M}_{k:0}\left(\mathrm{Im}(\mathbf{P}_0)\right). \tag{31}$$

Moreover, since from (4) (with $\mathbf{Q}_k = 0$)

$$\mathrm{rank}(\mathbf{P}_{k+1}) = \mathrm{rank}(\mathbf{P}_k), \tag{32}$$

we infer that

$$\mathrm{Im}(\mathbf{P}_k) = \mathbf{M}_{k:0}\left(\mathrm{Im}(\mathbf{P}_0)\right). \tag{33}$$

The moral is that the KF merely operates within the subspaces of the sequence $\mathbf{M}_{k:0}(\mathrm{Im}(\mathbf{P}_0))$, which do not depend on the observations. In the absence of model error, the rank of $\mathbf{P}_k$ cannot exceed that of $\mathbf{P}_0$ even if the dynamics are degenerate.

4.2. Collapse of the error covariance matrices onto the unstable-neutral subspace. The unstable-neutral subspace is defined as the subspace $\mathcal{U}_k$ spanned by the n_0 BLVs at t_k whose exponents, λ_i with $i = 1, \ldots, n_0$, are nonnegative. The stable subspace $\mathcal{S}_k$ is defined as the subspace spanned by the $n - n_0$ BLVs at t_k associated with negative exponents. The inequality equation (30), $\mathbf{P}_k \leq \mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^{\mathrm{T}}$, provides the convergence onto $\mathcal{U}_k$ in a sense that is made clear below. It also gives the rate of such convergence as shown in section 4.3.

Let us write the singular value decomposition (SVD) of $\mathbf{M}_{k:0} = \mathbf{U}_{k:0}\mathbf{\Sigma}_{k:0}\mathbf{V}_{k:0}^{\mathrm{T}}$, where $\mathbf{U}_{k:0}$ and $\mathbf{V}_{k:0}$ are both orthogonal matrices in $\mathbb{R}^{n\times n}$, and $\mathbf{\Sigma}_{k:0}$ in $\mathcal{C}_+^n$ is the diagonal matrix of the singular values. The left singular vectors are the columns of $\mathbf{U}_{k:0} = [\mathbf{u}_1^{k:0}, \ldots, \mathbf{u}_n^{k:0}]$ and when $k \to \infty$, they converge to the BLVs defined at t_k, denoted here as $\mathbf{u}_i^k$. The right singular vectors are the columns of $\mathbf{V}_{k:0} = [\mathbf{v}_1^{k:0}, \ldots, \mathbf{v}_n^{k:0}]$ which converge to the forward Lyapunov vectors (FLVs) at time t_0 as $k \to \infty$ denoted here as $\mathbf{v}_i^0$ [17, 29]. Let us write $[\mathbf{\Sigma}_{k:0}]_{i,i} = \exp(\lambda_i^k k)$ with λ_i^k being real numbers and for large k ordered as $\lambda_1^k > \cdots > \lambda_{n_0}^k \geq 0 > \lambda_{n_0+1}^k > \cdots > \lambda_n^k$, which is justified by the nondegeneracy hypothesis on the Lyapunov spectrum. Using the SVD we have

$$\mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^{\mathrm{T}} = \mathbf{U}_{k:0}\mathbf{\Sigma}_{k:0}\mathbf{V}_{k:0}^{\mathrm{T}}\mathbf{P}_0\mathbf{V}_{k:0}\mathbf{\Sigma}_{k:0}\mathbf{U}_{k:0}^{\mathrm{T}}. \tag{34}$$

Define $\mathfrak{S}_k$ as the set of indices i for which $\lambda_i^k < 0$ and $\mathfrak{S}_k^s$ to be the set of indices corresponding to the s smallest singular values in $\mathbf{\Sigma}_{k:0}$. Note also that $\mathfrak{S}_k^{n-n_0} = \mathfrak{S}_k$ for large k. Let the subspace $\mathcal{S}_{k:0}^s$ be the span of the left singular vectors $\mathbf{u}_i^{k:0}$, where $i \in \mathfrak{S}_k^s$. Let $\Pi_{\mathcal{S}_{k:0}^s}$ be the orthogonal projector onto $\mathcal{S}_{k:0}^s$ which, owing to the orthonormality of the left singular vectors, reads

$$\Pi_{\mathcal{S}_{k:0}^s} = \sum_{i\in\mathfrak{S}_k^s} \mathbf{u}_i^{k:0}\left(\mathbf{u}_i^{k:0}\right)^{\mathrm{T}}. \tag{35}$$

For large enough k, $\mathfrak{S}_k$ gets progressively closer and eventually coincides with the set $\mathfrak{S}$ of indices i for which $\lambda_i < 0$ and each of its subsets $\mathfrak{S}_k^s$ approaches its corresponding subset $\mathfrak{S}^s$ defined similarly. Note that $\mathfrak{S}^{n-n_0} = \mathfrak{S}$. Furthermore, the subspace $\mathcal{S}_{k:0}^s$ converges to $\mathcal{S}_k^s$ which is the span of the s most stable BLVs.

We are now interested in an upper bound in $\mathcal{C}^s$ for $(\mathbf{V}_{k:0}^s)^{\mathrm{T}}\mathbf{P}_0\mathbf{V}_{k:0}^s$, with $\mathbf{V}_{k:0}^s = [\mathbf{v}_{n-s+1}^{k:0}, \dots, \mathbf{v}_n^{k:0}]$ to be jointly used with (34). For this purpose we define

$$\alpha_s^k = \max_{\mathbf{h}\in\mathrm{Im}\left(\mathbf{V}_{k:0}^s\right),\, \|\mathbf{h}\|=1} \mathbf{h}^{\mathrm{T}}\mathbf{P}_0\mathbf{h}, \tag{36}$$

where $\|.\|$ denotes the Euclidean norm. As a consequence, we have

$$\left(\mathbf{V}_{k:0}^s\right)^{\mathrm{T}}\mathbf{P}_0\mathbf{V}_{k:0}^s \le \alpha_s^k\mathbf{I}_s. \tag{37}$$

From this inequality and from (34), we infer

$$\Pi_{\mathcal{S}_{k:0}^s}\mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^{\mathrm{T}}\Pi_{\mathcal{S}_{k:0}^s} \le \alpha_s^k\Pi_{\mathcal{S}_{k:0}^s}\mathbf{U}_{k:0}\mathbf{\Sigma}_{k:0}^2\mathbf{U}_{k:0}^{\mathrm{T}}\Pi_{\mathcal{S}_{k:0}^s}. \tag{38}$$

Note that, if σ_1^0 is the largest eigenvalue of $\mathbf{P}_0$, we have the uniform bound $\alpha_s^k \le \sigma_1^0$ for any k and s (see Appendix B, point 5). Hence, we can define a finite bound

$$\alpha_s = \sup_{k\ge 0}\alpha_s^k \tag{39}$$

which satisfies for any k and s: $\alpha_s^k \le \alpha_s \le \sigma_1^0$. Using this uniform bound, in conjunction with (30) and (38), we obtain

$$\Pi_{\mathcal{S}_{k:0}^s}\mathbf{P}_k\Pi_{\mathcal{S}_{k:0}^s} \le \alpha_s\sum_{i\in\mathfrak{S}_k^s}\exp\left(2\lambda_i^k k\right)\mathbf{u}_i^{k:0}\left(\mathbf{u}_i^{k:0}\right)^{\mathrm{T}}. \tag{40}$$

Hence, for every unit vector $\mathbf{h} \in \mathcal{S}_{k:0}^s$

$$\mathbf{h}^{\mathrm{T}}\mathbf{P}_k\mathbf{h} \le \alpha_s\exp\left(2\lambda_{n-s+1}^k k\right). \tag{41}$$

In particular, if $i \in \mathfrak{S}$, then $(\mathbf{u}_i^{k:0})^{\mathrm{T}}\mathbf{P}_k\mathbf{u}_i^{k:0} \to 0^+$ as $k \to \infty$. This defines a *weak* form of collapse of $\mathbf{P}_k$ onto the unstable-neutral subspace $\mathcal{U}_k$. A *strong* form of collapse is defined by the stable subspace $\mathcal{S}_k$ being in the null space of $\mathbf{P}_k$. This can be obtained under the hypothesis that $\mathbf{P}_k$ is uniformly bounded, which can in turn be satisfied if the system is sufficiently observed. Indeed, if $\mathbf{P}_k$ is uniformly bounded, and because of its positive semidefiniteness, it can be shown that $\|\mathbf{P}_k\mathbf{u}_i^{k:0}\| \to 0$ as $k \to \infty$ (see Appendix B, point 5). Hence, asymptotically, the stable subspace $\mathcal{S}_k$ is in the null space of $\mathbf{P}_k$. As described in the introduction, this property is at the core of the class of DA algorithms referred to as *AUS* [20, and references therein].

4.3. Rate of convergence of the eigenvalues. In the case of weak—a fortiori strong—collapse, the rate of convergence of each of the eigenvalues of $\mathbf{P}_k$ can be determined from (41) as follows. Let σ_i^k for $i = 1, \dots, n$ denote the eigenvalues of $\mathbf{P}_k$ ordered as $\sigma_1^k \geq \sigma_2^k \cdots \geq \sigma_n^k$. Equation (41) guarantees that (Appendix B, point 6) $\mathbf{P}_k$ has at least s of its eigenvalues less than or equal to $\alpha_s \exp(2\lambda_{n-s+1}^k k)$. It follows that

$$\sigma_i^k \leq \alpha_i \exp\left(2\lambda_i^k k\right) \tag{42}$$

which gives us an upper bound for all eigenvalues of $\mathbf{P}_k$ and a rate of convergence for the $n - n_0$ smallest ones.

4.4. Asymptotic rank of the error covariance matrix. A consequence of (40) is the upper bound of the asymptotic rank of the error covariance matrix $\mathbf{P}_k$. In fact, the asymptotic rank of $\mathbf{P}_k$ is bounded by the minimum between the rank of $\mathbf{P}_0$ and n_0. This mathematically reads

$$\lim_{k\to\infty} \mathrm{rank}(\mathbf{P}_k) \leq \min\left\{\mathrm{rank}(\mathbf{P}_0), n_0\right\}. \tag{43}$$

4.5. Observability and boundedness of the error statistics. As mentioned in section 2, we define the system to be observable if $\det(\mathbf{\Gamma}_k) \neq 0$ or, equivalently, given that $\mathbf{M}_{k:0}$ is assumed to be nonsingular, $\det(\mathbf{\Theta}_k) \neq 0$ [14]. If the system is observable, the inequalities (30) and (16) can be combined to obtain

$$\mathbf{P}_k \leq \min\left\{\mathbf{M}_{k:0}\mathbf{P}_0\mathbf{M}_{k:0}^{\mathrm{T}}, \mathbf{\Gamma}_k^{-1}\right\}, \tag{44}$$

where the accurate definition of the minimum in $\mathcal{C}^n$ is given in Appendix B (point 4). We note that if $\mathbf{\Gamma}_k$ is bounded by $\mathbf{L}$ in $\mathcal{C}_+^n$, $\mathbf{\Gamma}_k \geq \mathbf{L}$, we have $\mathbf{P}_k \leq \mathbf{\Gamma}_k^{-1} \leq \mathbf{L}^{-1}$ which bounds the error covariances. The existence of the bound $\mathbf{L}$ in $\mathcal{C}_+^n$ guarantees the observability of the system; it forces the precision of the observations to be spread in space and time. Interestingly, the inequality equation (44) reveals that the uncertainty in the state estimate cannot exceed that associated with the most precise ingredient of the assimilation, the forecast initial conditions or the observations. This is further explored in the following section.

5. Asymptotic behavior of $\mathbf{P}_k$ and its independence from $\mathbf{P}_0$. In this section, we study the asymptotic behavior of the forecast error covariance matrix $\mathbf{P}_k$ when $k \to \infty$. In particular, we are interested in the conditions for which the asymptotic sequence of $\mathbf{P}_k$ becomes independent of $\mathbf{P}_0$. The authors of [24] have provided an appealing and yet heuristic derivation of the asymptotic limit of $\mathbf{P}_k$ in the autonomous case, under some observability condition and assuming the absence of a neutral mode in the dynamics, but also assuming the nondegeneracy of the eigenspectrum of the dynamics. Here, we are interested in a rigorous, nonautonomous generalization in the possible presence of neutral modes using a generalized observability condition. As in the previous section, we assume that the Lyapunov spectrum of the dynamics is nondegenerate, i.e., there are n distinct Lyapunov exponents. The degenerate case will be discussed at a more heuristic level at the end of the section.

