Theory and Computation of Covariant Lyapunov Vectors

Pavel V. Kuptsov · Ulrich Parlitz

Abstract Lyapunov exponents are well-known characteristic numbers that describe growth rates of perturbations applied to a trajectory of a dynamical system in different state space directions. Covariant (or characteristic) Lyapunov vectors indicate these directions. Though the concept of these vectors has been known for a long time, they became practically computable only recently due to algorithms suggested by Ginelli et al. [Phys. Rev. Lett. 99, 2007, 130601] and by Wolfe and Samelson [Tellus 59A, 2007, 355]. In view of the great interest in covariant Lyapunov vectors and their wide range of potential applications, in this article we summarize the available information related to Lyapunov vectors and provide a detailed explanation of both the theoretical basics and numerical algorithms. We introduce the notion of adjoint covariant Lyapunov vectors. The angles between these vectors and the original covariant vectors are norm-independent and can be considered as characteristic numbers. Moreover, we present and study in detail an improved approach for computing covariant Lyapunov

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vectors. Also we describe how one can test for hyperbolicity of chaotic dynamics without explicitly computing covariant vectors.

Keywords Covariant Lyapunov vectors · Characteristic Lyapunov vectors · Forward and backward Lyapunov vectors · Lyapunov exponents · Lyapunov analysis · Tangent space · High-dimensional chaos

1 Introduction

High-dimensional nonlinear systems like coupled oscillators, dynamical networks, or extended excitable media often exhibit very complex dynamics that is difficult to analyze and to characterize. From a practical point of view there only a few concepts have been developed for studying low-dimensional systems that can efficiently be applied to high-dimensional attractors, too. An important example are Lyapunov exponents that describe growth rates of perturbations applied to a trajectory in different state space directions. These exponents are a central point in the investigation of chaotic dynamical systems. They are related to a number of different physical properties such as sensitivity to initial conditions or local entropy production and can be used to estimate the (Kaplan–Yorke) dimension of (even very high-dimensional) attractors (Eckmann and Ruelle 1985).

Mathematically, Lyapunov exponents are defined in tangent space. This space is spanned by all possible infinitesimal perturbations that can be applied to a state of the system. The dimension of the tangent space is equal to the dimension of the original phase space. In general, the tangent space is an inner product space, but often the tangent space is defined as an Euclidean space where the inner product is just the ordinary scalar (dot) product. The dynamics in this space is generated by linear operators that determine the evolution of perturbation vectors from one point on the trajectory to another. These operators are called tangent linear propagators or resolvents. The tangent space is a very important subject of study. On the one hand, the tangent space dynamics is closely related to the dynamics of the original system. One can obtain key characteristics of the original system observing the associated tangent space dynamics. On the other hand, the tangent space is linear and the dynamics in this space is determined by the action of linear operators. This means that analysis methods as well as results are universal for a wide class of systems.

Besides the growth rates of perturbations the directions of this growth are also important. There are various concepts identifying these directions, including bred vectors (Toth and Kalnay 1993, 1997), which are finite-amplitude perturbations initialized and periodically rescaled within the original phase space, singular or optimal vectors (Buizza et al. 1993; Buizza and Palmer 1995), which are the singular vectors of a finite-time propagator, or finite-time normal modes (Frederiksen 1997), defined as eigenvectors of the propagator.

Orthogonal sets of singular vectors related to the propagators operating on infinite time intervals were referred to by Legras and Vautard as forward and backward Lyapunov vectors (Legras and Vautard 1996). These vectors can be computed in parallel with the Lyapunov exponents (Legras and Vautard 1996; Ershov and Potapov 1998),

and, thus, are closely related to them. Unlike the exponents, the forward and backward Lyapunov vectors depend on time, i.e., they are different for different trajectory points. Analyzing the orientation of these vectors, one can expect to recover the local structure of an attractor. But unfortunately, the forward and backward Lyapunov vectors provide only limited information. They always remain orthogonal and thus cannot indicate directions of stable and unstable manifolds as well as their tangencies. These vectors are not invariant under time reversal and are not covariant with the dynamics. The latter means that forward (or backward) vectors at a given point are not mapped by tangent propagators to the forward (backward) vectors at the image point. Another drawback of these vectors is their norm-dependence, i.e., they depend on the definition of the inner products and norms in the tangent space (Legras and Vautard 1996).

The concept of norm-independent Lyapunov vectors has been known for a long time (Eckmann and Ruelle 1985; Vastano and Moser 1991; Legras and Vautard 1996; Trevisan and Pancotti 1998). However, only recently two efficient algorithms for computing these vectors were suggested almost simultaneously by Wolfe and Samelson (2007) and by Ginelli et al. (2007). After Ginelli et al. we call these vectors covariant Lyapunov vectors. Note that these vectors are also referred to as characteristic Lyapunov vectors (Legras and Vautard 1996; Wolfe and Samelson 2007). These vectors are not orthogonal; they are invariant under time reversal and covariant with the dynamics in the sense that they may, in principle, be computed once and then determined for all times using the tangent propagator. (Note that this is the case only for exact covariant vectors, while those computed numerically do not demonstrate perfect covariance due to the accumulation of numerical errors.) The covariant Lyapunov vectors can be considered as a generalization of the notion of "normal modes." They are reduced to Floquet vectors if the flow is time periodic and to stationary normal modes if the flow is stationary (Wolfe and Samelson 2007).

In view of potential wide applications to the analysis of complex, high-dimensional dynamics, the covariant Lyapunov vectors receive a lot of interest of researchers (Szendro et al. 2007; Kuptsov and Kuznetsov 2009; Pazó et al. 2008; Yang et al. 2009; Kuptsov and Parlitz 2010; Yang and Radons 2010; Pazó and López 2010). For these extensive studies to be productive, it is important to analyze the Lyapunov vectors systematically. In this paper we summarize features of forward, backward, and covariant Lyapunov vectors and provide a detailed explanation of both the theoretical basics and numerical algorithms. We present and study in detail an efficient method for computing covariant Lyapunov vectors, which can be considered as a modification of the method by Wolfe and Samelson. Moreover, our general approach reveals the existence of adjoint covariant Lyapunov vectors. This is *not an independent type of characteristic vectors*, because given the covariant vectors, one can always compute the adjoint ones. However, the angles between corresponding covariant and adjoint covariant vectors provide a compact representation of the information contained in the covariant vectors and can be used as characteristic numbers. In particular, the presence of homoclinic tangencies is indicated by orthogonality of corresponding original and adjoint covariant vectors. Since the covariant as well as the adjoint covariant vectors are norm-independent, their angles also are invariant with respect to the norm.

The structure of the article is as follows. In Sect. 2 we present the theory of Lyapunov exponents and forward and backward Lyapunov vectors, and in Sect. 3 we describe numerical methods for computing them. Section 4 presents the theoretical aspects of covariant Lyapunov vectors, and in Sect. 5 we describe different methods of computing covariant vectors. Finally, in Sect. 6 a simple illustrative example is presented. In Sect. 7 we summarize the results presented.

2 Lyapunov Exponents, Forward and Backward Lyapunov Vectors

2.1 Basic Definitions

Consider a system whose dynamics can be described by an ordinary differential equation,

$$\dot{\boldsymbol{u}} = \boldsymbol{g}(\boldsymbol{u}, t), \tag{1}$$

where $\boldsymbol{u} \equiv \boldsymbol{u}(t) \in \mathbb{R}^m$ is an m-dimensional state vector that changes in time t, and $\boldsymbol{g}(\boldsymbol{u}, t) \in \mathbb{R}^m$ is a nonlinear vector function. We are primarily interested in high-dimensional systems, so m is assumed to be large. Equation (1) can model a system with many interacting point-wise dynamical elements, or it can be a finite step size approximation of a spatially extended system that appears after discretization of spatial derivatives. Infinitesimal perturbations to a trajectory of this system are described by the following equation:

$$\dot{\boldsymbol{v}} = \mathbf{J}(\boldsymbol{u}, t)\boldsymbol{v}, \tag{2}$$

where $\mathbf{J}(\boldsymbol{u}, t) \in \mathbb{R}^{m \times m}$ is the Jacobian matrix composed of derivatives of the vector function $\boldsymbol{g}(\boldsymbol{u}, t)$ with respect to components of the vector $\boldsymbol{u}$. The fundamental matrix $\mathbf{M} \in \mathbb{R}^{m \times m}$ for Eq. (2) can be found as a solution of the matrix equation

$$\dot{\mathbf{M}} = \mathbf{J}(\boldsymbol{u}, t)\mathbf{M}, \tag{3}$$

where any non-singular matrix can be used as an initial condition.

The tangent linear propagator or resolvent is defined as

$$\mathcal{F}(t_1, t_2) = \mathbf{M}(t_2)\mathbf{M}(t_1)^{-1}, \tag{4}$$

and can be represented by a non-singular $m \times m$ matrix. The propagator evolves solutions of Eq. (2) from time t_1 to time t_2:

$$\boldsymbol{v}(t_2) = \mathcal{F}(t_1, t_2)\boldsymbol{v}(t_1), \tag{5}$$

where $\boldsymbol{v}(t_1)$ and $\boldsymbol{v}(t_2)$ are tangent vectors at times t_1 and t_2, respectively, computed along the same trajectory of the base system (1). According to Eq. (4), the propagator is always non-singular and $\mathcal{F}(t_1, t_2) = \mathcal{F}(t_2, t_1)^{-1}$. Furthermore we define the adjoint tangent propagator:

$$\mathcal{G}(t_1, t_2) = \mathcal{F}(t_1, t_2)^{-\mathrm{T}}, \tag{6}$$

where "−T" denotes matrix inversion and transposition. In general, a non-Euclidean norm can be defined in the tangent space, so that instead of the transposition a generalized adjoint with respect to the chosen norm has to be used. In this paper we do not consider such cases.

As follows from Eq. (5), the growth of the Euclidean norm of tangent vectors in forward-time dynamics is determined by the matrix $\mathcal{F}(t_1, t_2)^{\mathrm{T}} \mathcal{F}(t_1, t_2)$. We denote its eigenvectors and eigenvalues as $\boldsymbol{f}_i^+(t_1, t_2)$ and $\sigma_i(t_1, t_2)^2$, respectively, where $\sigma_1(t_1, t_2) \geq \sigma_2(t_1, t_2) \geq \cdots \geq \sigma_m(t_1, t_2) \geq 0$. The eigenvectors are termed optimal vectors because the maximal growth ratio is equal to $\sigma_1(t_1, t_2)$ and is achieved if the initial vector $\boldsymbol{v}(t_1)$ coincides with $\boldsymbol{f}_1^+(t_1, t_2)$. The same role for the backward-time dynamics plays the matrix $\mathcal{F}(t_1, t_2)^{-\mathrm{T}} \mathcal{F}(t_1, t_2)^{-1}$ with the reciprocal eigenvalues and the eigenvectors $\boldsymbol{f}_i^-(t_1, t_2)$.

The eigenvectors and eigenvalues can be found via singular value decompositions (SVD) (Golub and van Loan 1996) of the propagator matrix and its inverse, thus:

$$\mathcal{F}(t_1, t_2) \boldsymbol{f}_i^+(t_1, t_2) = \boldsymbol{f}_i^-(t_1, t_2) \sigma_i(t_1, t_2), \tag{7}$$

$$\mathcal{F}(t_1, t_2)^{-1} \boldsymbol{f}_i^-(t_1, t_2) = \boldsymbol{f}_i^+(t_1, t_2) \sigma_i(t_1, t_2)^{-1}. \tag{8}$$

Here $\sigma_i(t_1, t_2)$ are called singular values, and $\boldsymbol{f}_i^+(t_1, t_2)$ and $\boldsymbol{f}_i^-(t_1, t_2)$ are right and left singular vectors of $\mathcal{F}(t_1, t_2)$, respectively. The singular vectors are orthonormal. They are norm-dependent, i.e., they have different orientations with respect to different norms (Legras and Vautard 1996; Wolfe and Samelson 2007). Taking into account Eqs. (6), (7), and (8), one can write the SVD for the adjoint propagator $\mathcal{G}(t_1, t_2)$ and its inverse as

$$\mathcal{G}(t_1, t_2) \boldsymbol{f}_i^+(t_1, t_2) = \boldsymbol{f}_i^-(t_1, t_2) \sigma_i(t_1, t_2)^{-1}, \tag{9}$$

$$\mathcal{G}(t_1, t_2)^{-1} \boldsymbol{f}_i^-(t_1, t_2) = \boldsymbol{f}_i^+(t_1, t_2) \sigma_i(t_1, t_2). \tag{10}$$

Comparing Eq. (7) with (9) and Eq. (8) with (10) we see that the propagators $\mathcal{F}(t_1, t_2)$ and $\mathcal{G}(t_1, t_2)$ have identical singular vectors and reciprocal singular values.