If $\mathbf{C}_k$ is a matrix in $\mathbb{R}^{n\times n}$ whose columns are the normalized-to-one covariant Lyapunov vectors (CLVs) of the dynamics at t_k we have the defining relationship

$$\mathbf{M}_{k:l}\mathbf{C}_l = \mathbf{C}_k\mathbf{\Lambda}_{k:l}, \tag{45}$$

where $\mathbf{\Lambda}_{k:l}$ is a diagonal matrix because of the nondegeneracy of the Lyapunov spectrum. Its diagonal entries are the exponential of the local Lyapunov exponents between t_l and t_k. We will however distinguish between $\mathbf{\Lambda}_{k:l}$ and $\mathbf{\Lambda}_{k:l}^{\mathrm{T}}$ as if the matrix was not symmetric to ease the discussion on the degeneracy case. Assuming that the columns of $\mathbf{C}_k$ are ordered according to the associated decreasing Lyapunov exponents, we can decompose $\mathbf{C}_k$ into $\begin{bmatrix} \mathbf{C}_{+,k} & \mathbf{C}_{-,k} \end{bmatrix}$, where $\mathbf{C}_{+,k}$ contains the unstable and neutral CLVs and $\mathbf{C}_{-,k}$ contains the stable CLVs. The transpose of the inverse of $\mathbf{C}_k$ which, by construction, forms a dual basis for the CLVs can be decomposed accordingly:

$$\widetilde{\mathbf{C}}_k \triangleq \mathbf{C}_k^{-\mathrm{T}} \triangleq \begin{bmatrix} \widetilde{\mathbf{C}}_{+,k} & \widetilde{\mathbf{C}}_{-,k} \end{bmatrix}, \tag{46}$$

where $\widetilde{\mathbf{C}}_{+,k} \in \mathbb{R}^{n\times n_0}$ and $\widetilde{\mathbf{C}}_{-,k} \in \mathbb{R}^{n\times(n-n_0)}$. We decompose $\mathbf{\Lambda}_{k:l}$ into

$$\mathbf{\Lambda}_{k:l} \triangleq \begin{bmatrix} \mathbf{\Lambda}_{+,k:l} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_{-,k:l} \end{bmatrix}, \tag{47}$$

where $\mathbf{\Lambda}_{+,k:l} \in \mathbb{R}^{n_0\times n_0}$ and $\mathbf{\Lambda}_{-,k:l} \in \mathbb{R}^{(n-n_0)\times(n-n_0)}$. Thus, one has

$$\mathbf{M}_{k:l} = \mathbf{C}_{+,k}\mathbf{\Lambda}_{+,k:l}\widetilde{\mathbf{C}}_{+,l}^{\mathrm{T}} + \mathbf{C}_{-,k}\mathbf{\Lambda}_{-,k:l}\widetilde{\mathbf{C}}_{-,l}^{\mathrm{T}}. \tag{48}$$

Recall that the FLVs and BLVs are the columns of $\mathbf{V}_k = \lim_{k\to\infty}\mathbf{V}_{k:l}$ and $\mathbf{U}_k = \lim_{l\to-\infty}\mathbf{U}_{k:l}$, respectively. Moreover, the FLVs and BLVs associated with the unstable and neutral directions are the columns of $\mathbf{V}_{+,k} \in \mathbb{R}^{n\times n_0}$ and $\mathbf{U}_{+,k} \in \mathbb{R}^{n\times n_0}$, respectively, which correspond to the first n_0 columns of $\mathbf{V}_k$ and $\mathbf{U}_k$, respectively. Finally, the BLVs associated with the stable directions are the columns of $\mathbf{U}_{-,k} \in \mathbb{R}^{n\times(n-n_0)}$, which correspond to the last $n-n_0$ columns of $\mathbf{U}_k$. From [16], we have $\mathbf{C}_k = \mathbf{U}_k\mathbf{T}_k = \mathbf{V}_k\mathbf{L}_k$, where $\mathbf{T}_k$ and $\mathbf{L}_k$ are an invertible upper triangular matrix and an invertible lower triangular matrix, respectively. Hence, there is an invertible upper triangular matrix, $\mathbf{T}_{+,k} \in \mathbb{R}^{n_0\times n_0}$, such that $\mathbf{C}_{+,k} = \mathbf{U}_{+,k}\mathbf{T}_{+,k}$ yielding $\mathrm{Im}(\mathbf{C}_{+,k}) = \mathrm{Im}(\mathbf{U}_{+,k})$. Moreover, $\widetilde{\mathbf{C}}_k = \mathbf{U}_k\mathbf{T}_k^{-\mathrm{T}} = \mathbf{V}_k\mathbf{L}_k^{-\mathrm{T}}$, which implies that there is an invertible lower triangular matrix and an invertible upper triangular matrix, $\mathbf{T}_{-,k}^{-\mathrm{T}} \in \mathbb{R}^{(n-n_0)\times(n-n_0)}$ and $\mathbf{L}_{-,k}^{-\mathrm{T}} \in \mathbb{R}^{n_0\times n_0}$, respectively, such that $\widetilde{\mathbf{C}}_{-,k} = \mathbf{U}_{-,k}\mathbf{T}_{-,k}^{-\mathrm{T}}$ and $\widetilde{\mathbf{C}}_{+,k} = \mathbf{V}_{+,k}\mathbf{L}_{+,k}^{-\mathrm{T}}$. Consequently, $\mathrm{Im}(\widetilde{\mathbf{C}}_{-,k}) = \mathrm{Im}(\mathbf{U}_{-,k})$ and $\mathrm{Im}(\widetilde{\mathbf{C}}_{+,k}) = \mathrm{Im}(\mathbf{V}_{+,k})$. These identities will be used in the following.

An asymptotic sequence $\mathbf{S}_k$ such that $\lim_{k\to\infty}(\mathbf{P}_k - \mathbf{S}_k) = \mathbf{0}$ will be called an asymptote for $\mathbf{P}_k$ in the following. Our goal is to prove that the two following conditions are sufficient for the existence of an asymptote for $\mathbf{P}_k$ which is independent of $\mathbf{P}_0$. An additional condition may be required if neutral modes are present in the dynamics. Recall that $\mathbf{P}_0$ is possibly degenerate of rank $r_0 \leq n$. As in section 3, $\mathbf{P}_0$ can be factorized into $\mathbf{P}_0 = \mathbf{X}_0\mathbf{X}_0^{\mathrm{T}}$, where $\mathbf{X}_0$ is a matrix in $\mathbb{R}^{n\times r_0}$.

Condition 1. The condition reads

$$\mathrm{rank}\left(\widetilde{\mathbf{C}}_{+,0}^{\mathrm{T}}\mathbf{X}_0\right) = n_0. \tag{49}$$

The idea is to make the column space of $\mathbf{P}_0$ large enough so that the unstable and neutral CLVs at t_0 have nonzero projections onto this space. Since we showed that $\mathrm{Im}(\widetilde{\mathbf{C}}_{+,k}) = \mathrm{Im}(\mathbf{V}_{+,k})$, the condition is equivalent to $\mathrm{rank}(\mathbf{V}_{+,0}^{\mathrm{T}}\mathbf{X}_0) = n_0$. Consequently, the column space of $\mathbf{P}_k$ will asymptotically contain the unstable-neutral subspace. Note that (49) implies $r_0 \geq n_0$, but $r_0 \geq n_0$ does not imply (49).

Condition 2. The unstable and neutral directions of the model are uniformly observed, i.e., for k large enough there is $\varepsilon > 0$ such that

$$\mathbf{C}_{+,k}^{\mathrm{T}}\mathbf{\Gamma}_k\mathbf{C}_{+,k} > \varepsilon\mathbf{I}_{n_0}. \tag{50}$$

The condition is equivalent to $\mathbf{U}_{+,k}^{\mathrm{T}}\mathbf{\Gamma}_k\mathbf{U}_{+,k} > \varepsilon\mathbf{I}_{n_0}$ with a possibly different $\varepsilon > 0$, since we showed that $\mathrm{Im}(\mathbf{C}_{+,k}) = \mathrm{Im}(\mathbf{U}_{+,k})$.

We would like to project the degrees of freedom in $\mathbf{P}_0$ onto the unstable-neutral and stable subspaces. Since $\mathbf{C}_{+,0}\widetilde{\mathbf{C}}_{+,0}^{\mathrm{T}} + \mathbf{C}_{-,0}\widetilde{\mathbf{C}}_{-,0}^{\mathrm{T}} = \mathbf{I}_n$, we have

$$\mathbf{X}_0 = \mathbf{C}_{+,0}\widetilde{\mathbf{C}}_{+,0}^{\mathrm{T}}\mathbf{X}_0 + \mathbf{C}_{-,0}\widetilde{\mathbf{C}}_{-,0}^{\mathrm{T}}\mathbf{X}_0. \tag{51}$$

Define $\mathbf{Z}_+ \triangleq \widetilde{\mathbf{C}}_{+,0}^{\mathrm{T}}\mathbf{X}_0 \in \mathbb{R}^{n_0\times r_0}$ which is of rank n_0 by Condition 1. The column spaces of $\mathbf{C}_{+,0}\mathbf{Z}_+$ and of $\mathbf{C}_{-,0}\widetilde{\mathbf{C}}_{-,0}^{\mathrm{T}}\mathbf{X}_0$ are linearly independent and their sum spans the column space of $\mathbf{X}_0$. Hence, they are complementary subspaces in $\mathrm{Im}(\mathbf{X}_0)$. That is why $\mathbf{C}_{-,0}\widetilde{\mathbf{C}}_{-,0}^{\mathrm{T}}\mathbf{X}_0$ must be of dimension $r_0 - n_0$. Thus, a QR decomposition of rank $r_0 - n_0$ can be used: $\mathbf{C}_{-,0}\widetilde{\mathbf{C}}_{-,0}^{\mathrm{T}}\mathbf{X}_0 = \mathbf{W}_{-,0}\mathbf{Z}_-$, where $\mathbf{W}_{-,0} \in \mathbb{R}^{n\times(r_0-n_0)}$ is an orthonormal matrix such that $\mathbf{W}_{-,0}^{\mathrm{T}}\mathbf{W}_{-,0} = \mathbf{I}_{r_0-n_0}$ and $\mathbf{Z}_- \in \mathbb{R}^{(r_0-n_0)\times r_0}$ is a full-rank matrix. Note that $\widetilde{\mathbf{C}}_{+,0}^{\mathrm{T}}\mathbf{W}_{-,0} = \mathbf{0}$. Hence, we have

$$\mathbf{X}_0 = \mathbf{C}_{+,0}\mathbf{Z}_+ + \mathbf{W}_{-,0}\mathbf{Z}_- = \begin{bmatrix} \mathbf{C}_{+,0} & \mathbf{W}_{-,0} \end{bmatrix}\mathbf{Z}, \quad \text{where} \quad \mathbf{Z} \triangleq \begin{bmatrix} \mathbf{Z}_+ \\ \mathbf{Z}_- \end{bmatrix} \tag{52}$$

in $\mathbb{R}^{r_0\times r_0}$ is of rank r_0 since $\mathrm{rank}(\mathbf{X}_0) = r_0$, and hence $\mathbf{Z}$ is invertible. Let us define

$$\mathbf{W}_0 \triangleq \begin{bmatrix} \mathbf{C}_{+,0} & \mathbf{W}_{-,0} \end{bmatrix} \quad \text{and} \quad \mathbf{G} \triangleq \mathbf{Z}^{-\mathrm{T}}\mathbf{Z}^{-1}, \tag{53}$$

where $\mathbf{G} \in \mathcal{C}_+^{r_0}$. Thus $\mathbf{P}_0 = \mathbf{W}_0\mathbf{G}^{-1}\mathbf{W}_0^{\mathrm{T}}$. This factorization is applied to (20):

$$\begin{aligned}
\mathbf{P}_k &= \mathbf{M}_{k:0}\mathbf{W}_0\mathbf{G}^{-1}\mathbf{W}_0^{\mathrm{T}}\left(\mathbf{I}_n + \mathbf{\Theta}_k\mathbf{W}_0\mathbf{G}^{-1}\mathbf{W}_0^{\mathrm{T}}\right)^{-1}\mathbf{M}_{k:0}^{\mathrm{T}} \\
&= \mathbf{M}_{k:0}\mathbf{W}_0\mathbf{G}^{-1}\left(\mathbf{I}_{r_0} + \mathbf{W}_0^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{W}_0\mathbf{G}^{-1}\right)^{-1}\mathbf{W}_0^{\mathrm{T}}\mathbf{M}_{k:0}^{\mathrm{T}} \\
&= \mathbf{M}_{k:0}\mathbf{W}_0\left(\mathbf{G} + \mathbf{W}_0^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{W}_0\right)^{-1}\mathbf{W}_0^{\mathrm{T}}\mathbf{M}_{k:0}^{\mathrm{T}},
\end{aligned} \tag{54}$$

where Appendix C has been employed.

We now focus on the projection of $\mathbf{P}_k$ onto the forward unstable-neutral subspace, which reads, from (21), (48), (54),

$$\begin{aligned}\widetilde{\mathbf{C}}_{+,k}^{\mathrm{T}}\mathbf{P}_k\widetilde{\mathbf{C}}_{+,k} &= \mathbf{\Lambda}_{+,k:0}\widetilde{\mathbf{C}}_{+,0}^{\mathrm{T}}\mathbf{W}_0\left(\mathbf{G}+\mathbf{W}_0^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{W}_0\right)^{-1}\mathbf{W}_0^{\mathrm{T}}\widetilde{\mathbf{C}}_{+,0}\mathbf{\Lambda}_{+,k:0}^{\mathrm{T}} \\ &= \mathbf{\Lambda}_{+,k:0}\left[\left(\mathbf{G}+\mathbf{W}_0^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{W}_0\right)^{-1}\right]_{++}\mathbf{\Lambda}_{+,k:0}^{\mathrm{T}} \\ &= \mathbf{\Lambda}_{+,k:0}\left[\begin{pmatrix}\mathbf{G}_{++}+\mathbf{\Theta}_k^{++} & \mathbf{G}_{+-}+\mathbf{\Theta}_k^{+-}\\ \mathbf{G}_{-+}+\mathbf{\Theta}_k^{-+} & \mathbf{G}_{--}+\mathbf{\Theta}_k^{--}\end{pmatrix}^{-1}\right]_{++}\mathbf{\Lambda}_{+,k:0}^{\mathrm{T}} \\ &= \left[\begin{pmatrix}\mathbf{\Lambda}_{+,k:0}^{-\mathrm{T}}\mathbf{G}_{++}\mathbf{\Lambda}_{+,k:0}^{-1}+\mathbf{\Gamma}_{++,k} & \mathbf{\Lambda}_{+,k:0}^{-\mathrm{T}}\mathbf{G}_{+-}+\mathbf{\Lambda}_{+,k:0}^{-\mathrm{T}}\mathbf{\Theta}_k^{+-}\\ \mathbf{G}_{-+}\mathbf{\Lambda}_{+,k:0}^{-1}+\mathbf{\Theta}_k^{-+}\mathbf{\Lambda}_{+,k:0}^{-1} & \mathbf{G}_{--}+\mathbf{\Theta}_k^{--}\end{pmatrix}^{-1}\right]_{++},\end{aligned} \tag{55}$$

where $[\cdot]_{++}$ is the matrix block corresponding to the unstable-neutral modes, and

$$\mathbf{\Gamma}_{++,k}\triangleq\mathbf{C}_{+,k}^{\mathrm{T}}\mathbf{\Gamma}_k\mathbf{C}_{+,k}=\mathbf{\Lambda}_{+,k:0}^{-\mathrm{T}}\mathbf{\Theta}_k^{++}\mathbf{\Lambda}_{+,k:0}^{-1},\quad \mathbf{\Theta}_k^{++}\triangleq\mathbf{C}_{+,0}^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{C}_{+,0}, \tag{56}$$

$$\mathbf{\Theta}_k^{-+}\triangleq\mathbf{W}_{-,0}^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{C}_{+,0},\qquad \mathbf{\Theta}_k^{+-}\triangleq\mathbf{C}_{+,0}^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{W}_{-,0},\qquad \mathbf{\Theta}_k^{--}\triangleq\mathbf{W}_{-,0}^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{W}_{-,0}. \tag{57}$$

5.1. Asymptote in the absence of neutral modes. We first assume the absence of any neutral mode in the dynamics. In (55), the term $\mathbf{\Lambda}_{+,k:0}^{-\mathrm{T}}\mathbf{G}_{++}\mathbf{\Lambda}_{+,k:0}^{-1}$ asymptotically vanishes since in the absence of neutral modes,

$$\lim_{k\to\infty}\left\|\mathbf{\Lambda}_{+,k:l}^{-1}\right\|=\mathbf{0} \tag{58}$$

for any matrix norm $\|\cdot\|$ and any l. The behavior of $\mathbf{E}_{+,k}\triangleq\mathbf{G}_{-+}\mathbf{\Lambda}_{+,k:0}^{-\mathrm{T}}+\mathbf{\Theta}_k^{-+}\mathbf{\Lambda}_{+,k:0}^{-1}$ and $\mathbf{E}_{+,k}^{\mathrm{T}}$ as the unstable/stable off-diagonal blocks in (55) remain to be studied. To that end, we choose a submultiplicative matrix norm, and obtain

$$\begin{aligned}\|\mathbf{E}_{+,k}\| &\le \left\|\mathbf{G}_{-+}\right\|\left\|\mathbf{\Lambda}_{+,k:0}^{-\mathrm{T}}\right\| \\ &\quad+\sum_{l=0}^{k-1}\left\|\mathbf{W}_{-,0}^{\mathrm{T}}\right\|\left\|\widetilde{\mathbf{C}}_{-,0}\right\|\left\|\mathbf{\Lambda}_{-,l:0}^{\mathrm{T}}\right\|\left\|\mathbf{C}_{-,l}^{\mathrm{T}}\right\|\left\|\mathbf{\Omega}_l\right\|\left\|\mathbf{C}_{+,l}\right\|\left\|\mathbf{\Lambda}_{+,k:l}^{-1}\right\|.\end{aligned} \tag{59}$$

Since $\mathbf{\Omega}_l$ has been assumed uniformly bounded from above, and given that matrices with unitary columns are uniformly bounded (by $\sqrt{n}$ in the Frobenius norm), there is a constant c_+ such that for all k

$$\|\mathbf{E}_{+,k}\|\le\left\|\mathbf{G}_{-+}\right\|\left\|\mathbf{\Lambda}_{+,k:0}^{-\mathrm{T}}\right\|+c_+\sum_{l=0}^{k-1}\left\|\mathbf{\Lambda}_{-,l:0}\right\|\left\|\mathbf{\Lambda}_{+,k:l}^{-1}\right\|. \tag{60}$$

Here the matrix norm can be thought of as the spectral norm up to a multiplicative constant. Because the sum is dominated by the convergent series $\sum_{l=0}^{\infty}\|\mathbf{\Lambda}_{-,l:0}\|$ and because of (58) for each l, the majorant of $\mathbf{E}_{+,k}$ asymptotically vanishes so that $\lim_{k\to\infty}\|\mathbf{E}_{+,k}\|=\mathbf{0}$.

As a consequence, the off-diagonal terms of $\mathbf{G}+\mathbf{W}_0^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{W}_0$ in (55) asymptotically vanish. Moreover, the diagonal blocks are uniformly bounded from below by $\varepsilon\mathbf{I}_{n_0}$ by Condition 2 for the top-left block and $\mathbf{G}_{--} \in \mathcal{C}_{+}^{n-n_0}$ for the bottom-right block. Consequently, the inverse of $\mathbf{G}+\mathbf{W}_0^{\mathrm{T}}\boldsymbol{\Theta}_k\mathbf{W}_0$ is asymptotically given by the inverse of the diagonal blocks, up to a vanishing sequence of matrices, and for the unstable block one obtains

$$\lim_{k\to\infty}\left\{\widetilde{\mathbf{C}}_{+,k}^{\mathrm{T}}\mathbf{P}_k\widetilde{\mathbf{C}}_{+,k} - \left(\mathbf{C}_{+,k}^{\mathrm{T}}\boldsymbol{\Gamma}_k\mathbf{C}_{+,k}\right)^{-1}\right\} = \mathbf{0}. \tag{61}$$

This implies by Condition 2, that $\widetilde{\mathbf{C}}_{+,k}^{\mathrm{T}}\mathbf{P}_k\widetilde{\mathbf{C}}_{+,k}$ is asymptotically uniformly bounded. Moreover, we have proven in section 4 that $\lim_{k\to\infty}\mathbf{U}_{-,k}^{\mathrm{T}}\mathbf{P}_k\mathbf{U}_{-,k} = \mathbf{0}$, which by $\mathrm{Im}(\widetilde{\mathbf{C}}_{-,k}) = \mathrm{Im}(\mathbf{U}_{-,k})$, shows that $\lim_{k\to\infty}\widetilde{\mathbf{C}}_{-,k}^{\mathrm{T}}\mathbf{P}_k\widetilde{\mathbf{C}}_{-,k} = \mathbf{0}$.[1] As a consequence of Appendix B, point 5, and using the fact that $\mathbf{C}_k^{-1}\mathbf{P}_k\mathbf{C}_k^{-\mathrm{T}}$ is in $\mathcal{C}^n$, its off-diagonal blocks $\widetilde{\mathbf{C}}_{+,k}^{\mathrm{T}}\mathbf{P}_k\widetilde{\mathbf{C}}_{-,k}$ and $\widetilde{\mathbf{C}}_{-,k}^{\mathrm{T}}\mathbf{P}_k\widetilde{\mathbf{C}}_{+,k}$ also asymptotically vanish. We conclude (using the uniform boundedness of the $\mathbf{C}_k$)

$$\lim_{k\to\infty}\{\mathbf{P}_k - \mathbf{S}_k\} = \mathbf{0}, \quad \text{where} \quad \mathbf{S}_k = \mathbf{C}_{+,k}\left(\mathbf{C}_{+,k}^{\mathrm{T}}\boldsymbol{\Gamma}_k\mathbf{C}_{+,k}\right)^{-1}\mathbf{C}_{+,k}^{\mathrm{T}}. \tag{62}$$

Importantly, the asymptote $\mathbf{S}_k$ does not depend on $\mathbf{P}_0$. This generalizes the result in [24] to the nonautonomous case. Moreover, we will see later that this also generalizes their result to the case where the Lyapunov spectrum is degenerate.

The case where neutral modes are present is much more involved, and yet physically very important [32]. Indeed, there is a wide range of possible asymptotic behaviors for neutral CLVs, which could, for instance, grow, or decay, at a subexponential rate. They could intermittently behave as unstable or stable modes. To go further in the case where neutral modes are present, and only then, the neutral modes and their observability need to be characterized more precisely. Thus, an additional condition that complements Condition 2 needs to be introduced. Since several conditions are possible, we focus on one of them and discuss two others.

5.2. Asymptote in the presence of neutral modes. It is convenient to further split the unstable from the neutral CLVs as

$$\mathbf{C}_k \triangleq \begin{bmatrix} \mathbf{C}_{++,k} & \mathbf{C}_{+0,k} & \mathbf{C}_{-,k} \end{bmatrix}. \tag{63}$$

Accordingly, we refine the decomposition

$$\boldsymbol{\Lambda}_{k:l} \triangleq \begin{bmatrix} \boldsymbol{\Lambda}_{++,k:l} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Lambda}_{+0,k:l} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{\Lambda}_{-,k:l} \end{bmatrix}, \tag{64}$$

where $\boldsymbol{\Lambda}_{++,k:l} \in \mathbb{R}^{n_{0+}\times n_{0+}}$ and $\boldsymbol{\Lambda}_{+0,k:l} \in \mathbb{R}^{n_{00}\times n_{00}}$ are diagonal with $n_{0+} + n_{00} = n_0$. Furthermore, $\boldsymbol{\Lambda}_{+0,k:l}$ is factorized into growing and decaying contributions. First, $\boldsymbol{\Lambda}_{+0\uparrow,k:0} \in \mathbb{R}^{n_{00}\times n_{00}}$ is a diagonal matrix with entries: for $i = 1,\dots,n_{00}$,

$$[\boldsymbol{\Lambda}_{+0\uparrow,k:l}]_{ii} = [\boldsymbol{\Lambda}_{+0,k:l}]_{ii}\prod_{q=l+1}^{k}\max\left(\left|[\boldsymbol{\Lambda}_{+0,q:q-1}]_{ii}\right|^{-1}, 1\right). \tag{65}$$

This definition performs the factorization while transferring the transitivity property of $\boldsymbol{\Lambda}_{k:l}$,

[1] Alternatively, this can be recovered from (54) including the rate of convergence.

i.e., $\mathbf{\Lambda}_{k:0} = \mathbf{\Lambda}_{k:l}\mathbf{\Lambda}_{l:0}$ for $k \geq l \geq 0$, to $\mathbf{\Lambda}_{+0\uparrow,k:l}$, i.e., $\mathbf{\Lambda}_{+0\uparrow,k:0} = \mathbf{\Lambda}_{+0\uparrow,k:l}\mathbf{\Lambda}_{+0\uparrow,l:0}$ for $k \geq l \geq 0$. Second, we also define $\mathbf{\Lambda}_{+0\downarrow,k:0} \triangleq \mathbf{\Lambda}_{+0,k:0}\mathbf{\Lambda}^{-1}_{+0\uparrow,k:0}$ and

$$\mathbf{\Lambda}_{+\uparrow,k:0} \triangleq \begin{bmatrix} \mathbf{\Lambda}_{++,k:0} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_{+0\uparrow,k:0} \end{bmatrix}, \quad \mathbf{\Lambda}_{+\downarrow,k:0} \triangleq \begin{bmatrix} \mathbf{I}_{n_{0+}} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_{+0\downarrow,k:0} \end{bmatrix}. \tag{66}$$

Let us suggest a possible condition that supplements Conditions 1 and 2, in order to obtain an asymptote $\mathbf{S}_k$ for $\mathbf{P}_k$ which, in the presence of neutral modes, does not depend on $\mathbf{P}_0$.

Condition 3. We define

$$\mathbf{\Phi}_k = \mathbf{\Lambda}^{-\mathrm{T}}_{+0\uparrow,k:0}\mathbf{C}^{\mathrm{T}}_{+0,0}\mathbf{\Theta}_k\mathbf{C}_{+0,0}\mathbf{\Lambda}^{-1}_{+0\uparrow,k:0} \tag{67}$$

and require that for any $\mathbf{v} \in \mathbb{R}^{n_{00}}$, and using the Euclidean norm $\|\cdot\|$

$$\liminf_{k\to\infty} \|\mathbf{\Phi}_k\mathbf{v}\| = +\infty. \tag{68}$$

Let us give the example of a realistic setup that leads to condition 3. Assume that the dynamics is autonomous. Hence, there is at least one neutral CLV $\mathbf{v}$ for which the local Lyapunov exponents are 0. Suppose that there is a sequence ω_l of nonnegative numbers such that $\mathbf{\Omega}_l \geq \omega_l\mathbf{v}\mathbf{v}^{\mathrm{T}}$, and assume $\sum_{l=0}^{\infty}\omega_l = \infty$, then it is not difficult to show through equations (21), (67) that Condition 3 is satisfied. In particular, if the observation process is time invariant such that $\omega \triangleq \omega_l > 0$, then $\|\mathbf{\Phi}_k\mathbf{v}\| = \omega k\|\mathbf{v}\|$ which indeed diverges with k.