If all $\sigma_i(t_1, t_2)$ are distinct, the singular vectors are unique up to a simultaneous change of signs of elements of $\boldsymbol{f}_i^+(t_1, t_2)$ and $\boldsymbol{f}_i^-(t_1, t_2)$. In the presence of degeneracy, we still can find a set of orthonormal right singular vectors that are mapped according to Eq. (7) onto a set of orthonormal left singular vectors, but these sets are not unique and can be selected arbitrarily.

Strictly speaking, propagators and singular vectors as well as the Lyapunov vectors considered below can depend on time both explicitly, and implicitly via state vectors $\boldsymbol{u}(t)$. To avoid complicated notation, we shall use a compact form, like $\mathcal{F}(t_1, t_2)$.

2.2 Properties of Propagators. Transformation of Volumes Built on Singular Vectors

Let us discuss how $\mathcal{F}(t_1, t_2)$ transforms volumes of different dimensions: segments, squares, cubes, and so on. Being at a trajectory point at t_1 we construct a k-dimensional unit volume using the first k right singular vectors $\boldsymbol{f}_i^+(t_1, t_2)$. According to Eq. (7) $\mathcal{F}(t_1, t_2)$ transforms these vectors into the left singular vectors $\boldsymbol{f}_i^-(t_1, t_2)$ associated with the trajectory point at t_2 that are stretched/contracted by

factors $\sigma_i(t_1, t_2)$; see Fig. 1(a). The volume at t_2 is equal to the product of the first k singular values. Alternatively, we can consider a k-dimensional ball of unit radius at t_1. At t_2 this ball is transformed into an ellipsoid with axes along the vectors $\boldsymbol{f}_i^-$ and lengths σ_i. One can describe this transformation of volumes by

$$V_k(t_2) = V_k(t_1) \exp\left((t_2 - t_1) \sum_{i=1}^{k} \tilde{\mu}_i(t_1, t_2)\right), \tag{11}$$

where $V_k(t)$ is the k-dimensional volume, and $\tilde{\mu}_i(t_1, t_2) = \ln \sigma_i(t_1, t_2)/(t_2 - t_1)$ are stretch ratios that can be considered as local Lyapunov exponents. (Note that there are alternative definitions of local Lyapunov exponents, which shall be considered below.)

The backward transformation with $\mathcal{F}(t_1, t_2)^{-1}$ is symmetric. At $t = t_2$ we construct a unit volume using the first k left singular vectors $\boldsymbol{f}_i^-(t_1, t_2)$. According to Eq. (8), the right singular vectors span this volume at $t = t_1$, and the edges of this volume are stretched/contracted by factors σ_i^{-1}; see Fig. 1(b). In a similar manner we can consider a unit ball at t_2 that is transformed into an ellipsoid at t_1. Therefore, the volumes are again transformed in accordance with Eq. (11).

This discussion is also valid for the adjoint propagator $\mathcal{G}(t_1, t_2)$. But because the singular values are now reciprocal, the volumes are transformed as

$$V_k(t_2) = V_k(t_1) \exp\left(-(t_2 - t_1) \sum_{i=1}^{k} \tilde{\mu}_i(t_1, t_2)\right). \tag{12}$$

Fig. 1 Transformation of a volume. (**a**) Forward step by the propagator $\mathcal{F}(t_1, t_2)$, (**b**) backward step via $\mathcal{F}(t_1, t_2)^{-1}$
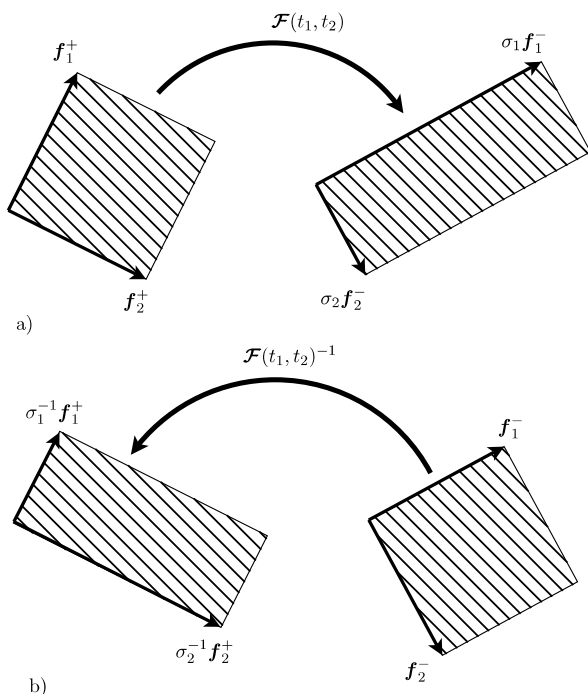
2.3 Far-past and Far-future Operators. Forward and Backward Lyapunov Vectors

For infinitely large time intervals we can expect to obtain limits for the stretch ratios and singular vectors. The Oseledec multiplicative ergodic theorem (Oseledec 1968) and its corollaries state that the limit indeed exists for $t_2 \to \infty$, and also a limit can be reached for $t_1 \to -\infty$. When $t_2 \to \infty$, the *far-future operator* is defined as

$$\mathbf{W}^+(t) = \lim_{t_2 \to \infty} \left[\mathcal{F}(t, t_2)^{\mathrm{T}} \mathcal{F}(t, t_2) \right]^{1/(2(t_2 - t))}$$

$$= \lim_{t_2 \to \infty} \left[\mathbf{F}^+(t, t_2) \mathbf{\Sigma}(t, t_2)^{1/(t_2 - t)} \mathbf{F}^+(t, t_2)^{\mathrm{T}} \right], \tag{13}$$

where $\mathbf{F}^+(t, t_2) = [\boldsymbol{f}_1^+(t, t_2), \ldots, \boldsymbol{f}_m^+(t, t_2)]$ and $\mathbf{\Sigma}(t, t_2) = \mathrm{diag}[\sigma_1(t, t_2), \ldots, \sigma_m(t, t_2)]$ are matrices of singular vectors and values, respectively. The eigenvectors of the far-future operator are the limits of vectors $\boldsymbol{f}_i^+(t, t_2)$. We denote them as $\boldsymbol{\varphi}_i^+(t)$ and refer to them as *forward Lyapunov vectors*. They are orthonormal and depend on t (Legras and Vautard 1996). The convergence of the singular vectors to the Lyapunov vectors is considered in Reynolds and Errico (1999). Logarithms of eigenvalues of $\mathbf{W}^+(t)$, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$, are called Lyapunov exponents. Regardless of time dependence of $\mathbf{W}^+(t)$, they do not depend on time.

The *far-past operator* is defined as

$$\mathbf{W}^-(t) = \lim_{t_1 \to -\infty} \left[\mathcal{F}(t_1, t)^{-\mathrm{T}} \mathcal{F}(t_1, t)^{-1} \right]^{1/(2(t - t_1))}$$

$$= \lim_{t_1 \to -\infty} \left[\mathbf{F}^-(t_1, t) \mathbf{\Sigma}(t_1, t)^{-1/(t - t_1)} \mathbf{F}^-(t_1, t)^{\mathrm{T}} \right], \tag{14}$$

where $\mathbf{F}^-(t_1, t) = [\boldsymbol{f}_1^-(t_1, t), \ldots, \boldsymbol{f}_m^-(t_1, t)]$. The eigenvectors of this matrix are the limits of the left singular vectors $\boldsymbol{f}_i^-(t_1, t)$ for $t_1 \to -\infty$. They are called *backward Lyapunov vectors*. These vectors are also referred to as Gram–Schmidt vectors, because they can be computed in the course of a procedure, which includes Gram–Schmidt orthogonalizations; see Sect. 3. We denote them by $\boldsymbol{\varphi}_i^-(t)$. Similar to the forward vectors, the backward Lyapunov vectors are orthonormal, and depend on t (Legras and Vautard 1996). As well as singular vectors, forward and backward Lyapunov vectors are norm-dependent (Legras and Vautard 1996; Wolfe and Samelson 2007). The logarithms of the eigenvalues of $\mathbf{W}^-(t)$ are equal to the Lyapunov exponents with opposite signs.

In analogy with the finite-time case, the k-dimensional volumes can be built on the forward Lyapunov vectors $\boldsymbol{\varphi}_i^+(t)$. Modifying Eq. (11), we find that average growth rates of these volumes are the sums of Lyapunov exponents,

$$\sum_{i=1}^{k} \lambda_i = \lim_{t_2 \to \infty} \left(\frac{1}{t_2 - t_1} \ln \frac{V_k(t_2)}{V_k(t_1)} \right). \tag{15}$$

As we shall see below, this formula is valid for almost any k-dimensional volume in the tangent space, not necessarily related to the forward Lyapunov vectors.

The Lyapunov exponents may not be all distinct. To take possible degeneracy into account we introduce an additional notation. Let s be a number of *distinct* Lyapunov exponents ($1 \leq s \leq m$), and let $\lambda^{(i)}$ ($i = 1, 2, \ldots, s$) denote the ith distinct Lyapunov exponent with the multiplicity $\nu^{(i)}$. So, we have $\lambda^{(1)} > \lambda^{(2)} > \cdots > \lambda^{(s)}$, and $\sum_{i=1}^{s} \nu^{(i)} = m$. In what follows, to address the whole spectrum of Lyapunov exponents as well as related vectors, we shall employ lower indices while paying special attention to the multiplicity, we shall use upper indices. The notation $\boldsymbol{\varphi}_{\lambda^{(i)}}^{\pm}$ will stand for a set of vectors, related to the ith distinct Lyapunov exponent, and $\boldsymbol{\varphi}_{\lambda^{(i)}, j}^{\pm}$, where $j = 1, 2, \ldots, \nu^{(i)}$, will denote the jth vector related to $\lambda^{(i)}$.

In presence of the degeneracy forward and backward Lyapunov vectors are not unique. But as we already mentioned for singular vectors, this is not an obstacle, because it is always sufficient to choose any orthonormal set of these vectors.

The adjoint propagator $\mathcal{G}$ can also be used to define far-past and far-future operators and forward and backward vectors, respectively. The Lyapunov exponents are the logarithms of the eigenvalues of the far-past operator, while the far-future operator is associated with the Lyapunov exponents with inverted signs.

2.4 Oseledec Subspaces. Asymptotic Behavior of Arbitrary Vectors and Volumes

Let us now discuss what happens with arbitrary vectors. The framework that helps to understand it is provided by the following set of subspaces:

$$
S_j^+(t) = \text{span}\{\boldsymbol{\varphi}_{\lambda^{(i)}}^+(t) | i = j, j+1, \ldots, s\}, \qquad S_{s+1}^+(t) = \emptyset,
$$
$$
S_s^+(t) \subset S_{s-1}^+(t) \subset \cdots \subset S_1^+(t) = \mathbb{R}^m. \tag{16}
$$

In other words, $S_j^+(t)$ is spanned by forward Lyapunov vectors $\boldsymbol{\varphi}_{\lambda^{(i)}}^+(t)$ ($i \geq j$) related to the distinct Lyapunov exponents starting from the jth one. Dimensions of these subspaces are $\dim S_j^+(t) = \sum_{i=j}^{s} \nu^{(i)}$, where $\nu^{(i)}$ is the multiplicity of $\lambda^{(i)}$. Analogous subspaces spanned by the backward Lyapunov vectors $\boldsymbol{\varphi}_{\lambda^{(i)}}^-(t)$ are defined by

$$
S_j^-(t) = \text{span}\{\boldsymbol{\varphi}_{\lambda^{(i)}}^-(t) | i = 1, 2, \ldots, j\}, \qquad S_0^-(t) = \emptyset,
$$
$$
S_1^-(t) \subset S_2^-(t) \subset \cdots \subset S_s^-(t) = \mathbb{R}^m, \tag{17}
$$

and their dimensions are $\dim S_j^-(t) = \sum_{i=1}^{j} \nu^{(i)}$. These sets of subspaces are referred to as Oseledec splitting (Oseledec 1968; Benettin et al. 1980; Legras and Vautard 1996).

Recall that the propagator $\mathcal{F}(t_1, t_2)$ maps each right singular vector onto the corresponding left singular vector and stretching rates are determined by singular values; see Eq. (7). When $(t_2 - t_1) \to \infty$, the right and left singular vectors converge to forward and backward Lyapunov vectors, respectively, and the stretching rates converge to the Lyapunov exponents. Hence, the Oseledec subspace $S_j^+(t)$ consists of vectors

that asymptotically grow or decay with rate $\lambda \leq \lambda^{(j)}$. In turn, the vectors from Oseledec subspace $S_j^-(t)$ grow or decay with exponential rates $\lambda \geq \lambda^{(j)}$ *backward in time*.