Analysis of (55) in the presence of neutral modes is not straightforward, and instead we use a Schur complement for the inverse of the top-left block,

$$\begin{aligned}\left[\left(\mathbf{G} + \mathbf{W}_0^{\mathrm{T}}\mathbf{\Theta}_k\mathbf{W}_0\right)^{-1}\right]^{-1}_{++} &= \mathbf{G}_{++} + \mathbf{\Theta}^{++}_k - \left(\mathbf{G}_{+-} + \mathbf{\Theta}^{+-}_k\right) \\ &\quad \times \left(\mathbf{G}_{--} + \mathbf{\Theta}^{--}_k\right)^{-1}\left(\mathbf{G}_{-+} + \mathbf{\Theta}^{-+}_k\right).\end{aligned} \tag{69}$$

Separating the growing and decaying trends of the neutral modes, this yields

$$\begin{aligned}\mathbf{\Lambda}^{\mathrm{T}}_{+\downarrow,k:0}\left(\widetilde{\mathbf{C}}^{\mathrm{T}}_{+,k}\mathbf{P}_k\widetilde{\mathbf{C}}_{+,k}\right)^{-1}\mathbf{\Lambda}_{+\downarrow,k:0} &= \mathbf{\Lambda}^{-\mathrm{T}}_{+\uparrow,k:0}\left(\mathbf{G}_{++} + \mathbf{\Theta}^{++}_k\right)\mathbf{\Lambda}^{-1}_{+\uparrow,k:0} \\ &\quad - \mathbf{E}^{\mathrm{T}}_k\left(\mathbf{G}_{--} + \mathbf{\Theta}^{--}_k\right)^{-1}\mathbf{E}_k,\end{aligned} \tag{70}$$

where $\mathbf{E}_k \triangleq \mathbf{G}_{-+}\mathbf{\Lambda}^{-1}_{+\uparrow,k:0} + \mathbf{\Theta}^{-+}_k\mathbf{\Lambda}^{-1}_{+\uparrow,k:0}$. $\mathbf{E}_k$ can be split into $\mathbf{E}_k = [\ \mathbf{E}_{+,k} \quad \mathbf{E}_{0,k}\ ]$, where $\mathbf{E}_{+,k} \triangleq \mathbf{W}^{\mathrm{T}}_{-,0}\mathbf{G}\mathbf{C}_{++,0}\mathbf{\Lambda}^{-1}_{++,k:0} + \mathbf{W}^{\mathrm{T}}_{-,0}\mathbf{\Theta}_k\mathbf{C}_{++,0}\mathbf{\Lambda}^{-1}_{++,k:0}$ is the stable/unstable matrix block and $\mathbf{E}_{0,k} \triangleq \mathbf{W}^{\mathrm{T}}_{-,0}\mathbf{G}\mathbf{C}_{+0,0}\mathbf{\Lambda}^{-1}_{+0\uparrow,k:0} + \mathbf{W}^{\mathrm{T}}_{-,0}\mathbf{\Theta}_k\mathbf{C}_{+0,0}\mathbf{\Lambda}^{-1}_{+0\uparrow,k:0}$ is the stable/neutral matrix block. This definition of $\mathbf{E}_{+,k}$ is consistent with that of $\mathbf{E}_{+,k}$ in section 5.1. For the same reasons as in section 5.1, we have $\lim_{k\to\infty}\|\mathbf{E}_{+,k}\| = \mathbf{0}$. Similarly, there is a constant c_0 such that for all k

$$\|\mathbf{E}_{0,k}\| \leq \left\|\mathbf{G}_{-+}\right\|\left\|\mathbf{\Lambda}^{-1}_{+0\uparrow,k:0}\right\| + c_0\sum_{l=0}^{k-1}\|\mathbf{\Lambda}_{-,l:0}\|\left\|\mathbf{\Lambda}_{+0\downarrow,l:0}\right\|\left\|\mathbf{\Lambda}^{-1}_{+0\uparrow,k:l}\right\|, \tag{71}$$

which, however, only ensures that $\|\mathbf{E}_{0,k}\|$ is uniformly bounded from above. Note that, in deriving (71), we used $\mathbf{\Lambda}_{+0,l:0}\mathbf{\Lambda}^{-1}_{+0\uparrow,k:0} = \mathbf{\Lambda}_{+0,l:0}\mathbf{\Lambda}^{-1}_{+0\uparrow,l:0}\mathbf{\Lambda}^{-1}_{+0\uparrow,k:l} = \mathbf{\Lambda}_{+0\downarrow,l:0}\mathbf{\Lambda}^{-1}_{+0\uparrow,k:l}$. Hence, the only case where the last term of (70), as well as $\mathbf{\Lambda}_{+\uparrow,k:0}^{-\mathrm{T}}\mathbf{G}_{++}\mathbf{\Lambda}_{+\uparrow,k:0}^{-1}$, do not asymptotically vanish but are uniformly bounded is for entries related to the neutral modes alone. Yet, in this case, the neutral subblock of $\mathbf{\Lambda}_{+\uparrow,k:0}^{-\mathrm{T}}\mathbf{\Theta}_k^{++}\mathbf{\Lambda}_{+\uparrow,k:0}^{-1}$, which is $\mathbf{\Phi}_k$, asymptotically dominates the bounded correction by Condition 3, so that, even in the presence of neutral modes, the correction term is negligible. More precisely, (70) has the asymptote

$$\begin{bmatrix} \mathbf{C}_{++,0}^{\mathrm{T}}\mathbf{\Gamma}_k\mathbf{C}_{++,0} & \mathbf{\Lambda}_{++,k:0}^{-\mathrm{T}}\mathbf{C}_{++,0}^{\mathrm{T}}\mathbf{\Theta}_k^{++}\mathbf{C}_{+0,0}\mathbf{\Lambda}_{+0\uparrow,k:0}^{-1} \\ \mathbf{\Lambda}_{+0\uparrow,k:0}^{-\mathrm{T}}\mathbf{C}_{+0,0}^{\mathrm{T}}\mathbf{\Theta}_k^{++}\mathbf{C}_{++,0}\mathbf{\Lambda}_{++,k:0}^{-1} & \mathbf{\Phi}_k+\mathbf{B}_k \end{bmatrix}, \tag{72}$$

where $\mathbf{B}_k$ is a bounded sequence. Its inverse, i.e., $\mathbf{\Lambda}_{+\downarrow,k:0}^{-1}\widetilde{\mathbf{C}}_{+,k}^{\mathrm{T}}\mathbf{P}_k\widetilde{\mathbf{C}}_{+,k}\mathbf{\Lambda}_{+\downarrow,k:0}^{-\mathrm{T}}$, is well-defined and obtained by the formula of the inverse of a matrix with 2×2 subblocks, which yields the asymptote

$$\begin{bmatrix} \left(\mathbf{C}_{++,0}^{\mathrm{T}}\mathbf{\Gamma}_k\mathbf{C}_{++,0}\right)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Phi}_k^{-1} \end{bmatrix}. \tag{73}$$

We can conclude similarly to the end of section 5.1 that (62) is still valid in the presence of neutral modes if Condition 3 is satisfied. In this case, the asymptotic sequence can further be simplified into

$$\mathbf{S}_k = \mathbf{C}_{++,0}\left(\mathbf{C}_{++,0}^{\mathrm{T}}\mathbf{\Gamma}_k\mathbf{C}_{++,0}\right)^{-1}\mathbf{C}_{++,0}^{\mathrm{T}}. \tag{74}$$

Note that we expect the rate of convergence to the neutral subspace to be possibly quite different from the exponential convergence to the stable subspace. For instance, considering again the example where $\|\mathbf{\Phi}_k\mathbf{v}_k\| = \omega k\|\mathbf{v}_k\|$, $\widetilde{\mathbf{C}}_{+0,k}^{\mathrm{T}}\mathbf{P}_k\widetilde{\mathbf{C}}_{+0,k}$ asymptotically behaves like $(\omega k)^{-1}\mathbf{I}_{n_{00}}$.

An alternative to Condition 3, but which does not exhaust all the possible behaviors of neutral dynamics, is to assume that the sequence $\mathbf{\Lambda}_{+0\uparrow,k:0}^{-1}$ has a limit and

$$\lim_{k\to\infty}\left\|\mathbf{\Lambda}_{+0\uparrow,k:0}^{-1}\right\| = \mathbf{0}. \tag{75}$$

If satisfied, $\mathbf{E}_{0,k}$ and $\mathbf{\Lambda}_{+\uparrow,k:0}^{\mathrm{T}}\mathbf{G}_{++}\mathbf{\Lambda}_{+\uparrow,k:0}^{-1}$ in (70) both asymptotically vanish. Therefore, the convergence is similar to that of section 5.1: the neutral modes are effectively unstable modes. Equation (62) remains valid but the neutral modes may have a nonnegligible contribution to $\mathbf{S}_k$ depending on the asymptotic behavior of $\mathbf{\Gamma}_{00,k} = \mathbf{C}_{+0,k}^{\mathrm{T}}\mathbf{\Gamma}_k\mathbf{C}_{+,0;k}$.

If the sequence $\|\mathbf{\Lambda}_{+0\uparrow,k:0}^{-1}\|$ does not have a limit or if its limit is distinct from 0, then the sequence has an adherence point in $]0,1]$.Then, the sequence $\|\mathbf{E}_{0,k}\|$ does not necessarily asymptotically vanish. However, it can be seen that if the neutral modes are observed with an $\mathbf{\Omega}_l$ bounded from below, $\mathbf{\Phi}_k$ necessarily diverges, which leads back to the asymptote equation (74).

Note that we have discussed criteria applying to all neutral modes. However, Condition 3 or its alternatives could be individualized to each neutral mode.

5.3. Degeneracy of the Lyapunov spectrum. At a more heuristic level, we discuss the case where there are multiplicities greater than one in the Lyapunov spectrum. In this case, (45) remains valid, up to some qualifications. While the Oseledec subspaces themselves are covariant, they may not be entirely decomposable into one dimensional covariant subspaces—one should immediately consider the analogy with generalized eigenvectors for Jordan blocks. Indeed, when there is a degenerate Lyapunov spectrum there may only be a single covariant vector per exponent. If we redefine $\mathbf{C}_k$ to be a matrix with columns composed of an ordered basis for each covariant Oseledec subspace then $\mathbf{\Lambda}_{k:l}$ is not necessarily a diagonal matrix but rather upper triangular over $\mathbb{C}$. In that case, the transpose operators in the above derivations should be understood as conjugate and transpose operators. This consideration only matters in the derivation where norms of $\mathbf{\Lambda}_{k:l}$ are to be computed when studying the convergence of sequences and sums. In this case, the spectral norm is not necessarily related to the eigenspectrum of $\mathbf{\Lambda}_{k:l}$ which is not necessarily self-adjoint (something that has been overlooked in the derivation in [24] in the autonomous case). However, we can heuristically expect a polynomial correction as a function of $k-l$ to the exponential growth or decay of $\mathbf{\Lambda}_{k:l}$ because of the impact of the Jordan blocks. By the Oseledec theorem, ones knows that $\lim_{k-l\to\infty}(\mathbf{\Lambda}_{k:l}^{\mathrm{T}}\mathbf{\Lambda}_{k:l})^{1/2(k-l)} = \exp(\mathbf{D})$, where $\mathbf{D}$ is the diagonal matrix of the Lyapunov exponents. Hence, $\mathbf{\Lambda}_{k:l}^{\mathrm{T}}\mathbf{\Lambda}_{k:l}$ asymptotically behaves like $\exp((k-l)\mathbf{D})$ up to a subexponential correction. To compute the matrix norm of $\mathbf{\Lambda}_{k:l}$, one can equivalently use the spectral norm and compute the square root of the spectral radius $\rho(\mathbf{\Lambda}_{k:l}^{\mathrm{T}}\mathbf{\Lambda}_{k:l})$ which is asymptotically equivalent to $\rho(\exp((k-l)\mathbf{D}))$ up to a subexponential correction which could be absorbed into the exponential trend if need be. This shows that the exponential trends in the above derivations are unchanged. As a consequence, we believe that the main results of this section are likely to be unaltered by the Lyapunov spectrum degeneracy. Only the neutral modes, that are not subject to exponential growth or decay, could be impacted. This will be studied and reported in a separate paper.

5.4. Role of the neutral modes. It is finally worth mentioning the particular role played by the neutral modes. In section 4, the exponential convergence to $\mathbf{0}$ of $\mathbf{P}_k$ for all stable directions was proven. Provided the three conditions equations (49), (50), (68) are met, the above discussion points to an exponential convergence of $\mathbf{P}_k$ onto $\mathbf{S}_k$ for all unstable directions. Nevertheless, the discussion also suggests a slower convergence of $\mathbf{P}_k$ to $\mathbf{0}$ for neutral directions. The critical importance of the neutral modes was originally observed by [27] in numerical experiments with assimilation in the unstable-neutral subspace in the context of variational DA with nonlinear dynamics. They numerically showed that it was necessary to include the neutral direction within the subspace where the assimilation was performed in order to efficiently control the error growth. The analysis carried out in the present section further corroborates their findings.

Moving away from the linear hypothesis towards nonlinear dynamics and in connection with this slow convergence of the neutral modes, it was recently argued [4] that the region of the Lyapunov spectrum around the neutral modes is critical in the convergence of the EnKF. The misestimation of the uncertainty in this region of the spectrum was shown to be the reason why the ad hoc technique known as inflation meant to stabilize the filter is very often required.

6. Numerical results.

We present here numerical results on the asymptotic properties of the analysis error covariance $\mathbf{P}_k^{\mathrm{a}}$ that corroborate and illustrate the theoretical findings. The convergence results obtained for $\mathbf{P}_k$ can easily be transferred to $\mathbf{P}_k^{\mathrm{a}}$ by (7), or by applying $\mathbf{P}_k^{\mathrm{a}} \leq \mathbf{P}_k$ which is readily obtained using the matrix shift lemma to (6) as in (23).

Three different experimental setups are considered, with different choices of the dynamical and observational models in (1), (2). In all cases the perfect model hypothesis is employed, $\mathbf{Q}_k = \mathbf{0}$.

Exp1: Autonomous system. The state- and observation-space dimensions are $n = 30$ and $d = 10$, respectively. The time-invariant matrices $\mathbf{M}_k \triangleq \mathbf{M} \in \mathbb{R}^{n\times n}$, $\mathbf{H}_k \triangleq \mathbf{H} \in \mathbb{R}^{d\times n}$, and $\mathbf{R}_k \triangleq \mathbf{R} \in \mathbb{R}^{d\times d}$ are chosen randomly, i.e., with entries which are indepedently and identically distributed (iid) standard normal random variables.

Exp2: Random nonautonomous system. The state- and observation-space dimensions are $n = 30$ and $d = 10$, respectively. The time-varying, invertible, propagators $\mathbf{M}_k \in \mathbb{R}^{n\times n}$, the observation error covariance matrices $\mathbf{R}_k \in \mathbb{R}^{d\times d}$, and the observation matrices $\mathbf{H}_k \in \mathbb{R}^{d\times n}$ are all randomly generated, i.e., the entries of these matrices are iid standard normal random variables.

Exp3: Nonautonomous system obtained by linearization around a trajectory of the Lorenz-95 model. The entries of the observation error covariance, $\mathbf{R}_k$ and $\mathbf{H}_k$ are generated as in Exp2 but with the state- and observation-space dimensions being $n = 40$ and $d = 15$, respectively. The propagators $\mathbf{M}_k$ are taken to be the linearization around a trajectory on the attractor of the $n = 40$-dimensional Lorenz-95 model [18], which is very commonly used in DA literature; see, e.g., [9, and references therein]. The equations read

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = x_{j-1}\left(x_{j+1} - x_{j-2}\right) - x_j + F, \qquad j = 1, \dots, n, \tag{76}$$

with periodic boundary conditions, $x_0 = x_n$, $x_{-1} = x_{n-1}$, and $x_{n+1} = x_1$. The standard value of the forcing, $F = 8$, is used in the following experiments. The observation interval is $\Delta t = 0.1$.

In another numerical experiment, we used a simpler observational network, by choosing $\mathbf{H}_k = [1, 0, \dots, 0]$, corresponding to observation of only the first component of the state vector. The numerical results for Exp3 (with randomly chosen elements of $\mathbf{H}_k$ of dimension 15×40) and for this much simpler observational network were qualitatively the same and thus the latter have not been presented here.

It must be emphasized that this case (Exp3) does not coincide with the nonlinear filtering problem of the Lorenz-95 model but it makes use of the linearization of the model to build up the propagator which is then used as a linear model in (1).

Note, furthermore, that in an extended Kalman filter (EKF, [14]) applied to a nonlinear system such as the Lorenz-95, the only place where the state estimate enters the computation of the covariance matrices is in the linearization of the model dynamics in which one needs to estimate the Jacobian of the model dynamics evaluated on the system's state. Therefore, for the Lorenz-95 model, the analysis and forecast covariances of the EKF will show asymptotic behavior similar to what is presented below. While this behavior was already observed and exploited in a reduced-order formulation of the EKF based on the unstable subspace [28], it does not give many hints about the asymptotic behavior of a fully nonlinear filter.

Each of the three experimental setups is representative of a class of systems. Numerical results (not shown) for other choices of the system and observational dimension as well as for other realizations of the random matrices $\mathbf{M}_k, \mathbf{H}_k, \mathbf{R}_k$ were found to be qualitatively equivalent to the results reported below.

For the three numerical experiments described above, it is very difficult to check the observability condition $\det(\mathbf{\Gamma}_k) \neq 0$ because the matrices $\mathbf{\Gamma}_k$ soon become very ill-conditioned. But we expect that the system would be observable with probability 1 for Exp1 and Exp2, while in Exp3 (the case of the Lorenz-95 model), we expect the system to be observable even with a single variable being observed, since each variable is coupled to those around it. Note that we are unable to numerically verify the above statements.

The QR method [23, 17] is adopted to numerically compute the Lyapunov vectors and exponents. Starting from a random positive semidefinite $\mathbf{P}_0^{\mathrm{a}}$, the sequence $(\mathbf{P}_k, \mathbf{P}_k^{\mathrm{a}})$ for $k > 0$ of forecast and analysis error covariance matrices was generated based on the KF equations (6), (7).

Recall that n_0 stands for the number of nonnegative Lyapunov exponents: in most cases, n_0 will correspond to the number of positive plus one zero exponent. Numerically, this zero Lyapunov exponent will not be exactly zero but it will fluctuate around it. Also recall that r_0 is the rank of the initial covariance matrices $\mathbf{P}_0$, or $\mathbf{P}_0^{\mathrm{a}}$.

6.1. Rate of convergence of the eigenvalues. The following numerical experiments show the relation between the rates of convergence of eigenvalues, σ_i^k, of the error covariance matrix $\mathbf{P}_k$, and the Lyapunov exponents of the dynamical system of (1), (2). The eigenvalues are ordered so that $\sigma_1^k \geq \sigma_2^k \cdots \geq \sigma_n^k$.

When $r_0 < n_0$, the rank of $\mathbf{P}_k$ as $k \to \infty$ generically remains r_0 for almost all initial conditions with no eigenvalues decaying to zero. Thus we consider here the relevant situation $r_0 \geq n_0$. From section 4.1, we know that in this case, $\sigma_{r_0+1}^k = \cdots = \sigma_n^k = 0$. Moreover, from section 4.4, (43), we know that $\sigma_1^k, \ldots, \sigma_{n_0}^k$ will remain nonzero even in the limit $k \to \infty$—except maybe for the neutral directions as discussed in section 5—whereas $\sigma_{n_0+1}^k, \ldots, \sigma_{r_0}^k$ will decay to zero. Recall from section 4.2 that $\exp(\lambda_i^k k)$ is a singular value of $\mathbf{M}_{k:0}$ so that λ_i^k approaches the Lyapunov exponent λ_i as $k \to \infty$; the Lyapunov exponents are ordered so that the first n_0 are nonnegative, $\lambda_1 > \lambda_2 > \cdots > \lambda_{n_0} \geq 0$, whereas the rest are negative with decreasing value, $0 > \lambda_{n_0+1} > \lambda_{n_0+2} > \cdots > \lambda_n$.

The results of section 4.3 and the inequality (42) can be used to derive the rate of convergence of the smallest $r_0 - n_0$ eigenvalues σ_i^k with $i = n_0 + 1, \ldots, r_0$. Using the largest eigenvalue at the initial time, σ_1^0, as for α_i in (42) we have

$$\sigma_i^k \leq \sigma_1^0 \exp\left(2\lambda_i^k k\right) \tag{77}$$

which implies that, asymptotically,

$$\ln(\sigma_i^k) \leq \ln(\sigma_1^0) + 2\lambda_i^k k \underset{k\to\infty}{\sim} \ln(\sigma_1^0) + 2\lambda_i k. \tag{78}$$

The equivalence in (78) is valid in the limit $k \to \infty$ since $\lambda_i^k \to \lambda_i$ as $k \to \infty$. Therefore for $i = n_0 + 1, \ldots, r_0$, the eigenvalues σ_i^k of $\mathbf{P}_k$ decay to zero exponentially fast with the exponential decay rate asymptotically being at least twice the Lyapunov exponent λ_i. Note that, as mentioned above, $\mathbf{P}_k^{\mathrm{a}} \leq \mathbf{P}_k$, so the aforementioned decay rate is also valid for the eigenvalues of the analysis error covariance matrix, $\mathbf{P}_k^{\mathrm{a}}$.

Figure 1(a) illustrates the decay of some of the eigenvalues of the analysis error covariance matrix in Exp3. Similar graphs have been obtained for Exp1 and Exp2 (not shown). Figure 1(b) shows the slopes of the best fit lines for the semi-log plot of σ_i^k versus k for the full

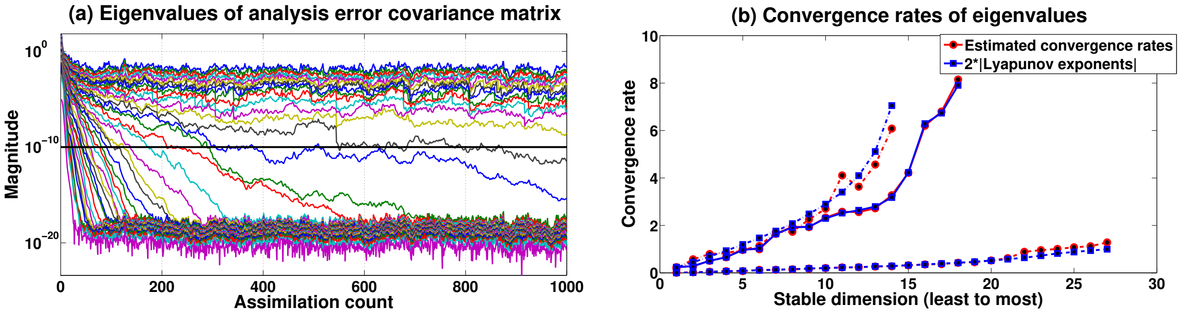

Figure 1. *Panel* (a) *shows the eigenvalues of* $\mathbf{P}_k^{\mathrm{a}}$ *in Exp*3 *and the decay of part of its spectrum. Panel* (b) *shows the comparison between the decay rate of the eigenvalues of the analysis covariance matrix (red lines) with twice the absolute value of the negative Lyapunov exponents (blue lines), for the autonomous system (solid line,* $n = 30, n_0 = 16$*), and for two examples of nonautonomous systems with random propagators (dash-dot line,* $n = 30, n_0 = 16$*) and with propagators derived from the Lorenz-*95 *system (dashed line,* $n = 40, n_0 = 14$*), for full rank* $\mathbf{P}_0$*.*

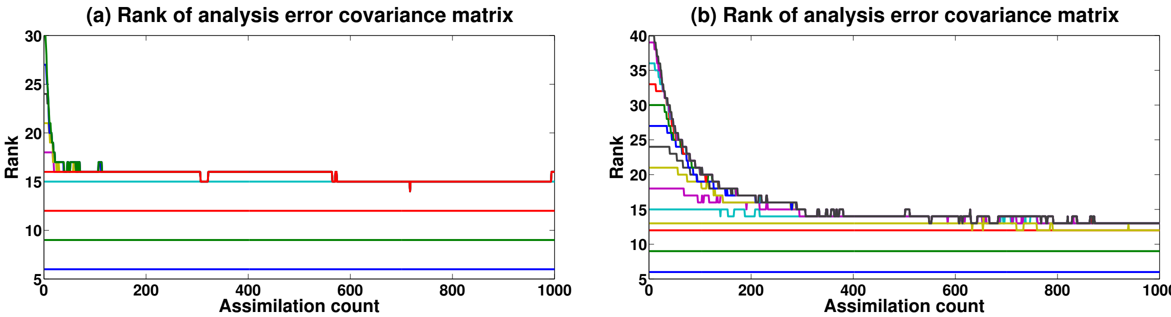

Figure 2. *Rank of* $\mathbf{P}_k^{\mathrm{a}}$ *as a function of* k *for several choices of the rank* r_0 *of* $\mathbf{P}_0^{\mathrm{a}}$ *(various colors) for two systems, one with random propagators* $\mathbf{M}_k$ (a) *with* $n_0 = 16$ *and another with propagators which are a linearization of Lorenz-*95 *around a trajectory on the attractor* (b) *with* $n_0 = 14$*.*

rank $\mathbf{P}_0$ (red dots), for all three experiments described above. The blue dots show the values of twice the absolute value of the corresponding negative Lyapunov exponents. We see that, indeed, the inequality (78) is saturated.

6.2. Existence of asymptotic sequences of low-rank covariance matrices. The next set of numerical results corroborate the results in section 4.2 about the projections of the covariance matrices onto the stable subspace vanishing and the results in section 5 about their asymptotic behavior.

Figure 2 plots the rank of $\mathbf{P}_k^{\mathrm{a}}$ as a function of k, where various choices of the rank r_0 of $\mathbf{P}_0^{\mathrm{a}}$ are shown by various colors in the figure. Note that we actually plot the number of eigenvalues greater than a threshold of 10^{-10}.

Panel (a) of Figure 2 shows the case of random propagators (Exp2) $\mathbf{M}_k$, which has $n = 30$ and $n_0 = 16$, i.e., the number of nonnegative Lyapunov exponents is 16. Panel (b) refers to the case Exp3 of linearization of Lorenz-95 with $F = 8$ around a trajectory on its attractor with $n = 40$ and $n_0 = 14$. We see that if $r_0 < n_0$, then the rank of $\mathbf{P}_k^{\mathrm{a}}$ is constant and equal to the initial rank r_0. On the other hand, if $r_0 \geq n_0$, then $r_0 - n_0$ eigenvalues values

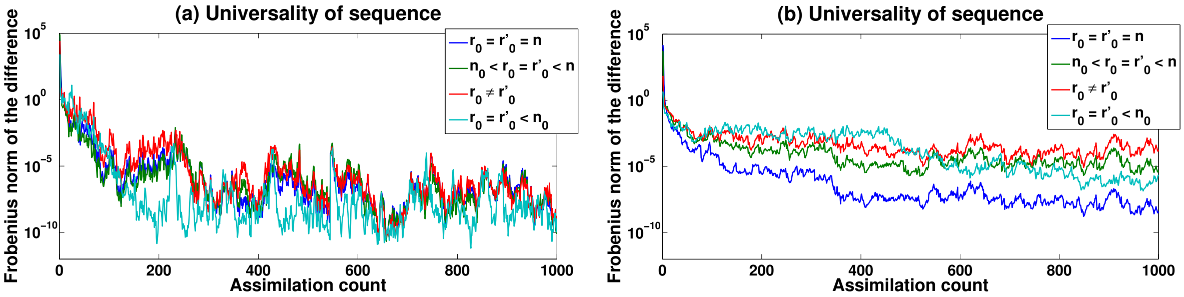

Figure 3. *Frobenius norm of the difference, i.e.,* $\|\mathbf{P}^{\mathrm{a}}_k - \mathbf{P}'^{\mathrm{a}}_k\|$ *for two sequences of analysis covariances matrices starting with different initial conditions* $\mathbf{P}^{\mathrm{a}}_0$ *and* $\mathbf{P}'^{\mathrm{a}}_0$ *for the case of random propagators* (a) *with* $n_0 = 16$ *and Lorenz-*95 *linearization* (b) *with* $n_0 = 14$.

approach zero, $n_0 - 1$ eigenvalues remain nonzero, while one eigenvalue fluctuates and it is unclear whether it will approach zero or indeed remain nonzero. It very likely corresponds to the neutral direction along which convergence of $\mathbf{P}_k$ is very slow even if well observed, as discussed in section 5.