Consider a vector $\boldsymbol{v}^{(j)}(t) \in S_j^+(t) \setminus S_{j+1}^+(t)$. This vector is orthogonal to each $\boldsymbol{\varphi}_{\lambda^{(i)}}^+(t)$, where $i < j$, and obligatory has a nonzero projection onto at least one of the vectors $\boldsymbol{\varphi}_{\lambda^{(j)}}^+(t)$, related to the jth distinct Lyapunov exponent. It means that being iterated for infinitely long time with the propagator $\mathcal{F}$, the vector $\boldsymbol{v}^{(j)}(t)$ exponentially grows with the average rate $\lambda^{(j)}$ (Oseledec 1968; Benettin et al. 1980; Shimada and Nagashima 1979),

$$\boldsymbol{v}^{(j)}(t_1) \in S_j^+(t_1) \setminus S_{j+1}^+(t_1) \Rightarrow \left\| \mathcal{F}(t_1, t_1 + t) \boldsymbol{v}^{(j)}(t_1) \right\| \sim \mathrm{e}^{\lambda^{(j)} t}. \qquad (18)$$

The vectors $\boldsymbol{v}^{(j)}(t) \in S_j^-(t) \setminus S_{j-1}^-(t)$ behave analogously in backward time:

$$\boldsymbol{v}^{(j)}(t_1) \in S_j^-(t_1) \setminus S_{j-1}^-(t_1) \Rightarrow \left\| \mathcal{F}(t_1 - t, t_1)^{-1} \boldsymbol{v}^{(j)}(t_1) \right\| \sim \mathrm{e}^{-\lambda^{(j)} t}. \qquad (19)$$

Vectors $\boldsymbol{v}^{(1)}(t) \in S_1^+(t) \setminus S_2^+(t)$ fill almost the whole tangent space, because the excluded subspace $S_2^+(t)$ has a measure zero in $\mathbb{R}^m$. It means that under the action of $\mathcal{F}$ almost any vector, i.e., 1-dimensional volume, asymptotically grows or decays with the exponent $\lambda^{(1)}$, and its image tends to the subspace $\mathrm{span}\{\boldsymbol{\varphi}_{\lambda^{(1)}}^-(t)\} = S_1^-(t)$. Consider now a square, i.e., a 2-dimensional volume. First we assume that $\lambda^{(1)}$ is not degenerate so that $\nu^{(1)} = 1$. Almost any such square has a 1-dimensional intersection with the subspace $S_2^+(t) \setminus S_3^+(t)$ of vectors $\boldsymbol{v}^{(2)}(t)$ that are dominated by the $\lambda^{(2)}$ (Benettin et al. 1980; Shimada and Nagashima 1979; Legras and Vautard 1996; Parker and Chua 1989). (Here "almost" means that there is a measure zero set of squares fully belonging to subspaces with $j > 1$.) Thus, the area of the square asymptotically grows or decays with the exponent $\lambda^{(1)} + \lambda^{(2)}$. All segments within this square except a single one approach the subspace $\mathrm{span}\{\boldsymbol{\varphi}_{\lambda^{(1)}}^-(t)\}$, while that one goes into $\mathrm{span}\{\boldsymbol{\varphi}_{\lambda^{(2)}}^-(t)\}$. As a result, this square tends into the subspace S_2^-. When $\nu^{(1)} = 2$, the area of the square grows/decays with $2\lambda^{(1)} = \lambda_1 + \lambda_2$ and the whole square is embedded into S_1^-. But when we take a cube, its volume grows or decays with $2\lambda^{(1)} + \lambda^{(2)} = \lambda_1 + \lambda_2 + \lambda_3$ and its image goes into S_2^-. In general this can be formulated as follows. Under the action of $\mathcal{F}$ almost any k-dimensional volume asymptotically grows or decays with average exponential rate $\sum_{i=1}^k \lambda_i$ and tends to settle down inside the subspace S_i^-, where i is defined from the inequalities $\dim S_{i-1}^- < k \leq \dim S_i^-$. In the same way considering vectors $\boldsymbol{v}^{(j)}(t) \in S_j^-(t) \setminus S_{j-1}^-(t)$ we see that almost any k-dimensional volume being iterated in backward time with the propagator $\mathcal{F}(t_1, t_2)^{-1}$ grows or decays with the exponential rate $\sum_{i=1}^k \lambda_i$ and settles down in $S_i^+(t)$, such that $\dim S_{i+1}^+(t) < k \leq \dim S_i^+(t)$. Formally, these asymptotic embeddings can be described as

$$\mathcal{F}(t_1, t) V_k(t_1) \underset{t_1 \to -\infty}{\subset} S_j^-(t), \quad \dim S_{j-1}^-(t) < k \leq \dim S_j^-(t), \qquad (20)$$

$$\mathcal{F}(t, t_2)^{-1} V_k(t_2) \underset{t_2 \to +\infty}{\subset} S_j^+(t), \quad \dim S_{j+1}^+(t) < k \leq \dim S_j^+(t). \qquad (21)$$

Let us now turn to the adjoint propagator $\mathcal{G}(t_1, t_2)$. We recall that its singular vectors coincide with the singular vectors for $\mathcal{F}$, while its singular values are reciprocal. Hence the adjoint Oseledec subspaces can be defined as

$$H_j^+(t) = \text{span}\{\boldsymbol{\varphi}_{\lambda^{(i)}}^+(t) | i = 1, 2, \ldots, j\}, \qquad H_0^+(t) = \emptyset,$$

$$H_1^+(t) \subset H_2^+(t) \subset \cdots \subset H_s^+(t) = \mathbb{R}^m, \tag{22}$$

$$H_j^-(t) = \text{span}\{\boldsymbol{\varphi}_{\lambda^{(i)}}^-(t) | i = j, j+1, \ldots, s\}, \qquad H_{s+1}^-(t) = \emptyset,$$

$$H_s^-(t) \subset H_{s-1}^-(t) \subset \cdots \subset H_1^-(t) = \mathbb{R}^m. \tag{23}$$

Note that $H_{j-1}^+(t) \perp S_j^+(t)$ and $H_{j+1}^-(t) \perp S_j^-(t)$. Reasoning in the same way as above, we find that the adjoint propagator $\mathcal{G}$ generates the following asymptotic behavior as $t \to \infty$:

$$\boldsymbol{v}^{(j)}(t_1) \in H_j^+(t_1) \setminus H_{j-1}^+(t_1) \Rightarrow \left\| \mathcal{G}(t_1, t_1 + t) \boldsymbol{v}^{(j)}(t_1) \right\| \sim e^{-\lambda^{(j)} t}, \tag{24}$$

$$\boldsymbol{v}^{(j)}(t_1) \in H_j^-(t_1) \setminus H_{j+1}^-(t_1) \Rightarrow \left\| \mathcal{G}(t_1 - t, t_1)^{-1} \boldsymbol{v}^{(j)}(t_1) \right\| \sim e^{\lambda^{(j)} t}, \tag{25}$$

and the asymptotic embeddings read

$$\mathcal{G}(t_1, t) V_k(t_1) \underset{t_1 \to -\infty}{\subset} H_j^-(t), \quad \dim H_{j+1}^-(t) < k \le \dim H_j^-(t), \tag{26}$$

$$\mathcal{G}(t, t_2)^{-1} V_k(t_2) \underset{t_2 \to +\infty}{\subset} H_j^+(t), \quad \dim H_{j-1}^+(t) < k \le \dim H_j^+(t). \tag{27}$$

2.5 Finite-Time Evolution of Forward and Backward Lyapunov Vectors

Now we need to discuss how orthogonal Lyapunov vectors are transformed in finite time intervals. First consider the action of $\mathcal{F}(t_1, t_2)$ on forward Lyapunov vectors. For any such vector related to the jth distinct Lyapunov exponent $\lambda^{(j)}$ we can write $\boldsymbol{\varphi}_{\lambda^{(j)}, i}^+(t_1) \in S_j^+(t_1) \setminus S_{j+1}^+(t_1)$, where $i = 1, 2, \ldots, \nu^{(j)}$; see Eq. (16). It means that this vector shows the asymptotic behavior (18), i.e., it grows or decays with the exponent $\lambda^{(j)}$ forward in time. In turn, it means that $\mathcal{F}(t_1, t_2) \boldsymbol{\varphi}_{\lambda^{(j)}, i}^+(t_1) = \boldsymbol{\psi}_{\lambda^{(j)}, i}^+(t_2) \in S_j^+(t_2) \setminus S_{j+1}^+(t_2)$. We see that the image of $\boldsymbol{\varphi}_{\lambda^{(j)}, i}^+(t_1)$ at t_2 is orthogonal to vectors $\boldsymbol{\varphi}_{\lambda^{(n)}}^+(t_2)$ with $n < j$. But this is not a forward Lyapunov vector anymore, because the subspaces $\text{span}\{\boldsymbol{\varphi}_{\lambda^{(j)}}^+(t_2)\}$ and $S_j^+(t_2) \setminus S_{j+1}^+(t_2)$ are not identical. Vectors from $S_j^+(t_2) \setminus S_{j+1}^+(t_2)$ obligatory have a nonzero projection inside $\text{span}\{\boldsymbol{\varphi}_{\lambda^{(j)}}^+(t_2)\}$ but typically do not belong to it and also have projections onto forward vectors with $n > j$.

Let us first assume that there is no degeneracy i.e., all Lyapunov exponents are distinct. In matrix form we have $\mathcal{F}(t_1, t_2) \boldsymbol{\Phi}^+(t_1) = \boldsymbol{\Psi}^+(t_2)$, where

$$\boldsymbol{\Phi}^+(t) = \left[\boldsymbol{\varphi}_1^+(t), \boldsymbol{\varphi}_2^+(t), \ldots, \boldsymbol{\varphi}_m^+(t) \right] \tag{28}$$

is the matrix consisting of the forward Lyapunov vectors. According to the above discussion of $\boldsymbol{\psi}_{\lambda^{(j)}, i}^+(t_2)$, the first vector-column of $\boldsymbol{\Psi}^+(t_2)$ is collinear with $\boldsymbol{\varphi}_1^+(t_2)$. The second one is orthogonal to $\boldsymbol{\varphi}_1^+(t_2)$, but can have nonzero projections onto all

others forward vectors. The third one is orthogonal both to $\boldsymbol{\varphi}_1^+(t_2)$ and to $\boldsymbol{\varphi}_2^+(t_2)$ and so on. Thus we can write

$$\boldsymbol{\Psi}^+(t_2) = \boldsymbol{\Phi}^+(t_2)\mathbf{L}, \qquad (29)$$

where $\mathbf{L}$ is a lower triangular matrix.

When the spectrum of Lyapunov exponents is degenerated, the matrix $\boldsymbol{\Phi}^+(t_2)$ is not unique. There exist subspaces span$\{\boldsymbol{\varphi}_{\lambda(j)}^+(t_2)\}$ corresponding to each unique Lyapunov exponent, such that any vector from these subspaces can be treated as a forward Lyapunov vector. This means that the decomposition (29) is also not unique, because there exists a variety of non-triangular matrices $\mathbf{L}$ satisfying this equation. But the representation of $\boldsymbol{\Psi}^+(t_2)$ as a product of an orthogonal and a lower triangular matrices exists and is unique regardless of the degeneracy of Lyapunov exponents. In fact, this is the well-known QL factorization (Golub and van Loan 1996). The analysis of the details of the factorization procedure shows that the orthogonal matrix can always be treated as a matrix of forward Lyapunov vectors. Hence, regardless of the degeneracy, Eq. (29) remains valid.

Altogether, the propagator $\mathcal{F}$ maps forward Lyapunov vectors onto new vectors that are not Lyapunov vectors. In other words, forward Lyapunov vectors are non-covariant with the dynamics. To recover forward Lyapunov vectors, we have to perform a QL factorization. For the subsequent analysis it is convenient to represent it as a mapping backward in time:

$$\mathcal{F}(t_1, t_2)^{-1}\boldsymbol{\Phi}^+(t_2) = \boldsymbol{\Phi}^+(t_1)\mathbf{L}^{\mathcal{F}}(t_1, t_2), \qquad (30)$$

where $\mathbf{L}^{\mathcal{F}}(t_1, t_2) \in \mathbb{R}^{m \times m}$ is a lower triangular matrix. Because the propagator is non-singular and QL factorization is unique (if one requires for all diagonal elements of $\mathbf{L}^{\mathcal{F}}(t_1, t_2)$ to be positive), this equation determines $\boldsymbol{\Phi}^+(t_1)$ via $\boldsymbol{\Phi}^+(t_2)$ in a unique way. By definition, the diagonal elements of $\mathbf{L}^{\mathcal{F}}(t_1, t_2)$ do not vanish, i.e., this matrix is non-singular.

Repeating the above discussion for the backward Lyapunov vectors, we see that, regardless of the degeneracy, the following relation is always valid:

$$\mathcal{F}(t_1, t_2)\boldsymbol{\Phi}^-(t_1) = \boldsymbol{\Phi}^-(t_2)\mathbf{R}^{\mathcal{F}}(t_1, t_2), \qquad (31)$$

where

$$\boldsymbol{\Phi}^-(t) = \left[\boldsymbol{\varphi}_1^-(t), \boldsymbol{\varphi}_2^-(t), \ldots, \boldsymbol{\varphi}_m^-(t)\right], \qquad (32)$$

and $\mathbf{R}^{\mathcal{F}}(t_1, t_2)$ is an upper triangular matrix with a nonzero diagonal. Like the forward vectors, the backward vectors are non-covariant with the dynamics.