In the next numerical experiment, we generate two sequences of analysis covariances $\mathbf{P}^{\mathrm{a}}_k$ and $\mathbf{P}'^{\mathrm{a}}_k$ starting from two different initial conditions $\mathbf{P}^{\mathrm{a}}_0$ and $\mathbf{P}'^{\mathrm{a}}_0$, respectively. Figure 3 shows the Frobenius norm of the difference between analysis covariances, i.e., $\|\mathbf{P}^{\mathrm{a}}_k - \mathbf{P}'^{\mathrm{a}}_k\|$, as a function of k. Four cases are considered in Figure 3:

1. $r_0 = r'_0 = n$ when the initial ranks are the same and equal to the state dimension (blue line);
2. $n_0 < r_0 = r'_0 < n$ when the initial covariance matrices are rank deficient with the same rank greater than n_0 (green line);
3. $r_0 \neq r'_0$ and $n_0 < r_0, r'_0 < n$ when the initial ranks are unequal but both ranks are greater than n_0 (red line);
4. $r_0 = r'_0 < n_0$ when the initial ranks are the same and less than n_0 (teal line).

In all these cases, we see that the norm of the difference approaches zero within the numerical accuracy, fluctuating between 10^{-8} and 10^{-3}, i.e., for large k, $\mathbf{P}^{\mathrm{a}}_k \approx \mathbf{P}'^{\mathrm{a}}_k$. Thus the sequence $\mathbf{P}^{\mathrm{a}}_k$ is equivalent to a sequence of covariance matrices all of rank $s = \min\{r_0, n_0\}$, independent of the initial condition $\mathbf{P}^{\mathrm{a}}_0$, but of course dependent on the dynamics $\mathbf{M}_k$, the observations $\mathbf{H}_k$, and their error covariances $\mathbf{R}_k$.

The asymptotic covariance matrices are most easily represented in the basis of the BLVs. As proven mathematically in section 4.2 in the case of strong collapse which occurs here because the systems are sufficiently observed, these covariance matrices have column spaces corresponding to the span of the most unstable BLVs and their null space subsumes the span of the stable BLVs. This can be seen by looking at the projection of these covariance matrices $\mathbf{P}^{\mathrm{a}}_k$ onto the BLVs $\mathbf{u}^k_1, \ldots, \mathbf{u}^k_n$ at time t_k.

Figure 4 shows these projections for four different values of $k = 2500$, 3000, 3500, 4000 for the cases $r_0 \geq n_0$ (top row) and $r_0 < n_0$ (middle row). The Exp2 and Exp3 cases are displayed in the left and right column panels, respectively. Note that the Lyapunov vectors are ordered from the largest to the smallest Lyapunov exponents. This is also clearly seen from the bottom row of the same Figure 4 which shows these projections at a fixed time $k = 5000$ for various initial ranks r_0 which are equal to or less than n_0.

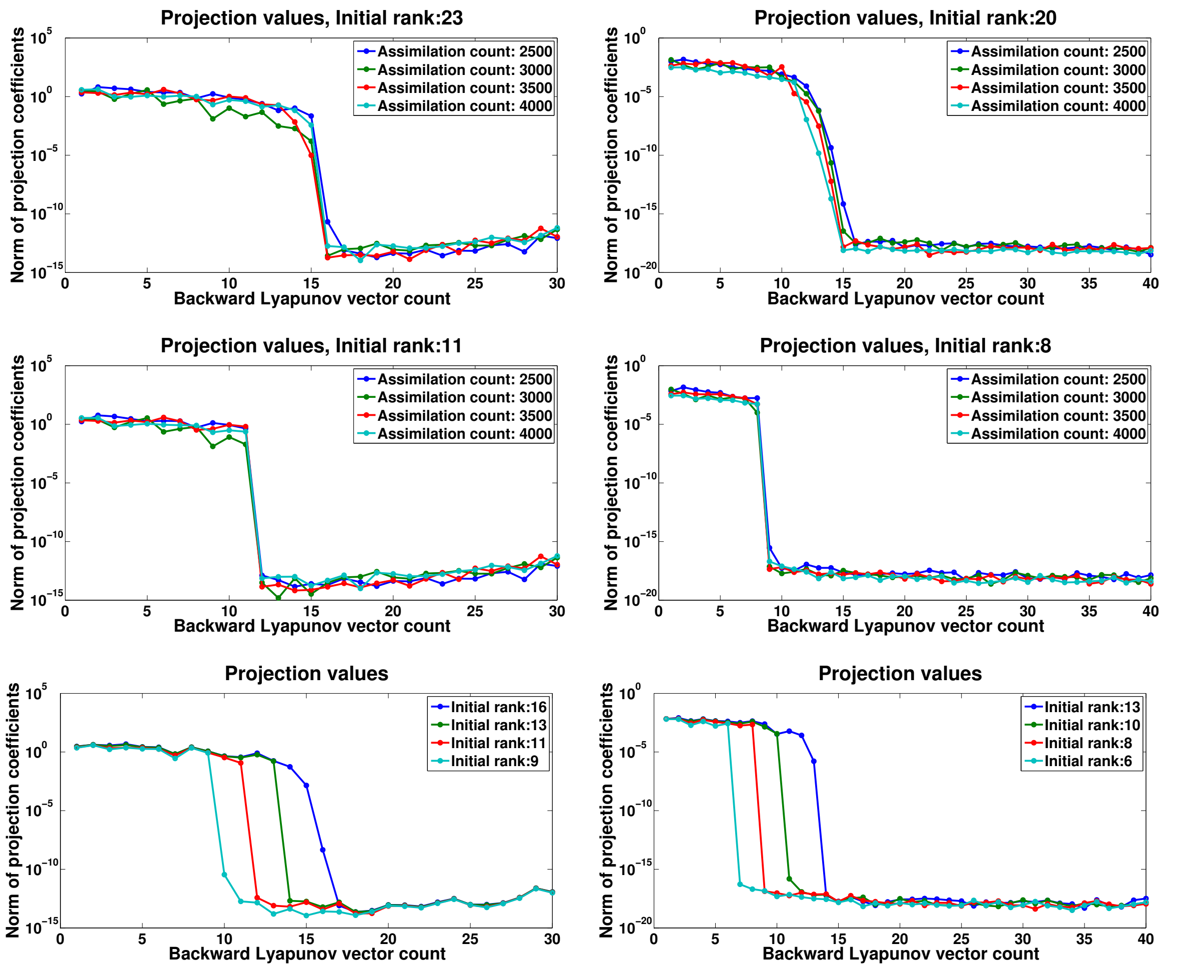

Figure 4. *Projections of covariance matrices* $\mathbf{P}_k^{\mathrm{a}}$ *onto the BLVs* $\mathbf{u}_1^k, \ldots, \mathbf{u}_n^k$ *for system with random propagators (left column,* $n = 30, n_0 = 16$*) and linearization of Lorenz-*95 *(right column,* $n = 40, n_0 = 14$*).*

6.3. Low-rank asymptotic covariance for autonomous systems. The last set of numerical results illustrates the asymptotic convergence of the analysis covariances for the case of autonomous systems. The results are very similar to those of the nonautonomous systems and a summary is presented in Figure 5. The left panel shows the Frobenius norm of the difference $\mathbf{P}_{k+1}^{\mathrm{a}} - \mathbf{P}_k^{\mathrm{a}}$ of the analysis covariance matrices at consecutive time instances. The figure clearly shows this difference going to zero and thus by Cauchy's convergence criterion, the sequence of the analysis covariance matrices converges. Different lines are meant for cases of different initial ranks. The right panel shows the projections onto the BLVs which also span the generalized eigenspace of $\mathbf{M}^{\mathrm{T}}$ [13], for four cases with different initial rank r_0, and these results are very similar to those shown in the bottom row of Figure 4.

7. Conclusion. We have shown that, for perfect linear dynamics and observation operator, and for any initial error covariance matrix, the solution of the KF covariance equation converges onto the unstable-neutral subspace of the dynamics. The rate of such convergence

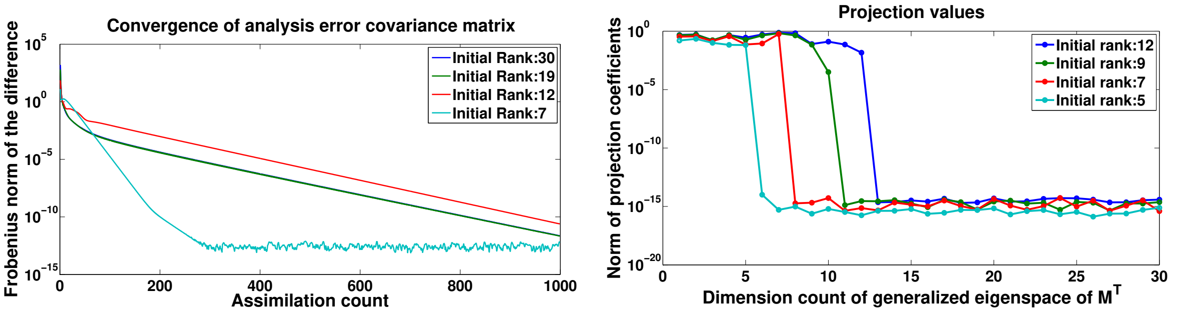

Figure 5. *Frobenius norm of the consecutive difference, i.e.,* $\|\mathbf{P}_k^{\mathrm{a}} - \mathbf{P}_{k-1}^{\mathrm{a}}\|$ *for several choices of rank* r_0 *of the initial condition* $\mathbf{P}_0^{\mathrm{a}}$ *(left panel) and projections onto the generalized eigenspace of* $\mathbf{M}^{\mathrm{T}}$ *(right panel) for the autonomous system with* $n = 30, n_0 = 13$.

has also been provided. Moreover, we have shown that under reasonable assumptions there exists a universal sequence, independent of the initial condition, toward which the KF error covariance converges if the system is sufficiently observed and if the column space of the initial error covariance has a nonzero projection on all the unstable and neutral FLVs. These results were obtained after proving an analytical expression of the covariances at any time in terms of the initial covariances. Numerical experiments were used to further corroborate and illustrate the mathematical statements. These results complete and generalize those in [13] and altogether lay the mathematical foundation of the methods that rely on the assimilation in the unstable subspace [20].

It should be stressed in this conclusion that we have also obtained alternative square root formulas for equations (18), (20), (30), (62), which means that those are written in terms of $\mathbf{X}_k$ the square root factor of $\mathbf{P}_k = \mathbf{X}_k\mathbf{X}_k^{\mathrm{T}}$ rather than $\mathbf{P}_k$. Those would have made an even stronger connection with ensemble filters since the columns of $\mathbf{X}_k$ can be seen as state perturbations associated with an ensemble of state vectors. However, the derivations that use the square root factors turned out to be equivalent or longer compared to working on $\mathbf{P}_k$ directly. They do not bring in new insights for the purposes of this paper compared to the derivations presented here. That is why we did not opt for the square root approach in this paper. Square root generalizations of these formulas will be introduced elsewhere [2] in a nonlinear context where they are more relevant.

Yet, this work leaves unresolved some key issues that are worth investigating in the perspective of the design of reduced-order algorithms applicable to practical situations. Specific lines of development include the treatment of model error and the extension to nonlinear dynamics. This latter problem stimulates indeed an intriguing, albeit necessary, direction of study whose main difficulty stands on the fact that the unstable subspace is, in this nonlinear case, no longer globally defined but a function of the underlying trajectory. Both lines of research may lead to interesting methodological and mathematical developments and are central in DA.

In our view the present results are also relevant to the field of ensemble-based DA algorithms for the geosciences or, more generally, to the uncertainty quantification and DA methods in complex high-dimensional and big data problems, of which DA for the geosciences is a prototypical example. We believe so for two distinctive reasons. First the present findings on the error covariance projection onto the unstable-neutral subspace provide a natural rationale to interpret a stream of numerical evidence that relates the minimum ensemble size to achieve a satisfactorily estimate of the system's state, with the number of unstable directions of the underlying dynamics [9, 19, 5]. Second, this study encourages a research effort toward EnKF formulations that incorporate the information on the unstable subspace explicitly in the design and choice of the ensemble, possibly in combination with localization techniques widely used to artificially increase the rank of the ensemble-based error covariance matrices.

While a specific recipe for a formulation of the EnKF under this framework is still part of the authors' ongoing research, some preliminary considerations can nevertheless be put forward. First, the convergence onto the unstable subspace for EnKF covariance can only be obtained for the class of the deterministic EnKFs, as confirmed by the numerical results performed by the authors [2]. Second, for the sake of the feasibility, the explicit use of the unstable subspace in the filter design for high-dimensional applications, must necessarily rely on an efficient computation of such a subspace. Recent developments along this line [34, 12] thus appear favorable and further support our current research.

It is finally worth mentioning another appealing research direction: the extension of the present framework to fully Bayesian DA methods typically preferable in the presence of strong nonlinearities and/or non-Gaussian error [3]. Besides the aforesaid difficulty inherent to nonlinear dynamics, the additional problem here is on how to link the geometrical (in the phase-space) features of the unstable subspace to the conditioning of a pdf, that is, the generalization to the fully Bayesian framework, of projecting the error covariances onto the unstable subspace.

Appendix A. Deriving $\mathbf{P}_k$ using the symplectic symmetry.