For the adjoint propagator $\mathcal{G}(t_1, t_2)$ we obtain

$$\mathcal{G}(t_1, t_2)^{-1}\boldsymbol{\Phi}^+(t_2) = \boldsymbol{\Phi}^+(t_1)\mathbf{R}^{\mathcal{G}}(t_1, t_2), \qquad (33)$$

$$\mathcal{G}(t_1, t_2)\boldsymbol{\Phi}^-(t_1) = \boldsymbol{\Phi}^-(t_2)\mathbf{L}^{\mathcal{G}}(t_1, t_2), \qquad (34)$$

where $\mathbf{R}^{\mathcal{G}}(t_1, t_2)$ and $\mathbf{L}^{\mathcal{G}}(t_1, t_2)$ are upper and lower non-singular triangular matrices, respectively.

Fig. 2 The idea of
orthogonalization. The vectors
v_i are the result of mapping (5)
and vectors q_i are their
orthogonalization: q_1 is
collinear to v_1, q_2 belongs to
the plane spanned by v_1 and v_2,
and q_3 belongs to the space
spanned by vectors v_1, v_2,
and v_3
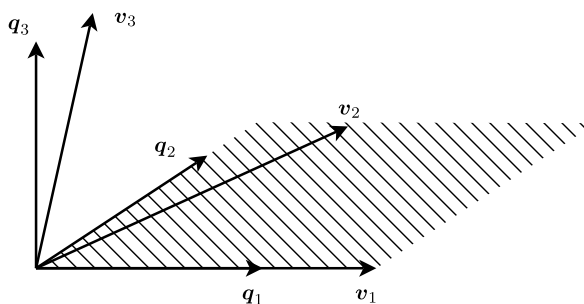
3 Numerical Computation of Lyapunov Exponents and Forward and Backward Vectors

The definition of the Lyapunov exponents and vectors cannot be implemented directly as a numerical algorithm. It is impossible to solve Eq. (3) for a sufficiently long time interval $t_2 - t_1$, to calculate the propagator $\mathcal{F}(t_1, t_2)$, and then to find a good approximation for the limit matrix $\mathbf{W}^+$. As we already discussed above, when we move away from the starting point t_1 almost any vector approaches the first backward Lyapunov vector $\boldsymbol{\varphi}_1^-(t)$, i.e., falls into subspace $S_1^-(t)$. Hence, in this way we can compute only the largest Lyapunov exponent and the corresponding vector.

Equation (31) determines a mapping of backward Lyapunov vectors at t_1 onto backward Lyapunov vectors at t_2. A set of all backward vectors at different times can be considered as a kind of limit set, attracting or repelling, and the mapping (31) can be treated as stationary dynamics on this set. This gives an idea for an iterative computation of the backward Lyapunov vectors. One can initialize an arbitrary orthogonal matrix and start iterations including mapping by $\mathcal{F}$ and QR factorization as described by Eq. (31). These iterations converge to the backward Lyapunov vectors where convergence is guaranteed by Eq. (20). One sees that the forward in time mapping embeds an arbitrary volume into the subspace spanned by backward Lyapunov vectors. It means that in the course of forward iterations $\mathcal{F}(t_n, t_{n+1})\mathbf{Q}(t_n) = \mathbf{Q}(t_{n+1})\mathbf{R}^{\mathcal{F}}(t_{n+1}, t_n)$ columns of $\mathbf{Q}(t_n) \in \mathbb{R}^{m \times m}$ converge to backward Lyapunov vectors. In fact this idea was suggested almost simultaneously by Benettin et al. (1978, 1980) and by Shimada and Nagashima (1979) to compute the Lyapunov exponents. The convergence of these iterations towards the backward Lyapunov vectors is discussed in Legras and Vautard (1996), and Ershov and Potapov (1998).

Consider the iterations in more detail; see Fig. 2. Suppose we have an orthogonal matrix $\mathbf{Q}(t_n)$. First we determine $\mathcal{F}(t_n, t_{n+1})$ for some interval $t_{n+1} - t_n$, which typically is not very large, and perform the mapping $\mathbf{V}(t_{n+1}) = \mathcal{F}(t_n, t_{n+1})\mathbf{Q}(t_n)$. The first vector-column v_1 of $\mathbf{V}(t_{n+1})$ behaves as we need, namely it approaches the subspace S_1^-. So, we only normalize it to prevent overflow or underflow: $v_1 \to q_1$, $\|q_1\| = 1$. The plane spanned by vectors v_1 and v_2 approaches the subspace S_2^- if $\lambda_1 \neq \lambda_2$, or it goes into S_1^- otherwise. In the first case we need to prevent the collapse of the plane due to the alignment of v_2 along $\boldsymbol{\varphi}_1^-$, and also the orientation of the plane has to be preserved to support the convergence. These two goals can be achieved by finding a new vector q_2 which is orthogonal to q_1 and belongs to the

plane originally spanned by v_1 and v_2. This vector is also normalized. In the second case, when $\lambda_1 = \lambda_2$, there is no alignment and, in principle, there are more options how to define q_2. But it is allowed anyway to compute q_2 as if the degeneracy was absent, and this is the most reasonable choice, making the procedure most transparent. In a similar manner we find the third normalized vector q_3 that is orthogonal to q_1 and q_2 and belongs to the space spanned by v_1, v_2 and v_3. Doing so for all the remaining columns of $\mathbf{V}(t_{n+1})$ we compose the matrix $\mathbf{Q}(t_{n+1})$ whose columns are vectors q_i. Then we use this $\mathbf{Q}(t_{n+1})$ as an initial value for the next mapping with $\mathcal{F}(t_{n+1}, t_{n+2})$ and repeat the procedure. After many recursions the columns of $\mathbf{Q}(t_n)$ converge to the backward Lyapunov vectors. This procedure works not only for the whole set of vectors, but allows one to compute any number of the first backward Lyapunov vectors.

The described procedure eliminates the ambiguity of backward Lyapunov vectors that emerge when not all Lyapunov exponents are distinct. Particular directions of backward Lyapunov vectors corresponding to each degenerate Lyapunov exponent $\lambda^{(j)}$ depend on the choice of the initial matrix $\mathbf{Q}(t_0)$. But these variations remain within subspace $\mathrm{span}\{\varphi^-_{\lambda^{(j)}}\}$ so that any choice is appropriate. Moreover, in practical computations the degeneracy manifests itself very weakly, because typically the degenerate Lyapunov exponents converge to identical values very slowly. In fact, dealing with a high-dimensional system one needs to know in advance which of the exponents are expected to be identical to identify them in the computed spectrum.

The computation of the Lyapunov exponents is illustrated in Fig. 3. An initial unit square composed of vectors $q_i(t_n)$ is transformed into the parallelogram spanned by the vectors $v_i(t_{n+1})$. After the orthogonalization we obtain $q_i(t_{n+1})$. To compute the area of the parallelogram we can construct a rectangle with identical area by projecting $v_j(t_{n+1})$ onto $q_i(t_{n+1})$: $r_{ij} = q_i v_j$. As we see from the figure, the area is $r_{11}r_{22}$. Similarly, a k-dimensional unit volume after the mapping is equal to $r_{11}r_{22} \ldots r_{kk}$. Thus, we can define the local Lyapunov exponents as

$$\tilde{\lambda}_i = \ln(r_{ii})/(t_{n+1} - t_n). \tag{35}$$

In the course of the mapping/orthogonalization iterations we need to accumulate and average $\tilde{\lambda}_i$ to obtain the Lyapunov exponents.

By construction, the first vector v_1 has only one nonzero projection onto q_1, the second vector v_2 has two nonzero projections, onto q_1 and q_2, the third vector v_3 has three nonzero projections onto first three vectors q_i and so on. It means that r_{ij} are elements of an upper triangular matrix. So, the procedure described above represents the matrix $\mathbf{V}$ as the product $\mathbf{V} = \mathbf{QR}$. Here $\mathbf{Q}$ is an orthogonal matrix such that $\mathrm{span}\{q_1, q_2, \ldots, q_k\} = \mathrm{span}\{v_1, v_2, \ldots, v_k\}$ for any $k \leq m$, and $\mathbf{R}$ is an upper triangular matrix consisting of the projections of columns of $\mathbf{V}$ onto columns of $\mathbf{Q}$. This procedure is called QR factorization (Golub and van Loan 1996). There are different numerical algorithms of the QR factorization. Note that the often used Gram–Schmidt algorithm as well as its modified version are not very accurate when the dimension of the tangent space is large (Kuptsov 2010). Most high precision QR algorithms are based on so called Householder transformations (Geist et al. 1990; Golub and van Loan 1996).

Fig. 3 Computation of a volume after the mapping by $\mathcal{F}(t_n, t_{n+1})$
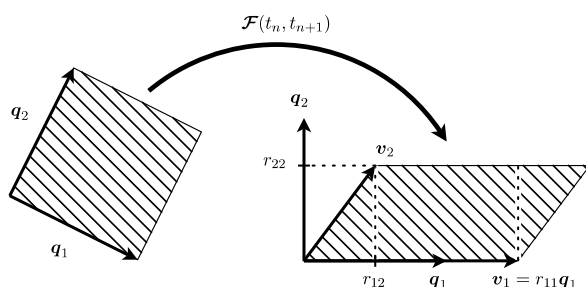
Another way to compute backward Lyapunov vectors is based on the adjoint propagator $\mathcal{G}$. Equation (34) determines the stationary dynamics, and Eq. (26) indicates that the forward iterations converge to this dynamics. Because $\mathcal{G}(t_n, t_{n+1})$ has reciprocal singular values, the value $\sigma_m(t_n, t_{n+1})^{-1}$ dominates in the course of forward iterations with the adjoint propagator. It means that columns of $\mathbf{Q}$ converge to the backward Lyapunov vectors in the reverse order. If we rearrange columns of $\mathbf{\Phi}^-$ in Eq. (34) in the reverse order, we also have to transpose $\mathbf{L}^{\mathcal{G}}$ with respect to its diagonal and with respect to the antidiagonal. As a result we obtain an upper triangular matrix. Thus, the algorithm is identical to the one previously described. We perform the mapping by $\mathcal{G}(t_n, t_{n+1})$, find a QR factorization of the resulting matrix, take $\mathbf{Q}(t_{n+1})$, and do the next recursion.

Consider now the computation of the forward Lyapunov vectors. The first algorithm is based on Eqs. (27) and (33). We need to move backward in time alternating mappings with $\mathcal{G}(t_n, t_{n+1})^{-1}$ and QR factorizations. The matrices $\mathbf{Q}$ converge to $\mathbf{\Phi}^+$, and the forward Lyapunov vectors come up in the correct order. Note that $\mathcal{G}^{-1}$ is merely the transposition of $\mathcal{F}$; see Eq. (6). In the course of this procedure we can compute local Lyapunov exponents as logarithms of diagonal elements of triangular matrices per unit time. For short time intervals these local exponents will differ from those given by Eq. (35), but being averaged over many times steps they also converge to the Lyapunov exponents.

Another algorithm for the forward Lyapunov vectors is based on Eqs. (30) and (21). The procedure is the same as above except using the inverted propagator $\mathcal{F}^{-1}$. This method computes the vectors in the reversed order, and, hence, the previous one is usually more applicable. The idea to apply the transposed propagator instead of the inverted one was suggested in Legras and Vautard (1996).

The implementation of the algorithm with the transposed propagator $\mathcal{F}^{\mathrm{T}}$ is straightforward for discrete time systems (e.g. coupled map lattices), where the action of $\mathcal{F}^{\mathrm{T}}$ on a set of (Lyapunov) vectors can be computed using the transposed Jacobian matrix of the system. In principle, one can do the same with continuous systems, but in that case one would have to compute the full propagator $\mathcal{F}$ first by solving m copies of the linearized ODE (2) and then use its transpose $\mathcal{F}^{\mathrm{T}}$ to evolve the desired number of tangent vectors. This implementation is inefficient if the system is very high dimensional ($m \gg 1$) and if only a few Lyapunov vectors are to be computed. As an alternative, the action of $\mathcal{F}^{\mathrm{T}}$ can reformulated as follows. Using the Magnus expansion (Magnus 1954), we can represent the propagator of Eq. (2) via matrix exponential functions as $\mathcal{F}(t_1, t_2) = \exp[\mathbf{\Omega}^{\mathcal{F}}(t_1, t_2)]$. Here $\mathbf{\Omega}^{\mathcal{F}}(t_1, t_2)$ is a matrix that is given

as a series expansion $\mathbf{\Omega}^{\mathcal{F}}(t_1, t_2) = \sum_{i=1}^{\infty} \mathbf{\Omega}_i^{\mathcal{F}}(t_1, t_2)$, with $\mathbf{\Omega}_1^{\mathcal{F}}(t_1, t_2) = \int_{t_1}^{t_2} \mathbf{J}(\tau_1) \, d\tau_1$, $\mathbf{\Omega}_2^{\mathcal{F}}(t_1, t_2) = \frac{1}{2} \int_{t_1}^{t_2} d\tau_1 \int_{t_1}^{\tau_1} d\tau_2 [\mathbf{J}(\tau_1), \mathbf{J}(\tau_2)]$, and so on, see Magnus (1954), $\mathbf{J}(\tau) \equiv \mathbf{J}(\boldsymbol{u}, \tau)$ is the Jacobian matrix, and $[\cdot, \cdot]$ denotes the matrix commutator. The adjoint propagator reads $\mathcal{G}(t_1, t_2) = \mathcal{F}(t_1, t_2)^{-\mathrm{T}} = \exp\{-[\mathbf{\Omega}^{\mathcal{F}}(t_1, t_2)]^{\mathrm{T}}\} = \exp[\mathbf{\Omega}^{\mathcal{G}}(t_1, t_2)]$. The matrix $\mathbf{\Omega}^{\mathcal{G}}(t_1, t_2) = -[\mathbf{\Omega}^{\mathcal{F}}(t_1, t_2)]^{\mathrm{T}}$ generating $\mathcal{G}(t_1, t_2)$ is obtained with a Magnus expansion where the Jacobian matrix $\mathbf{J}(\boldsymbol{u}, t)$ is replaced by $-\mathbf{J}(\boldsymbol{u}, t)^{\mathrm{T}}$. So, to compute the action of $\mathcal{G}(t_1, t_2)$ on a tangent vector we have to solve the following linear ODE:

$$\dot{\boldsymbol{v}} = -\mathbf{J}(\boldsymbol{u}, t)^{\mathrm{T}} \boldsymbol{v} \qquad (36)$$

forward in time (from t_1 to $t_2 > t_1$, because the action of the adjoint propagator $\mathcal{G}(t_1, t_2)$ corresponds to moving forward in time). To compute forward Lyapunov vectors using $\mathcal{F}(t_1, t_2)^{\mathrm{T}} = \mathcal{G}(t_1, t_2)^{-1}$ we have to invert $\mathcal{G}(t_1, t_2)$. This can be done by integrating the required number of copies of Eq. (36) and the basic system (1) backward in time (from t_2 to t_1).

All four algorithms compute the dominating Lyapunov exponents and corresponding vectors with the highest precision, while the remaining part of the spectrum is not very accurate. Namely, $\mathcal{F}$- and $\mathcal{G}^{-1}$-algorithms do the best for the first Lyapunov exponent and vectors, while $\mathcal{F}^{-1}$- and $\mathcal{G}$-algorithms achieve the highest accuracy for the mth exponent and vectors. One can perform $\mathcal{F}$- and $\mathcal{G}$-algorithms in parallel, and then construct weighted sums of computed exponents and backward vectors to obtain the whole spectrum with very high precision. Similarly, performing backward iterations simultaneously with $\mathcal{F}^{-1}$ and $\mathcal{G}^{-1}$ one can compute the forward Lyapunov vectors with improved accuracy.

4 Covariant Lyapunov Vectors

Orthogonal matrices computed according to QR decomposition preserve subspaces spanned by each *first k* columns of a factorized matrix. The QL decomposition preserves subspaces spanned by each *last k* columns of a factorized matrix. It means that considering Eqs. (30) and (31), we can conclude that Oseledec subspaces (16) and (17) are preserved under the tangent flow (Eckmann and Ruelle 1985; Legras and Vautard 1996). The same conclusion follows from Eqs. (33) and (34) for the subspaces (22) and (23):

$$\mathcal{F}(t_1, t_2) S_j^+(t_1) = S_j^+(t_2), \qquad \mathcal{F}(t_1, t_2) S_j^-(t_1) = S_j^-(t_2), \qquad (37)$$

$$\mathcal{G}(t_1, t_2) H_j^+(t_1) = H_j^+(t_2), \qquad \mathcal{G}(t_1, t_2) H_j^-(t_1) = H_j^-(t_2). \qquad (38)$$

So, the Oseledec subspaces are invariant under time reversal and covariant with the dynamics. But this is not the case for the forward and backward Lyapunov vectors themselves. Being multiplied by $\mathcal{F}$ and $\mathcal{G}$ they also have to be multiplied by lower or upper triangular matrices to be mapped to new forward and backward Lyapunov vectors; see Eqs. (30), (31), (33), and (34).

Given the covariant subspaces, it is natural to search for some vectors inside these subspaces that are also covariant with the dynamics and are invariant with respect to

time reversal. These vectors are referred to as *covariant Lyapunov vectors* (Ginelli et al. 2007). We denote them by $\boldsymbol{\gamma}_j(t)$. The basic property of these vectors (which are covariant with respect to the propagator $\mathcal{F}$) can be written as

$$\left\| \mathcal{F}(t_1, t_1 \pm t)\boldsymbol{\gamma}_j(t_1) \right\| \sim \exp(\pm\lambda_j t) \tag{39}$$

for any t_1 and $t \to \infty$. The covariant Lyapunov vectors are norm-independent (Legras and Vautard 1996; Wolfe and Samelson 2007). Also we can introduce norm-independent adjoint vectors $\boldsymbol{\theta}_j(t)$ that are covariant with respect to the adjoint dynamics:

$$\left\| \mathcal{G}(t_1, t_1 \pm t)\boldsymbol{\theta}_j(t_1) \right\| \sim \exp(\mp\lambda_j t). \tag{40}$$

Equation (39) means that Eqs. (18) and (19) are fulfilled simultaneously, and Eq. (40) implies the simultaneous validity of Eqs. (24) and (25). It means that the covariant Lyapunov vectors belong to the intersection of the Oseledec subspaces (Ruelle 1979; Eckmann and Ruelle 1985; Legras and Vautard 1996), and the adjoint covariant vectors can be found within the intersections of the adjoint subspaces:

$$\boldsymbol{\gamma}_j(t) \in S_j^+(t) \cap S_j^-(t), \tag{41}$$

$$\boldsymbol{\theta}_j(t) \in H_j^+(t) \cap H_j^-(t). \tag{42}$$

These intersections are always nonempty because the sum of dimensions of Oseledec subspaces is always higher than the dimension of the whole tangent space.

Consider arbitrary vectors $\boldsymbol{v}^{(j)}(t_1) \in S_j^+(t_1) \setminus S_{j+1}^+(t_1)$, where $j = 1, 2, \ldots, s$, and s is the number of distinct Lyapunov exponents. There are $\nu^{(j)}$ linearly independent vectors corresponding to the jth Lyapunov exponent $\lambda^{(j)}$, and the total number of such vectors is $\sum_{j=1}^s \nu^{(j)} = m$. Representing the whole set of these vectors as a matrix $\mathbf{V}$, we obtain $\mathbf{V} = \boldsymbol{\Phi}^+\mathbf{A}^+$, where $\mathbf{A}^+$ is a lower triangular matrix, and $\boldsymbol{\Phi}^+$ is a matrix of forward Lyapunov vectors (28). As follows from Eq. (18), when the forward propagator $\mathcal{F}$ is applied to these vectors, the first $\nu^{(1)}$ of them grow or decay asymptotically with the exponent $\lambda^{(1)}$, the next $\nu^{(2)}$ vectors grow / decay with the exponent $\lambda^{(2)}$ and so on. In a similar manner we can consider arbitrary vectors $\boldsymbol{v}^{(j)}(t_1) \in S_j^-(t_1) \setminus S_{j-1}^-(t_1)$. The matrix of these vectors $\mathbf{V}$ can be found as $\mathbf{V} = \boldsymbol{\Phi}^-\mathbf{A}^-$, where $\mathbf{A}^-$ is an upper triangular matrix, and $\boldsymbol{\Phi}^-$ is defined by Eq. (32). According to Eq. (19), acting upon these vectors by the inverted propagator $\mathcal{F}^{-1}$, we can observe that the first $\nu^{(1)}$ of them grow or decay asymptotically with the exponent $-\lambda^{(1)}$, the next $\nu^{(2)}$ vectors grow / decay with the exponent $-\lambda^{(2)}$ and so on. Let $\boldsymbol{\Gamma}(t) = [\boldsymbol{\gamma}_1(t), \boldsymbol{\gamma}_2(t), \ldots, \boldsymbol{\gamma}_m]$ be a matrix consisting of the covariant Lyapunov vectors, and let $\boldsymbol{\Theta}(t) = [\boldsymbol{\theta}_1(t), \boldsymbol{\theta}_2(t), \ldots, \boldsymbol{\theta}_m]$ be a matrix of adjoint covariant vectors. As follows from Eq. (39), the covariant vectors have to demonstrate both forward (18) and backward (19) asymptotic behavior. It means that there exist an upper triangular matrix $\mathbf{A}^-$ and a lower triangular matrix $\mathbf{A}^+$, such that

$$\boldsymbol{\Gamma}(t) = \boldsymbol{\Phi}^-(t)\mathbf{A}^-(t) = \boldsymbol{\Phi}^+(t)\mathbf{A}^+(t). \tag{43}$$

Reasoning in a similar manner one obtains for the adjoint vectors:

$$\boldsymbol{\Theta}(t) = \boldsymbol{\Phi}^+(t)\mathbf{B}^+(t) = \boldsymbol{\Phi}^-(t)\mathbf{B}^-(t), \tag{44}$$

where $\mathbf{B}^+(t)$ and $\mathbf{B}^-(t)$ are upper and lower triangular matrices, respectively. Note that Eqs. (43) and (44) convey, in fact, the same property of covariant vectors as Eqs. (41) and (42), respectively. Multiplying Eq. (43) by $[\boldsymbol{\Phi}^+(t)]^T$ and Eq. (44) by $[\boldsymbol{\Phi}^-(t)]^T$ we obtain the relations between triangular matrices that will be required later:

$$\mathbf{P}(t)\mathbf{A}^-(t) = \mathbf{A}^+(t), \tag{45}$$

$$\mathbf{P}(t)^T\mathbf{B}^+(t) = \mathbf{B}^-(t), \tag{46}$$

where

$$\mathbf{P}(t) = \left[\boldsymbol{\Phi}^+(t)\right]^T\boldsymbol{\Phi}^-(t) \tag{47}$$

is a $m \times m$ orthogonal matrix.

If the Lyapunov exponents are degenerated, the covariant vectors are not unique. Let us discuss what Eq. (43) implies in this case (Eq. (44) can be considered in the same way). If $\boldsymbol{\Gamma}(t)$ is known, then we can compute $\boldsymbol{\Phi}^-(t)$ and $\mathbf{A}^-(t)$, and $\boldsymbol{\Phi}^+(t)$ and $\mathbf{A}^+(t)$ via QR and QL decompositions, respectively, in a unique way. However, Eq. (43) does not determine $\boldsymbol{\Gamma}(t)$ via $\boldsymbol{\Phi}^+(t)$ and $\boldsymbol{\Phi}^-(t)$ in a unique way. In principle, there exist orthogonal matrices $\boldsymbol{\Phi}^-$ and $\boldsymbol{\Phi}^+$ that allow one to fulfill Eq. (43) with several couples $\mathbf{A}^-(t)$ and $\mathbf{A}^+(t)$, resulting in different matrices $\boldsymbol{\Gamma}$, and, hence, in different covariant Lyapunov vectors. As an example one can consider a matrix $\boldsymbol{\Phi}^+$ that consists of columns of $\boldsymbol{\Phi}^-$ arranged in the reverse order. Ambiguity of $\mathbf{A}^-(t)$ and $\mathbf{A}^+(t)$ means that there are Lyapunov exponents associated with several covariant vectors. But on the other hand, the total number of covariant vectors is equal to the total number of Lyapunov exponents m, and there are no exponents without vectors. It means that the ambiguity can occur if and only if the Lyapunov exponents are degenerate. The covariant vectors associated with a k times degenerated Lyapunov exponent can have arbitrary orientation within a k-dimensional subspace corresponding to this exponent. But because any set of linearly independent covariant vectors from the subspace corresponding to the degenerated exponent is as good as any other, this ambiguity can be ignored: we just need to have any linear independent set of vectors. (We recall that though forward and backward vectors are also subject to the degeneracy, their ambiguity is eliminated in the course of the computations, see Sect. 3.)