This appendix gives an account of the linear representation of the recurrence equation (4), which had initially been developed as a way to solve the Riccati equation in the autonomous case [1, and references therein]. We use it to give an alternative derivation of (18) and to discuss in more detail the analytic expression in the autonomous case. The underlying symplectic structure of the KF has been, for instance, explored in [6, 33].

A.1. General linear representation using symplectic matrices.

Let us rewrite the recurrence equation (4):

$$\begin{aligned}
\mathbf{P}_k &= \mathbf{M}_k \left(\mathbf{I}_n + \mathbf{P}_{k-1}\boldsymbol{\Omega}_{k-1}\right)^{-1} \mathbf{P}_{k-1}\mathbf{M}_k^{\mathrm{T}} + \mathbf{Q}_k \\
&= \mathbf{M}_k\mathbf{P}_{k-1} \left(\mathbf{I}_n + \boldsymbol{\Omega}_{k-1}\mathbf{P}_{k-1}\right)^{-1} \mathbf{M}_k^{\mathrm{T}} + \mathbf{Q}_k \\
&= \mathbf{M}_k\mathbf{P}_{k-1} \left(\mathbf{M}_k^{-\mathrm{T}} + \mathbf{M}_k^{-\mathrm{T}}\boldsymbol{\Omega}_{k-1}\mathbf{P}_{k-1}\right)^{-1} + \mathbf{Q}_k \\
&= \left(\mathbf{M}_k\mathbf{P}_{k-1} + \mathbf{Q}_k \left\{\mathbf{M}_k^{-\mathrm{T}} + \mathbf{M}_k^{-\mathrm{T}}\boldsymbol{\Omega}_{k-1}\mathbf{P}_{k-1}\right\}\right) \left(\mathbf{M}_k^{-\mathrm{T}} + \mathbf{M}_k^{-\mathrm{T}}\boldsymbol{\Omega}_{k-1}\mathbf{P}_{k-1}\right)^{-1} \\
&= \left(\left\{\mathbf{M}_k + \mathbf{Q}_k\mathbf{M}_k^{-\mathrm{T}}\boldsymbol{\Omega}_{k-1}\right\} \mathbf{P}_{k-1} + \mathbf{Q}_k\mathbf{M}_k^{-\mathrm{T}}\right) \left(\mathbf{M}_k^{-\mathrm{T}}\boldsymbol{\Omega}_{k-1}\mathbf{P}_{k-1} + \mathbf{M}_k^{-\mathrm{T}}\right)^{-1} \\
&\triangleq \left(\mathbf{A}_k\mathbf{P}_{k-1} + \mathbf{B}_k\right) \left(\mathbf{C}_k\mathbf{P}_{k-1} + \mathbf{D}_k\right)^{-1}, \qquad (79)
\end{aligned}$$

where we used the matrix shift lemma from the first to the second line, and we defined block matrices $\mathbf{A}_k$, $\mathbf{B}_k$, $\mathbf{C}_k$, $\mathbf{D}_k$ in the fourth line. Let us define [1]

$$\mathbf{Z}_k \triangleq \begin{pmatrix} \mathbf{A}_k & \mathbf{B}_k \\ \mathbf{C}_k & \mathbf{D}_k \end{pmatrix} = \begin{pmatrix} \mathbf{M}_k + \mathbf{Q}_k \mathbf{M}_k^{-\mathrm{T}} \boldsymbol{\Omega}_{k-1} & \mathbf{Q}_k \mathbf{M}_k^{-\mathrm{T}} \\ \mathbf{M}_k^{-\mathrm{T}} \boldsymbol{\Omega}_{k-1} & \mathbf{M}_k^{-\mathrm{T}} \end{pmatrix}, \tag{80}$$

which is valid in the presence of model noise. This matrix belongs to the symplectic group $\mathrm{Sp}(2n, \mathbb{R})$ since $\mathbf{Z}_k^{-1} = -\mathbf{J}\mathbf{Z}_k^{\mathrm{T}}\mathbf{J}$, where $\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{I}_n \\ -\mathbf{I}_n & \mathbf{0} \end{pmatrix}$. It has a simple expression in the perfect model case:

$$\mathbf{Z}_k \triangleq \begin{pmatrix} \mathbf{A}_k & \mathbf{B}_k \\ \mathbf{C}_k & \mathbf{D}_k \end{pmatrix} = \begin{pmatrix} \mathbf{M}_k & \mathbf{0} \\ \mathbf{M}_k^{-\mathrm{T}} \boldsymbol{\Omega}_{k-1} & \mathbf{M}_k^{-\mathrm{T}} \end{pmatrix}. \tag{81}$$

Furthermore, let us introduce the following matrix in $\mathbb{R}^{2n\times n}$:

$$\mathbf{W}_k = \begin{pmatrix} \mathbf{X}_k \\ \mathbf{Y}_k \end{pmatrix}, \tag{82}$$

where $\mathbf{Y}_k$ is assumed to be invertible, which can and will be checked a posteriori, and we define the ratio $\boldsymbol{\omega}_k = \mathbf{X}_k \mathbf{Y}_k^{-1}$ in $\mathbb{R}^{n\times n}$. The $\mathbf{W}_k$ are related by the defining recurrence

$$\mathbf{W}_{k+1} \triangleq \mathbf{Z}_k \mathbf{W}_k. \tag{83}$$

We explicitly have

$$\begin{pmatrix} \mathbf{X}_{k+1} \\ \mathbf{Y}_{k+1} \end{pmatrix} \triangleq \mathbf{Z}_k \mathbf{W}_k = \begin{pmatrix} \mathbf{A}_k & \mathbf{B}_k \\ \mathbf{C}_k & \mathbf{D}_k \end{pmatrix} \begin{pmatrix} \mathbf{X}_k \\ \mathbf{Y}_k \end{pmatrix} = \begin{pmatrix} \mathbf{A}_k \mathbf{X}_k + \mathbf{B}_k \mathbf{Y}_k \\ \mathbf{C}_k \mathbf{X}_k + \mathbf{D}_k \mathbf{Y}_k \end{pmatrix}, \tag{84}$$

from which it is possible to infer the following recurrence on $\boldsymbol{\omega}_k$:

$$\begin{aligned} \boldsymbol{\omega}_{k+1} &= \mathbf{X}_{k+1} \mathbf{Y}_{k+1}^{-1} = (\mathbf{A}_k \mathbf{X}_k + \mathbf{B}_k \mathbf{Y}_k)(\mathbf{C}_k \mathbf{X}_k + \mathbf{D}_k \mathbf{Y}_k)^{-1} \\ &= (\mathbf{A}_k \mathbf{X}_k \mathbf{Y}_k^{-1} + \mathbf{B}_k)(\mathbf{C}_k \mathbf{X}_k \mathbf{Y}_k^{-1} + \mathbf{D}_k)^{-1} \\ &= (\mathbf{A}_k \boldsymbol{\omega}_k + \mathbf{B}_k)(\mathbf{C}_k \boldsymbol{\omega}_k + \mathbf{D}_k)^{-1}. \end{aligned} \tag{85}$$

Hence, we can represent the nonlinear update of $\boldsymbol{\omega}_k$ by the linear recurrence equation (83).

Now, we choose

$$\mathbf{X}_0 = \mathbf{P}_0 \quad \text{and} \quad \mathbf{Y}_0 = \mathbf{I}_n \tag{86}$$

in order to have $\boldsymbol{\omega}_k = \mathbf{P}_k$ for all $k \geq 0$, which implies that the nonlinear recurrence on $\mathbf{P}_k$ can be represented by the linear recurrence equation (83).

Insofar, no assumption on the rank of $\mathbf{P}_k$ was required and, even in the presence of model noise, the linear representation implies that $\mathbf{P}_k$ has the following dependence on $\mathbf{P}_0$:

$$\mathbf{P}_k = (\mathbf{A}^{(k)} \mathbf{P}_0 + \mathbf{B}^{(k)})(\mathbf{C}^{(k)} \mathbf{P}_0 + \mathbf{D}^{(k)})^{-1}, \tag{87}$$

where the $\mathbf{A}^{(k)}$, $\mathbf{B}^{(k)}$, $\mathbf{C}^{(k)}$, $\mathbf{D}^{(k)}$ only depend on $\boldsymbol{\Omega}_l$, $\mathbf{Q}_l$, and $\mathbf{M}_l$, $1 \leq l \leq k$. Our purpose now is to compute $\mathbf{P}_k$ for any t_k *in the perfect model* case using the linear representation equation (81). This is the focus of the rest of this appendix.

A.2. Solution in the autonomous case. We consider first the autonomous case, where $\mathbf{M}_k$, $\mathbf{\Omega}_k$, and $\mathbf{Z}_k$ are all independent of time, and we can suppress the time index from the notation. Hence, we would compute the power iterates $\mathbf{Z}^k$ of $\mathbf{Z}$ (not to be confused with the $\mathbf{Z}_k$ defined in (81). Let us assume that $\mathbf{Z}^k$ has the form

$$\mathbf{Z}^k \triangleq \begin{pmatrix} \mathbf{M}^k & \mathbf{0} \\ \left(\mathbf{M}^k\right)^{-\mathrm{T}} \mathbf{\Theta}'_k & \left(\mathbf{M}^k\right)^{-\mathrm{T}} \end{pmatrix}. \tag{88}$$

Note that we want $\mathbf{Z}^0 = \left(\begin{smallmatrix} \mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_n \end{smallmatrix}\right)$, so that $\mathbf{\Theta}'_0 = \mathbf{0}$. Then the recurrence on $\mathbf{Z}^k$ imposes the recurrence on the $\mathbf{\Theta}'_k$:

$$\mathbf{\Theta}'_{k+1} = \mathbf{M}^{\mathrm{T}} \mathbf{\Theta}'_k \mathbf{M} + \mathbf{\Omega}, \tag{89}$$

which identifies $\mathbf{\Theta}'_k$ with $\mathbf{\Theta}_k$ as defined by (21). Because $\mathbf{\Theta}_0$ and $\mathbf{\Omega}$ are symmetric, all $\mathbf{\Theta}_k$ for $k \geq 1$ are also symmetric. We can see it as an arithmetico-geometric recurrence and to solve it define by $\mathbf{\Psi}$ the solution of

$$\mathbf{\Psi} = \mathbf{M}^{\mathrm{T}} \mathbf{\Psi} \mathbf{M} + \mathbf{\Omega}. \tag{90}$$

This is the so-called discrete algebraic Lyapunov equation. Because a solution of this equation does not always exist [11], we consider instead the recurrence

$$e^{i\varepsilon} \mathbf{\Theta}^{\varepsilon}_{k+1} = \mathbf{M}^{\mathrm{T}} \mathbf{\Theta}^{\varepsilon}_k \mathbf{M} + \mathbf{\Omega}, \tag{91}$$

where $0 < \varepsilon < 2\pi$. By continuity, $\mathbf{\Theta}_k = \lim_{\varepsilon \to 0^+} \mathbf{\Theta}^{\varepsilon}_k$. The corresponding Lyapunov equation is

$$e^{i\varepsilon} \mathbf{\Psi}_{\varepsilon} = \mathbf{M}^{\mathrm{T}} \mathbf{\Psi}_{\varepsilon} \mathbf{M} + \mathbf{\Omega}. \tag{92}$$

It is formally equivalent to

$$\left(e^{i\varepsilon} \mathbf{I}_n - \mathbf{M}^{\mathrm{T}} \otimes \mathbf{M}^{\mathrm{T}}\right) \mathrm{vec}\left(\mathbf{\Psi}\right) = \mathrm{vec}\left(\mathbf{\Omega}\right), \tag{93}$$

where vec($\mathbf{\Psi}$) is the vector made from the stacked columns of $\mathbf{\Psi}$. Since

$$\det\left(e^{i\varepsilon} \mathbf{I}_n - \mathbf{M}^{\mathrm{T}} \otimes \mathbf{M}^{\mathrm{T}}\right) \neq 0 \tag{94}$$

for any real $\mathbf{M}$ and $0 < \varepsilon < 2\pi$, there exists a unique solution $\mathbf{\Psi}_{\varepsilon}$ of (93) in $\mathbb{C}$. Then, we obtain

$$\mathbf{\Theta}^{\varepsilon}_k = \mathbf{\Psi}_{\varepsilon} - (\mathbf{M}^k)^{\mathrm{T}} \mathbf{\Psi}_{\varepsilon} \mathbf{M}^k, \tag{95}$$

by subtracting (92) from (91) and then iterating. As a consequence, the following construction of a solution is always valid:

$$\mathbf{\Theta}_k = \lim_{\varepsilon \to 0^+} \left\{ \mathbf{\Psi}_{\varepsilon} - e^{-ik\varepsilon} \left(\mathbf{M}^k\right)^{\mathrm{T}} \mathbf{\Psi}_{\varepsilon} \mathbf{M}^k \right\}. \tag{96}$$

Hence,

$$\mathbf{Z}^k = \begin{pmatrix} \mathbf{M}^k & \mathbf{0} \\ \left(\mathbf{M}^k\right)^{-\mathrm{T}} \mathbf{\Theta}_k & \left(\mathbf{M}^k\right)^{-\mathrm{T}} \end{pmatrix}. \tag{97}$$

Using the linear representation leads to

$$\begin{aligned} \begin{pmatrix} \mathbf{X}_k \\ \mathbf{Y}_k \end{pmatrix} &= \begin{pmatrix} \mathbf{M}^k & \mathbf{0} \\ \left(\mathbf{M}^k\right)^{-\mathrm{T}} \mathbf{\Theta}_k & \left(\mathbf{M}^k\right)^{-\mathrm{T}} \end{pmatrix} \begin{pmatrix} \mathbf{P}_0 \\ \mathbf{I}_n \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{M}^k \mathbf{P}_0 \\ \left(\mathbf{M}^k\right)^{-\mathrm{T}} \mathbf{\Theta}_k \mathbf{P}_0 + \left(\mathbf{M}^k\right)^{-\mathrm{T}} \end{pmatrix}. \end{aligned} \tag{98}$$