Let us find how $\boldsymbol{\Gamma}(t_1)$ is transformed by $\mathcal{F}(t_1, t_2)$. In general, we can write

$$\mathcal{F}(t_1, t_2)\boldsymbol{\Gamma}(t_1) = \boldsymbol{\Gamma}(t_2)\mathbf{C}^{\mathcal{F}}(t_1, t_2), \tag{48}$$

where $\mathbf{C}^{\mathcal{F}}(t_1, t_2)$ is a matrix whose structure should be determined. When the Lyapunov spectrum is not degenerated, Eq. (41) immediately implies that $\mathbf{C}^{\mathcal{F}}(t_1, t_2)$ is diagonal. To show that this is the case regardless of the degeneracy, we substitute $\boldsymbol{\Gamma}(t) = \boldsymbol{\Phi}^+(t)\mathbf{A}^+(t)$, see Eq. (43), in Eq. (48) and, taking into account Eq. (30), we obtain

$$\mathbf{L}^{\mathcal{F}}(t_1, t_2)\mathbf{A}^+(t_2)\mathbf{C}^{\mathcal{F}}(t_1, t_2) = \mathbf{A}^+(t_1). \tag{49}$$

Since all known matrices here are lower triangular, $\mathbf{C}^{\mathcal{F}}(t_1, t_2)$ is also lower triangular. Analogously substituting $\boldsymbol{\Gamma}(t) = \boldsymbol{\Phi}^-(t)\mathbf{A}^-(t)$ in Eq. (48) and using Eq. (31) we

obtain

$$\mathbf{R}^{\mathcal{F}}(t_1, t_2)\mathbf{A}^-(t_1) = \mathbf{A}^-(t_2)\mathbf{C}^{\mathcal{F}}(t_1, t_2), \tag{50}$$

i.e., $\mathbf{C}^{\mathcal{F}}(t_1, t_2)$ is an upper triangular matrix. Simultaneous upper and lower triangular structure has only a diagonal matrix: $\mathbf{C}^{\mathcal{F}}(t_1, t_2) = \mathrm{diag}[c_1(t_1, t_2), c_2(t_1, t_2), \ldots, c_m(t_1, t_2)]$. Hence, the vectors $\boldsymbol{\gamma}_j$ can freely evolve under the tangent flow (48) so that the tangent flow preserves their directions. The direction, represented by $\boldsymbol{\gamma}_j(t_1)$ at t_1 is mapped onto the direction pointed by $\boldsymbol{\gamma}_j(t_2)$ at t_2, and the backward step maps $\boldsymbol{\gamma}_j(t_2)$ onto the direction of $\boldsymbol{\gamma}_j(t_1)$. The vectors themselves are stretched or contracted by factors $c_i^{\mathcal{F}}(t_1, t_2)$. (Recall that the directions of the forward and the backward Lyapunov vectors are not preserved.) The adjoint vectors freely evolve under the tangent flow generated by the adjoint propagator:

$$\mathcal{G}(t_1, t_2)\boldsymbol{\Theta}(t_1) = \boldsymbol{\Theta}(t_2)\big[\mathbf{C}^{\mathcal{G}}(t_1, t_2)\big]^{-1}. \tag{51}$$

One can say that the vectors $\boldsymbol{\gamma}_j$ are covariant with the tangent dynamics generated by $\mathcal{F}$ and the adjoint vectors $\boldsymbol{\theta}_j$ are covariant with the tangent dynamics of $\mathcal{G}$. This is the reason why these vectors are referred to as covariant vectors.

Since the covariant vectors are defined up to an arbitrary length, the diagonal elements of $\mathbf{C}^{\mathcal{F}}$ can be defined in various ways. In particular, to fulfill Eq. (39) we should not normalize the vectors, and $\mathbf{C}^{\mathcal{F}} \equiv \mathbf{I}$ in this case. However, in the course of numerical computations we need to avoid overflows and underflows. Hence, constant lengths of $\boldsymbol{\gamma}_j(t)$ have to preserved with respect to the chosen norm. In this case $c_j^{\mathcal{F}}(t_1, t_2) = \|\mathcal{F}(t_1, t_2)\boldsymbol{\gamma}_j(t_1)\| / \|\boldsymbol{\gamma}_j(t_1)\|$, and

$$\ln\big[c_j^{\mathcal{F}}(t_1, t_2)\big]/(t_2 - t_1) \tag{52}$$

can be treated as local Lyapunov exponent. The values of these local Lyapunov exponents depend on the norm, but being averaged over many / long time intervals (t_1, t_2), regardless of the norm they converge to the Lyapunov exponents λ_j. Consider an important particular case. As follows from the discussions in Sect. 3, one can build unit volumes using the covariant Lyapunov vectors when the diagonal elements of the upper triangular matrix $\mathbf{A}^-$ are equal to 1; see Eq. (43). Equation (50) describes the dynamics of $\mathbf{A}^-$ corresponding to the tangent dynamics of the covariant Lyapunov vectors. When two upper triangular matrices are multiplied, the resulting matrix is also upper triangular and its diagonal elements are the products of the diagonal elements of the multipliers. Thus, if the covariant Lyapunov vectors are rescaled to preserve ones on the diagonal of $\mathbf{A}^-$, then the $c_j^{\mathcal{F}}$ are equal to the diagonal elements of $\mathbf{R}^{\mathcal{F}}$, and the local Lyapunov exponents (52) coincide with those defined by Eq. (35): $\ln[c_j^{\mathcal{F}}(t_1, t_2)]/(t_2 - t_1) = \tilde{\lambda}_j(t_1, t_2)$.

Let us now discuss what it means if covariant vectors merge. The phase space of dynamical systems can contain structures called "wild hyperbolic sets" that are responsible for the existence of structurally stable and unavoidable homoclinic tangencies between stable and unstable manifolds. In turn, the presence of these tangencies results in formation of non-hyperbolic chaotic attractors (Guckenheimer

and Holmes 1983). Since covariant vectors are associated with invariant manifolds of trajectories, in points of tangencies the corresponding vectors become collinear (Eckmann and Ruelle 1985; Ginelli et al. 2007; Wolfe and Samelson 2007; Yang et al. 2009). The same happens with the corresponding adjoint covariant vectors. Collinear vectors result in a singularity of the matrices $\mathbf{\Gamma}(t)$, and $\mathbf{\Theta}(t)$. The triangular matrices $\mathbf{A}^{\pm}(t)$ and $\mathbf{B}^{\pm}(t)$ also become singular. Note that this property is time-invariant: as follows from Eqs. (48) and (51) if some of covariant vectors are identical at $t = t_1$, they remain identical for all time. In practice, selecting an arbitrary trajectory we almost never hit exactly the trajectory with the tangencies. But if a trajectory with tangencies exists, the arbitrarily selected orbit will pass infinitely close to it and we will encounter with a nonzero frequency ill-conditioned matrices of covariant vectors. Note that this is not the case for orthogonal forward and backward vectors, which are not affected by tangencies.

Now we consider how covariant and adjoint covariant vectors are related to each other. First of all notice that given $\mathbf{\Gamma}(t)$, one can always compute $\mathbf{\Phi}^{-}(t)$ and $\mathbf{A}^{-}(t)$ as its QR decomposition and $\mathbf{\Phi}^{+}(t)$ and $\mathbf{A}^{+}(t)$ as a QL decomposition. Then one can construct the matrix $\mathbf{P}(t) = [\mathbf{\Phi}^{+}(t)]^{\mathrm{T}}\mathbf{\Phi}^{-}(t)$ and compute $\mathbf{\Theta}(t)$ via the LU method as described below in Sect. 5.2. It means that these two sets of vectors are not independent from each other. However, the mutual orientation of these vectors can help to recover some new data.

Transposing Eq. (44) and multiplying it with Eq. (43), we obtain $\mathbf{B}^{+}(t)^{\mathrm{T}}\mathbf{A}^{+}(t) = \mathbf{B}^{-}(t)^{\mathrm{T}}\mathbf{A}^{-}(t)$. The left hand side of this equation is a lower triangular matrix, while the matrix on the right hand side is upper triangular. Hence,

$$\mathbf{B}^{\pm}(t)^{\mathrm{T}}\mathbf{A}^{\pm}(t) = \mathbf{A}^{\pm}(t)^{\mathrm{T}}\mathbf{B}^{\pm}(t) = \mathbf{D}(t), \tag{53}$$

where $\mathbf{D}(t)$ is a diagonal matrix. Again take into account Eqs. (44) and (43) to write

$$\mathbf{\Theta}(t)^{\mathrm{T}}\mathbf{\Gamma}(t) = \mathbf{\Gamma}(t)^{\mathrm{T}}\mathbf{\Theta}(t) = \mathbf{D}(t). \tag{54}$$

The diagonal structure of $\mathbf{D}$ indicates that each adjoint covariant vector $\boldsymbol{\theta}_j(t)$, $j = 1, 2, \ldots, m$ is always orthogonal to the covariant vectors $\boldsymbol{\gamma}_i(t)$, where $i \neq j$. In presence of the tangency $\boldsymbol{\gamma}_j(t) = \boldsymbol{\gamma}_{j+1}(t)$ the jth and the $(j+1)$th diagonal elements of $\mathbf{D}$ vanish, i.e., corresponding adjoint and original vectors also become orthogonal: $\boldsymbol{\gamma}_{j+i}(t) \perp \boldsymbol{\theta}_{j+i}(t)$, where $i = 0, 1$. It means that given the vectors $\boldsymbol{\gamma}_i(t)$, one can find the adjoint vectors $\boldsymbol{\theta}_j(t)$ as null vectors of the matrix consisting of all $\boldsymbol{\gamma}_i(t)$ except the jth one. Notice that even if a tangency occurs, one still can compute $\boldsymbol{\theta}_j(t)$ in this way. To find how $\mathbf{D}(t)$ is varying in time, we transpose Eq. (48), multiply it with Eq. (51), and take into account Eq. (6): $\mathbf{\Gamma}(t_1)^{\mathrm{T}}\mathbf{\Theta}(t_1) = \mathbf{C}^{\mathcal{F}}(t_1, t_2)\mathbf{\Gamma}(t_2)^{\mathrm{T}}\mathbf{\Theta}(t_2)[\mathbf{C}^{\mathcal{G}}(t_1, t_2)]^{-1}$. Hence, $\mathbf{D}(t_1) = \mathbf{C}^{\mathcal{F}}(t_1, t_2)\mathbf{D}(t_2)[\mathbf{C}^{\mathcal{G}}(t_1, t_2)]^{-1}$ (recall that all matrices here are diagonal). Altogether, the elements of the diagonal matrix $\mathbf{D}$ are cosines of angles between corresponding covariant and adjoint covariant vectors. Since these angles are affected by tangencies, their time averages as well as their temporal fluctuations; i.e., the first and other moments, can be considered as characteristic numbers describing the structure of an attractor. The angles are norm-independent, because they are defined in terms of covariant and adjoint covariant Lyapunov vectors which share this property.

If the covariant vectors are computed with a non-ideal accuracy, the errors will grows in course of the tangent dynamics. The same is the case for the adjoint covariant vectors. In particular, it means that if we have found numerically covariant vectors at t_1, we cannot compute them at $t > t_1$ via Eq. (48) because numerical errors results in the divergence from the true directions. But nevertheless, Pazó et al. (2010) shows that this divergence is actually sufficiently slow. Hence, Eq. (48) can be used to find an estimate for the covariant vectors at $t > t_1$ when $t - t_1$ is not very large.

The covariant Lyapunov vectors are defined locally, according to Eqs. (43) and (44), and asymptotically, as follows from Eqs. (39) and (40). These equations provide two basic ideas for computing these vectors. The first one is to find backward and forward Lyapunov vectors for some point of the trajectory and compute an intersection of corresponding Oseledec subspaces. The straightforward implementation of this approach, though possible, takes a lot of computational resources. We discuss it in Sect. 5.1. In Sects. 5.2 and 5.3 more "clever" implementations are considered.

The second approach is to try to arrive at asymptotic behavior described by Eq. (39) or (40). If we initialize a vector, satisfying Eq. (19) and start iterations backward in time, after a long time we closely approach the limiting vectors that evolve as $\mathcal{F}(t_n, t_{n+1})^{-1} \boldsymbol{v}_j(t_{n+1}) = \boldsymbol{v}_j(t_n) c_j(t_n, t_{n+1})^{-1}$, where $c_j(t_n, t_{n+1})$ are related to the local Lyapunov exponents (52). This equation is reversible, so that when the limit is reached, we can turn forward and arrive the opposite limit too. It means that the limiting vectors $\boldsymbol{v}_j$ found in this way satisfy Eq. (39) and coincide with $\boldsymbol{\gamma}_j$. The forward iterations defined by Eq. (18) also converge to the covariant Lyapunov vectors. Similarly, the iterations initialized according to Eqs. (24) and (25) converge to the adjoint covariant vectors. The straightforward numerical implementation of this approach is impossible. Due to numerical noise, vectors $\boldsymbol{v}^{(j)}$ cannot be initialized exactly as required, and the numerical routines always converge to the single dominating vector. But a way to avoid this obstacle is known, and we consider it in Sect. 5.4.

5 Numerical Methods for Computing Covariant Lyapunov Vectors

5.1 Intersection of Oseledec Subspaces

A straightforward way to find covariant Lyapunov vectors is based on Eq. (41). Given forward and backward Lyapunov vectors, one can construct intersections of the Oseledec subspaces and find the covariant vectors. To compute the intersection of two subspaces one can compute so called principle angles between subspaces (Golub and van Loan 1996; Knyazev and Argentati 2002). In brief, this method is associated with computation of the singular values and vectors of submatrices of the matrix (47).

To compute the jth covariant vector one needs the first j backward vectors and $m - j + 1$ last forward vectors. The first backward vectors can be computed in the course of the iterations with the propagator $\mathcal{F}$, and the last forward vectors are the result of the iterations with the inverted propagator $\mathcal{F}^{-1}$, see Sect. 3.

Regardless of j, $m + 1$ forward and backward Lyapunov vectors are always required. So, this method is applicable for computation of the whole spectrum, but this is not an efficient approach if one needs only a few first covariant vectors. Because

the forward Lyapunov vectors are computed in the reverse order, this method has a "flattened" accuracy along the spectrum: the backward vectors have higher accuracy in first part of the spectrum, and the forward one are more accurate in its last part. So, the resulting covariant vectors have approximately the same accuracy for the whole spectrum.

5.2 Method of LU Factorization

It is possible to avoid computation of the whole spectrum of the forward or backward Lyapunov vectors to get only a few first covariant vectors. Two original ideas, which were reported by Wolfe and Samelson (2007), and Ginelli et al. (2007), are discussed in Sects. 5.3 and 5.4. In the current section we present a new approach to this problem.

Consider Eq. (45). Matrices $\mathbf{A}^+$ and $\mathbf{A}^-$ are lower and upper triangular, respectively. If $\mathbf{A}^-$ is non-singular, we can rewrite Eq. (45) as $\mathbf{P} = \mathbf{A}^+(\mathbf{A}^-)^{-1}$. This equation can be considered as an LU factorization of $\mathbf{P}$, i.e., representation of a matrix as a product of a lower and an upper triangular matrix (Golub and van Loan 1996). If the factorization exists, it is unique up to the diagonal elements of one of the matrices (factors). For us it means that if we find the LU decomposition of $\mathbf{P}$, we find the covariant vectors up to arbitrary lengths.

There are many well developed standard routines computing the LU factorization. But for us the serious disadvantage is that they work well only as long as the assumption of non-singularity of $\mathbf{A}^-$ remains valid. If matrices $\mathbf{A}^\pm$ are singular, the straightforward factorization of $\mathbf{P}$ does not exist. The standard routines for LU decomposition avoid this obstacle performing preliminary permutations of rows and columns of $\mathbf{P}$. This is not suitable for us, because the order of rows and columns in $\mathbf{P}$ is essential. Moreover, the standard routines find both $\mathbf{A}^-$, and $\mathbf{A}^+$, while it is enough for us to have only $\mathbf{A}^-$.

Let us return to Eq. (45). We shall demonstrate now that the required elements of $\mathbf{A}^-$ can be found from this equation regardless of a possible singularity of $\mathbf{A}^\pm$. To compute the jth covariant vector we need to find the top j elements of the jth column of $\mathbf{A}^-$. This fragment of the column can be denoted as $\mathbf{A}^-(1:j, j)$. The remaining fragment $\mathbf{A}^-(j+1:m, j)$ contains zeros. Note that here we omit the time dependence and use parentheses to indicate submatrices. The matrix equation for nonzero elements reads $\mathbf{P}(1:j, 1:j)\mathbf{A}^-(1:j, j) = \mathbf{A}^+(1:j, j)$, where $\mathbf{P}(1:j, 1:j)$ is the top left square submatrix of $\mathbf{P}$. Because $\mathbf{A}^+$ is lower triangular, the fragment $\mathbf{A}^+(1:j, j)$ of its jth column contains zeros except for the diagonal element $\mathbf{A}^+(j, j)$. As already mentioned above, the LU decomposition is unique up to diagonal elements of one of the matrices. It means that we can eliminate the equation, corresponding to the jth row of $\mathbf{P}(1:j, 1:j)$ and write the following homogeneous matrix equation:

$$\mathbf{P}(1:j-1, 1:j)\mathbf{A}^-(1:j, j) = \mathbf{0}. \tag{55}$$

This equation allows to compute nonzero elements of the jth column of $\mathbf{A}^-$ as the null space of the rectangular submatrix $\mathbf{P}(1:j-1, 1:j)$. To obtain covariant unit vectors the solutions have to be normalized.

Equation (55) can, in principle, have multiple solutions for $\mathbf{A}^-(1:j, j)$. (In this case the rank of $\mathbf{P}(1:j-1, 1:j)$ is less than $(j-1)$.) As we discussed above, this

ambiguity can occur only due to the degeneracy of the Lyapunov exponents, and we can arbitrarily choose one of the multiple solutions.

As follows from Eq. (46), the adjoint covariant vectors can be computed analogously, using the equation

$$\left(\mathbf{P}^{\mathrm{T}}\right)(1:j-1,1:j)\mathbf{B}^{+}(1:j,j)=\mathbf{0}. \tag{56}$$

Let us now consider the submatrix $\mathbf{P}(1:j,1:j)$. If this is singular, then Eq. (55) provides for the $(j+1)$th column the solution $\mathbf{A}^{-}(1:m,j+1)=\mathbf{A}^{-}(1:m,j)$, i.e., the jth and $(j+1)$th covariant vectors coincide. The inverse is also true, and, hence, the singularity of the submatrix $\mathbf{P}(1:j,1:j)$ is a sufficient and necessary condition for merging of the jth and $(j+1)$th covariant vectors.

As discussed above, the merging of covariant Lyapunov vectors indicates tangencies of invariant manifolds of an attractor that, in particular, occur when the attractor is chaotic and non-hyperbolic (Guckenheimer and Holmes 1983). To detect the violation of hyperbolicity, one usually studies a distribution of angles between expanding and contracting subspaces spanned by corresponding covariant vectors (Lai et al. 1993; Anishchenko et al. 2000; Ginelli et al. 2007; Kuptsov and Kuznetsov 2009). (Another method for a numerical test of hyperbolicity, which does not employ covariant vectors, is based on the so called cone criterion Kuznetsov and Sataev 2007.) Analyzing properties of submatrices of $\mathbf{P}$ one can test for hyperbolicity without explicit computation of covariant vectors. Let the number of positive Lyapunov exponents be k. Moving along a trajectory, we need to compute some characteristic number whose small value indicates the nearness of $\mathbf{P}(1:k,1:k)$ to singularity. It can be, for instance, the determinant or the smallest singular value. A small characteristic number means that the trajectory passes close to the tangency. So, if the distribution of characteristic numbers computed for many trajectory points is well separated from the origin, then the chaos is hyperbolic, and if it approaches the origin violations of hyperbolicity occur.

One can also study the statistics of nearness to singularity of all submatrices $\mathbf{P}(1:j,1:j)$, where $j=1,2,\ldots,m-1$. This can provide detailed information concerning properties of various limit sets embedded in an attractor.

Another way to characterize an attractor is to compute the matrix $\mathbf{D}$ containing cosines of angles between covariant and adjoint covariant vectors. As discussed above, each merged couple of vectors, i.e., each tangency, is represented as a couple of zeros of the corresponding matrix elements. To compute $\mathbf{D}$, first we find the matrix $\mathbf{A}^{-}$, then using Eq. (45) compute only the diagonal elements of $\mathbf{A}^{+}$, and after that compute $\mathbf{B}^{+}$ using Eq. (56). (Though only its diagonal elements are required, we cannot get them without computing the rests of the columns.) Finally, we obtain the elements of $\mathbf{D}$ as products of diagonal elements of $\mathbf{A}^{+}$ and $\mathbf{B}^{+}$; see Eq. (53). Note that it is not required to compute the whole matrix $\mathbf{D}$. The method allows one to find only a few first elements.

Normally, one has to compute the covariant Lyapunov vectors for a series of subsequent points of a trajectory. A practical implementation of the algorithm in this case can be the following. We start the procedure for Lyapunov exponents forward in time including the iterations with $\mathcal{F}(t_1,t_2)$ and QR factorizations, and perform it as long as required for the orthogonal matrices $\mathbf{Q}(t)$ to converge to the matrices of
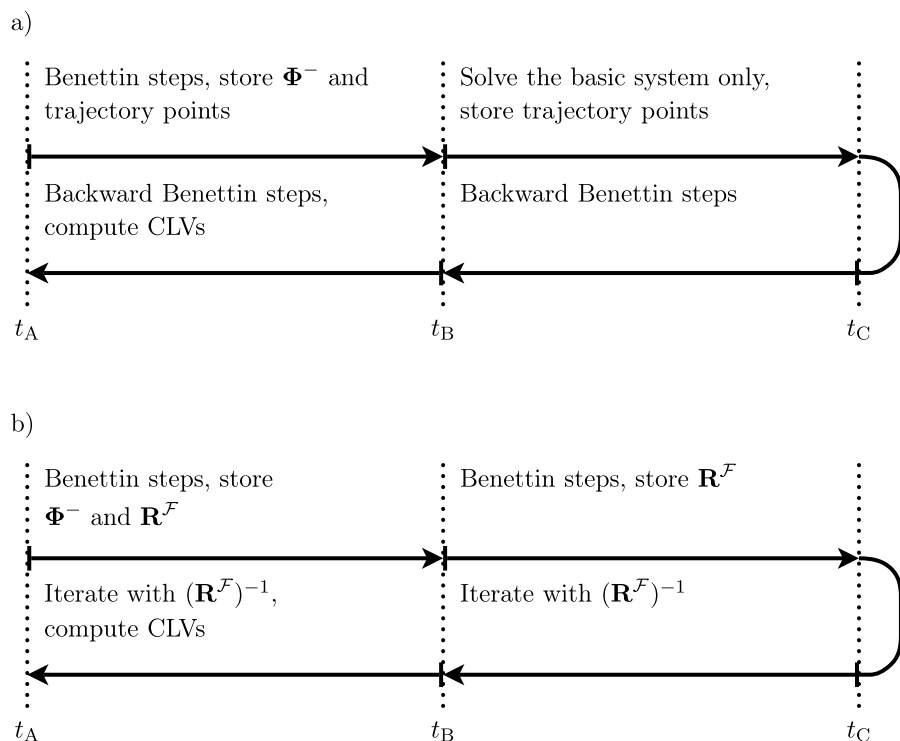
a)

b)

Fig. 4 Computation of covariant Lyapunov vectors (CLVs). (**a**) Method of LU factorization (see Sect. 5.2), and orthogonal complement method of Wolfe and Samelson (see Sect. 5.3). (**b**) Iterative method of Ginelli et al. (see Sect. 5.4)

the backward Lyapunov vectors $\boldsymbol{\Phi}^-(t)$. Denote the end of the preliminary stage as t_A. After this point the iterations are continued, but now we store trajectory points of the basic system and the backward vectors $\boldsymbol{\Phi}^-(t_n)$, see the diagram in Fig. 4(a). The duration of this stage depends on the number of points where we need to know the covariant vectors. At t_B we stop the storing of $\boldsymbol{\Phi}^-(t_n)$ and, moreover, stop the procedure for Lyapunov exponents and continue to solve only the basic system saving the trajectory points. This stage lasts from t_B to t_C. Its duration must be long enough for the subsequent backward procedure to converge. At t_C we start moving back along the saved trajectory performing the backward procedure for Lyapunov exponents including iterations with the adjoint propagator $\mathcal{G}^{-1}$ and QR factorizations. Upon the arrival at t_B we have the forward Lyapunov vectors $\boldsymbol{\Phi}^+(t)$. Now we pass the interval from t_B to t_A given both the backward vectors $\boldsymbol{\Phi}^-(t_n)$ that were saved in the course of the forward pass, and the forward vectors $\boldsymbol{\Phi}^+(t_n)$. These vectors can be used to compute the matrices $\mathbf{A}^-(t_n)$ by means of $\mathbf{P}$ (Eq. (47)), as explained before. In turn, these matrices can be used to find the covariant vectors $\boldsymbol{\Gamma}(t_n)$, according to Eq. (43). Note that it is not necessary to perform this procedure with the whole set of vectors. To compute j first covariant vectors we need j first backward vectors and $j-1$ first

forward vectors. In the appendix we provide a pseudocode implementation of the presented algorithm.

Columns of $\mathbf{A}^-(t_n)$ can also be considered as covariant Lyapunov vectors written with respect to the basis $\mathbf{\Phi}^-(t_n)$. The covariant vectors in the form of $\mathbf{A}^-(t_n)$ have a mutual orientation that is identical to $\mathbf{\Gamma}(t_n)$. Therefore, if for example the angles between covariant Lyapunov vectors are required, they can be computed with respect to columns of $\mathbf{A}^-(t_n)$. This allows us to save some machine time.