Using $\mathbf{P}_k = \mathbf{X}_k \mathbf{Y}_k^{-1}$, we conclude

$$\mathbf{P}_k = \mathbf{M}^k \mathbf{P}_0 \left[\mathbf{\Theta}_k \mathbf{P}_0 + \mathbf{I}_n\right]^{-1} \left(\mathbf{M}^k\right)^{\mathrm{T}}. \tag{99}$$

A.3. Solution in the nonautonomous case. In the nonautonomous case, we need to define

$$\mathbf{Z}^{(k)} \triangleq \mathbf{Z}_k \mathbf{Z}_{k-1} \cdots \mathbf{Z}_0. \tag{100}$$

The product is still in the symplectic group and of the form

$$\mathbf{Z}^{(k)} \triangleq \begin{pmatrix} \mathbf{M}_{k:0} & \mathbf{0} \\ \mathbf{\Gamma}'_k \mathbf{M}_{k:0} & \mathbf{M}_{k:0}^{-\mathrm{T}} \end{pmatrix}, \tag{101}$$

which leads to the following recurrence on $\mathbf{\Gamma}'_k$:

$$\mathbf{\Gamma}'_{k+1} = \mathbf{M}_{k+1}^{-\mathrm{T}} \left(\mathbf{\Gamma}'_k + \mathbf{\Omega}_k\right) \mathbf{M}_{k+1}^{-1}. \tag{102}$$

The finite-time solution to this recurrence is

$$\mathbf{\Gamma}'_k = \sum_{l=0}^{k-1} \mathbf{M}_{k:l}^{-\mathrm{T}} \mathbf{\Omega}_l \mathbf{M}_{k:l}^{-1} \tag{103}$$

which coincides with the definition of $\mathbf{\Gamma}_k$ in (14). Hence, we have an expression for $\mathbf{Z}^{(k)}$. We can use it to obtain a solution for the recurrence on $\mathbf{P}_k$ using the linear representation

$$\mathbf{Z}^{(k)} \begin{pmatrix} \mathbf{P}_0 \\ \mathbf{I}_n \end{pmatrix} = \begin{pmatrix} \mathbf{M}_{k:0} \mathbf{P}_0 \\ \mathbf{\Gamma}_k \mathbf{M}_{k:0} \mathbf{P}_0 + \mathbf{M}_{k:0}^{-\mathrm{T}} \end{pmatrix} \tag{104}$$

from which we obtain

$$\begin{aligned} \mathbf{P}_k &= \mathbf{M}_{k:0} \mathbf{P}_0 \left[\mathbf{\Gamma}_k \mathbf{M}_{k:0} \mathbf{P}_0 + \mathbf{M}_{k:0}^{-\mathrm{T}}\right]^{-1} \\ &= \mathbf{M}_{k:0} \mathbf{P}_0 \mathbf{M}_{k:0}^{\mathrm{T}} \left[\mathbf{I}_n + \mathbf{\Gamma}_k \mathbf{M}_{k:0} \mathbf{P}_0 \mathbf{M}_{k:0}^{\mathrm{T}}\right]^{-1} \\ &= \mathbf{M}_{k:0} \mathbf{P}_0 \left[\mathbf{I}_n + \mathbf{M}_{k:0}^{\mathrm{T}} \mathbf{\Gamma}_k \mathbf{M}_{k:0} \mathbf{P}_0\right]^{-1} \mathbf{M}_{k:0}^{\mathrm{T}} \end{aligned} \tag{105}$$

which coincides with (18) and (19).

Appendix B. A few useful properties of the symmetric positive (semi)definite matrices. Here we provide a selection of definitions and results about the symmetric positive (semi)definite matrices that we use in this paper. An introduction and detailed proofs of several of these results can be found in [35, chapter 6].

1. The partial ordering on $\mathcal{C}^n$ is defined by, for any $\mathbf{A}$ and $\mathbf{B}$ in $\mathcal{C}^n$, $\mathbf{A} \le \mathbf{B}$ if and only if for all $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} \le \mathbf{x}^{\mathrm{T}}\mathbf{B}\mathbf{x}$.
2. If $\mathbf{A}$ and $\mathbf{B}$ are in $\mathcal{C}^n$ and $\mathbf{G}$ is in $\mathbb{R}^{q\times n}$, $q \in \mathbb{N}$, we have that $\mathbf{A} \le \mathbf{B}$ implies $\mathbf{G}\mathbf{A}\mathbf{G}^{\mathrm{T}} \le \mathbf{G}\mathbf{B}\mathbf{G}^{\mathrm{T}}$ which is immediate from the previous definition of the partial ordering.
3. If $\mathbf{A}$ and $\mathbf{B}$ are in $\mathcal{C}^n_+$, $\mathbf{A} \le \mathbf{B}$ is equivalent to $\mathbf{A}^{-1} \ge \mathbf{B}^{-1}$. This can be shown using the double diagonalization theorem which states that there exists an invertible matrix $\mathbf{G}$ such that $\mathbf{G}\mathbf{A}\mathbf{G}^{\mathrm{T}}$ and $\mathbf{G}\mathbf{B}\mathbf{G}^{\mathrm{T}}$ are both diagonal.
4. If $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are in $\mathcal{C}^n$, by $\mathbf{A} \le \min\{\mathbf{B}, \mathbf{C}\}$ we mean that for all $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} \le \min\{\mathbf{x}^{\mathrm{T}}\mathbf{B}\mathbf{x}, \mathbf{x}^{\mathrm{T}}\mathbf{C}\mathbf{x}\}$.
5. If $\mathbf{A}$ is in $\mathcal{C}^n$, it has the eigendecomposition $\mathbf{A} = \sum_{i=1}^n \sigma_i \mathbf{v}_i \mathbf{v}_i^{\mathrm{T}}$, with $\sigma_i \ge 0$ and $\{\mathbf{v}_i\}_{1\le i\le n}$ an orthonormal basis. Let $\sigma_{\max} = \max_{1\le i\le n} \sigma_i$ and $\sigma_{\min} = \min_{1\le i\le n} \sigma_i$. Any $\mathbf{x}$ in $\mathbb{R}^n$ can decompose on the eigenvectors of $\mathbf{A}$: $\mathbf{x} = \sum_{i=1}^n (\mathbf{v}_i^{\mathrm{T}}\mathbf{x})\mathbf{v}_i$. As a consequence, one has

$$\begin{aligned} \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} = \sum_{i=1}^n \sigma_i \left(\mathbf{v}_i^{\mathrm{T}}\mathbf{x}\right)^2 &\le \sigma_{\max} \sum_{i=1}^n \left(\mathbf{v}_i^{\mathrm{T}}\mathbf{x}\right)^2 = \sigma_{\max}\mathbf{x}^{\mathrm{T}}\mathbf{x} \\ &\ge \sigma_{\min} \sum_{i=1}^n \left(\mathbf{v}_i^{\mathrm{T}}\mathbf{x}\right)^2 = \sigma_{\min}\mathbf{x}^{\mathrm{T}}\mathbf{x} \end{aligned} \tag{106}$$

which leads to $\sigma_{\min}\mathbf{I}_n \le \mathbf{A} \le \sigma_{\max}\mathbf{I}_n$. Further, as

$$\|\mathbf{A}\mathbf{x}\|^2 = \sum_{i=1}^n \sigma_i^2 \left(\mathbf{v}_i^{\mathrm{T}}\mathbf{x}\right)^2, \tag{107}$$

it follows that $\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} = 0 \iff \mathbf{A}\mathbf{x} = \mathbf{0}$.

Now, assume $\{\mathbf{A}_k\}_{k\in\mathbb{N}}$ is a uniformly bounded sequence in $\mathcal{C}^n$ and $\{\mathbf{x}_k\}_{k\in\mathbb{N}}$ is a uniformly bounded sequence in $\mathbb{R}^n$. Then $\lim_{k\to\infty} \mathbf{A}_k\mathbf{x}_k = \mathbf{0}$ implies that $\lim_{k\to\infty} \mathbf{x}_k^{\mathrm{T}}\mathbf{A}_k\mathbf{x}_k = 0$ by virtue of the boundedness of $\mathbf{x}_k$. Owing to the uniform boundedness of $\mathbf{A}_k$, we introduce $\sigma = \sup_{k\in\mathbb{N},1\le i\le n} \sigma_{k,i} < \infty$ and obtain

$$\begin{aligned} \|\mathbf{A}_k\mathbf{x}_k\|^2 &= \sum_{i=1}^n \sigma_{k,i}^2 \left(\mathbf{v}_{k,i}^{\mathrm{T}}\mathbf{x}_k\right)^2 \\ &\le \sigma \sum_{i=1}^n \sigma_{k,i} \left(\mathbf{v}_{k,i}^{\mathrm{T}}\mathbf{x}_k\right)^2 \le \sigma \mathbf{x}_k^{\mathrm{T}}\mathbf{A}_k\mathbf{x}_k. \end{aligned} \tag{108}$$

Hence, $\lim_{k\to\infty} \mathbf{x}_k^{\mathrm{T}}\mathbf{A}_k\mathbf{x}_k = 0$ implies that $\lim_{k\to\infty} \mathbf{A}_k\mathbf{x}_k = \mathbf{0}$. It follows that $\lim_{k\to\infty} \mathbf{x}_k^{\mathrm{T}}\mathbf{A}_k\mathbf{x}_k = 0 \iff \lim_{k\to\infty} \mathbf{A}_k\mathbf{x}_k = \mathbf{0}$. In particular, if the diagonal entry $[\mathbf{A}_k]_{ii}$ asymptotically vanishes, the associated row $[\mathbf{A}_k]_{i\cdot}$ and column $[\mathbf{A}_k]_{\cdot i}$ asymptotically vanish. Accordingly, if a given diagonal block of the $\mathbf{A}_k$ asymptotically vanishes, the off-diagonal blocks with the same row and column indices as the diagonal block asymptotically vanish.

6. Let $\mathbf{A} \in \mathcal{C}^n$ and $\alpha \geq 0$ be a constant. If there is a subspace $\mathcal{W} \subseteq \mathbb{R}^n$ of dimension $s \geq 1$ such that for all unit vectors $\mathbf{h} \in \mathcal{W}$, $\mathbf{h}^{\mathrm{T}}\mathbf{A}\mathbf{h} \leq \alpha$, then $\mathbf{A}$ has at least s of its eigenvalues less than or equal to α.
   To see this, decompose $\mathbf{A} = \sum_{i=1}^{n} \sigma_i \mathbf{v}_i \mathbf{v}_i^{\mathrm{T}}$ in its orthonormal eigenbasis, where $\sigma_i \geq 0$ and ordered as $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$. Consider $\mathcal{V}$ the $(s-1)$-dimensional subspace span of $\{\mathbf{v}_{n-s+2}, \ldots, \mathbf{v}_n\}$, which we take to be the null space if $s = 1$. The orthogonal subspace $\mathcal{V}^{\perp}$ of $\mathcal{V}$ is of dimension $n - s + 1$. The intersection $\mathcal{W} \cap \mathcal{V}^{\perp}$ is of dimension at least 1. Let us pick $\mathbf{h}$ of Euclidean norm 1 in this intersection. We have

$$\alpha \geq \mathbf{h}^{\mathrm{T}}\mathbf{A}\mathbf{h} = \sum_{i=1}^{n} \sigma_i (\mathbf{h}^{\mathrm{T}}\mathbf{v}_i)^2 = \sum_{i=1}^{n-s+1} \sigma_i (\mathbf{h}^{\mathrm{T}}\mathbf{v}_i)^2$$

$$\geq \sigma_{n-s+1} \sum_{i=1}^{n-s+1} (\mathbf{h}^{\mathrm{T}}\mathbf{v}_i)^2 = \sigma_{n-s+1}. \quad (109)$$

   Hence $\alpha \geq \sigma_{n-s+1} \geq \cdots \geq \sigma_n$.

Appendix C. Matrix shift lemma. Let $\mathbf{A} \in \mathbb{R}^{n\times m}$ and $\mathbf{B} \in \mathbb{R}^{m\times n}$. Assuming $x \mapsto f(x)$ can be written as a formal power series, i.e., $f(x) = \sum_{i=0}^{\infty} a_i x^i$, one has $\mathbf{A}f(\mathbf{B}\mathbf{A}) = \sum_{i=0}^{\infty} a_i \mathbf{A}(\mathbf{B}\mathbf{A})^i = \sum_{i=0}^{\infty} a_i (\mathbf{A}\mathbf{B})^i \mathbf{A} = f(\mathbf{A}\mathbf{B})\mathbf{A}$. This proves the matrix shift lemma, i.e., $\mathbf{A}f(\mathbf{B}\mathbf{A}) = f(\mathbf{A}\mathbf{B})\mathbf{A}$. In the special case that $f(x) = (1+x)^{-1}$, this property in fact holds for any matrix without consideration of the radius of convergence of the power series. Assuming $(\mathbf{I}_m + \mathbf{B}\mathbf{A})^{-1}$ and $(\mathbf{I}_n + \mathbf{A}\mathbf{B})^{-1}$ exist then

$$\mathbf{A}(\mathbf{I}_m + \mathbf{B}\mathbf{A})^{-1} = (\mathbf{I}_n + \mathbf{A}\mathbf{B})^{-1}(\mathbf{A} + \mathbf{A}\mathbf{B}\mathbf{A})(\mathbf{I}_m + \mathbf{B}\mathbf{A})^{-1} = (\mathbf{I}_n + \mathbf{A}\mathbf{B})^{-1}\mathbf{A}. \quad (110)$$

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