The numerical implementation of the described procedure includes well established numerical routines. To perform the forward procedure for Lyapunov exponents, besides of numerically solving the dynamical equations, one also needs to compute QR decompositions. For high-dimensional systems good results are obtained with algorithms based on Householder transformations (Geist et al. 1990; Golub and van Loan 1996). The backward steps may in addition require an interpolation of the stored trajectory to find a solution of variational equations with variable time steps. Finally, each column of $\mathbf{A}^-(t_n)$ is the null space of a corresponding rectangular submatrix of $\mathbf{P}$. One of the most reliable methods of computation of the null space is based on the SVD (Golub and van Loan 1996). The null vector is identified as a right singular vector corresponding to the vanishing singular value. Above we discussed that in principle in the case of degeneracy of Lyapunov exponents one can obtain more than one null vector for one column $\mathbf{A}^-(t_n)$. But exactly identical Lyapunov exponents are unlikely to occur in numerical computations, and, hence, multiple null vectors can (practically) never appear. It means that among right singular vectors we always have a preferable candidate with the smallest singular value.

Implementations of QR decomposition and SVD in Fortran can, for example, be found in the well-known LAPACK library (Anderson et al. 1999). For a C++ implementations we refer to the ALGLIB NET library (Bochkanov and Bystritsky 1999). Also this library provides implementations for many other platforms, such as Delphi and VBA.

5.3 Orthogonal Complement Method of Wolfe and Samelson

One of two first methods for the efficient computation of covariant Lyapunov vectors was suggested by Wolfe and Samelson (2007). Just as the LU method, their approach utilizes the local property of the covariant vectors determined by Eq. (43). This equation can be written for the jth vector as

$$\boldsymbol{\gamma}_j = \sum_{i=1}^{j} \boldsymbol{\varphi}_i^- \alpha_{ij}^-, \tag{57}$$

$$\boldsymbol{\gamma}_j = \sum_{i=j}^{m} \boldsymbol{\varphi}_i^+ \alpha_{ij}^+. \tag{58}$$

As above, the time dependence is not explicitly shown. Equating Eqs. (58) and (57) and multiplying them by $\boldsymbol{\varphi}_k^+$ we can find

$$\alpha_{kj}^+ = \sum_{n=1}^{j} \langle \boldsymbol{\varphi}_k^+ \boldsymbol{\varphi}_n^- \rangle \alpha_{nj}^-. \tag{59}$$

Now we substitute this α_{kj}^+ in Eq. (58) and multiply the resulting equation by $\boldsymbol{\varphi}_k^-$. Taking into account that $\langle \boldsymbol{\varphi}_k^- \boldsymbol{\gamma}_j \rangle = \alpha_{kj}^-$, we obtain

$$\alpha_{kj}^- = \sum_{n=1}^{j} \left(\sum_{i=j}^{m} p_{ik} p_{in} \right) \alpha_{nj}^-, \quad k \le j, \tag{60}$$

where $p_{ik} = \langle \boldsymbol{\varphi}_i^+ \boldsymbol{\varphi}_k^- \rangle$ are elements of the matrix $\mathbf{P}$ (47).

In principle, this equation allows one to compute α_{kj}^- and to find the covariant vectors via Eq. (57). But this straightforward approach is not efficient. To compute the jth covariant vector, the coefficients α_{kj}^- are required, where $k = 1, 2, \ldots, j$. These coefficients depend on $p_{ik} = \langle \boldsymbol{\varphi}_i^+ \boldsymbol{\varphi}_k^- \rangle$, where $i = j, j+1, \ldots, m$. So, we need $m - j + 1$ last vectors $\boldsymbol{\varphi}^+$, and j first vectors $\boldsymbol{\varphi}^-$. The total number is always $m + 1$.

The key idea of Wolfe and Samelson to avoid this obstacle utilizes the orthogonality of $\mathbf{P}$ (Wolfe and Samelson 2007; Samelson and Wolfe 2010). One can obtain the needed subspace spanned by the last $(m - j + 1)$ vectors by taking the orthogonal complement to the subspace of the first $(j - 1)$ vectors. In more detail, columns of $\mathbf{P}$ are orthogonal to each other, i.e., $\sum_{i=1}^{m} p_{ik} p_{in} = \delta_{kn}$, where $\delta_{kn} = 1$ if $k = n$ and 0 otherwise. This sum can be split at $i = j$ as follows:

$$\sum_{i=j}^{m} p_{ik} p_{in} = \delta_{kn} - \sum_{i=1}^{j-1} p_{ik} p_{in}. \tag{61}$$

The sum at the left hand side of this equation includes elements from the last rows of $\mathbf{P}$, while the sum at the right hand side consists of the elements of the first rows. So, the sum in parentheses in Eq. (60) can be substituted as

$$\alpha_{kj}^- = \sum_{n=1}^{j} \left(\delta_{kn} - \sum_{i=1}^{j-1} p_{ik} p_{in} \right) \alpha_{nj}^- = \alpha_{kj}^- - \sum_{n=1}^{j} \left(\sum_{i=1}^{j-1} p_{ik} p_{in} \right) \alpha_{nj}^-.$$

Thus, to compute j unknown coefficients α_{nj}^-, where $n \le j$, we have to solve a set of j linear homogeneous equations,

$$\sum_{n=1}^{j} \left(\sum_{i=1}^{j-1} p_{ik} p_{in} \right) \alpha_{nj}^- = 0 \quad (j = 1, 2, \ldots, m, \; k \le j). \tag{62}$$

(We remind the reader that $\alpha_{nj}^- = 0$ for $n > j$.) Equation (62) was suggested by Wolfe and Samelson to compute $\mathbf{A}^-$. It does not depend on the last rows of $\mathbf{P}$, so that one needs j first backward vectors and $j - 1$ first forward vectors to compute j first covariant vectors.

Later the method of Wolfe and Samelson was modified by Pazó et al. (2008) using the standard approach of computation of the forward and backward Lyapunov vectors, based on QR factorizations and on the backward iterations with the transposed propagator (these ideas were discussed in Sect. 3).

Changing the order of sums in Eq. (62), we can write it in matrix form as

$$\mathbf{P}(1:j-1,1:j)^{\mathrm{T}}\mathbf{P}(1:j-1,1:j)\mathbf{A}^{-}(1:j,j)=0. \tag{63}$$

Compare this equation with Eq. (55). We can see that solutions of Eq. (55) constitute a subset of solutions of Eq. (63). But because we need only one solution at each j, and because our LU method finds such solution, we can conclude that the LU method works in the same way as the Wolfe and Samelson method, avoiding redundant matrix multiplication.

5.4 Backward Iterations, Method of Ginelli et al.

Almost simultaneously with Wolfe and Samelson, Ginelli et al. (2007) suggested a method based on asymptotic properties of covariant vectors (39). The underlying idea of this method was described in the end of Sect. 4, but it cannot be directly implemented. Assume that we have backward Lyapunov vectors at t_1. Theoretically we can initialize $\boldsymbol{v}_j(t_1)$ satisfying Eq. (19), and start the backward iterations using $\mathcal{F}^{-1}$. But in practice, due to numerical noise all these vectors shall belong to $S_m^-(t_1) \setminus S_{m-1}^-(t_1)$, because this set has the largest measure. Hence, these iterations can provide only $\boldsymbol{\gamma}_m$. Due to the same reasons the forward iterations converge to $\boldsymbol{\gamma}_1$. The same is also true for the adjoint propagator.

The key idea of Ginelli et al. is to perform the iterations in the space of projections onto backward Lyapunov vectors $\boldsymbol{\Phi}^-(t)$. For a set of vectors initialized according to Eq. (19), the matrix of projections onto $\boldsymbol{\Phi}^-(t)$ is upper triangular and the iterations converge in the backward time. As follows from Eq. (50), the backward iterations with $\mathcal{F}(t_1,t_2)^{-1}$ in the space of projections onto $\boldsymbol{\Phi}^-(t)$ are equivalent to backward iterations with the upper triangular matrix $\mathbf{R}^{\mathcal{F}}(t_1,t_2)^{-1}$. This mapping preserves the triangular structure of the matrix of projections, and we can perform as many backward iterations as we need always staying within subspaces $S_j^-(t_1) \setminus S_{j-1}^-(t_1)$. In other words, any upper triangular matrix iterated backward in time with $\mathbf{R}^{\mathcal{F}}(t_1,t_2)^{-1}$ converges to $\mathbf{A}^-(t)$. Note that, since the subspaces $S_j^-(t)$ are spanned by the first j backward Lyapunov vectors, we are allowed to compute only j first covariant vectors without computing the rest of them.

In a similar way we can compute the first j adjoint covariant vectors, using the forward-time asymptotic (24). We start the procedure moving backward in time with the transposed propagator and computing forward Lyapunov vectors as described in Sect. 3. The triangular matrices $\mathbf{R}^{\mathcal{G}}(t_1,t_2)$ have to be stored. Then we turn round and start forward iterations $\mathbf{R}^{\mathcal{G}}(t_n,t_{n+1})^{-1}\mathbf{B}(t_n)=\mathbf{B}(t_{n+1})[\mathbf{C}^{\mathcal{G}}(t_n,t_{n+1})]^{-1}$ that converge to $\mathbf{B}^+(t)$.

A practical implementation of the method of Ginelli et al. might be the following; see the illustration in Fig. 4(b). First, we perform the procedure for Lyapunov exponents including forward iterations with $\mathcal{F}(t_1,t_2)$ and QR factorizations. This stage is preliminary and it is finished at t_A when we decide that the orthogonal matrices $\mathbf{Q}(t)$ have converged to the matrices of backward Lyapunov vectors $\boldsymbol{\Phi}^-(t)$. Starting from t_A, we continue the procedure, but now all the matrices $\boldsymbol{\Phi}^-(t_n)$ and $\mathbf{R}^{\mathcal{F}}(t_n,t_{n+1})$, see Eq. (31), are stored. This stage continues until t_B. The length of this stage depends on

the number of points where we later want to compute the covariant vectors. After t_B we still proceed with the procedure, but store only $\mathbf{R}^{\mathcal{F}}(t_n, t_{n+1})$. This stage must be sufficiently long to provide the convergence of the subsequent backward procedure and it finishes at t_C. At this point we initialize a set of arbitrary vectors, for which the property (19) is fulfilled. In fact, we just generate a random upper triangular matrix $\mathbf{A}$. Using the stored matrices $\mathbf{R}^{\mathcal{F}}(t_n, t_{n+1})$, we perform the backward iterations on the interval from t_C to t_B:

$$\mathbf{R}^{\mathcal{F}}(t_n, t_{n+1})^{-1}\mathbf{A}(t_{n+1}) = \mathbf{A}(t_n)\mathbf{C}(t_n, t_{n+1})^{-1}, \tag{64}$$

where the diagonal matrix $\mathbf{C}(t_n, t_{n+1})^{-1}$ contains column norms of $\mathbf{A}$. If $t_C - t_B$ is sufficiently large, $\mathbf{A}(t_n)$ converges to $\mathbf{A}^-(t_n)$. Now we pass the stage from t_B to t_A computing the covariant Lyapunov vectors via Eq. (43) and using them as we need. Note that this procedure allows one to compute not only the whole set of m covariant vectors, but also as many of them as we want.

As we already mentioned above, the columns of $\mathbf{A}^-(t_n)$ can also be considered as covariant Lyapunov vectors, so that in some cases it is enough to consider these vectors without computation of $\mathbf{\Gamma}(t_n)$. In this case the matrices $\mathbf{\Phi}^-(t_n)$ do not have to be stored.

The algorithm of backward iterations can suffer from ill-conditioned $\mathbf{R}^{\mathcal{F}}$, which manifests itself if one computes many (i.e., not just a few first) covariant Lyapunov vectors for a system with strong contraction. Typically, high-dimensional chaotic dissipative systems have several positive Lyapunov exponents of moderate magnitude while negative exponents can have large absolute values. Because logarithms of diagonal elements of $\mathbf{R}^{\mathcal{F}}$ are proportional to local Lyapunov exponents, they can be sufficiently small. So, if a lot of covariant vectors corresponding to negative Lyapunov exponents are computed, the diagonal elements of $\mathbf{R}^{\mathcal{F}}$ can become small, and the whole matrix $\mathbf{R}^{\mathcal{F}}$, whose determinant is the product of its diagonal elements, can potentially be ill-conditioned. In turn this can influence the accuracy of computations.

To avoid or at least minimize this problem one should first try to decrease the interval between QR orthogonalizations. Another, also almost obvious recommendation is not to employ Eq. (64) as it is, but compute iterations implicitly. Note that the implicit method is preferable regardless of the presence of ill-conditioned $\mathbf{R}^{\mathcal{F}}$. Namely, nonzero elements of the ith column of $\mathbf{A}(t_n)$ can be computed as a solution of equation

$$\mathbf{R}^{\mathcal{F}}(1:i, 1:i)\mathbf{A}_n(1:i, i) = \mathbf{A}_{n+1}(1:i, i), \tag{65}$$

where $\mathbf{R}^{\mathcal{F}}(1:i, 1:i)$ is a top left submatrix of $\mathbf{R}^{\mathcal{F}}$ and $\mathbf{A}_n(1:i, i)$ top fragment of the ith column of $\mathbf{A}(t_n)$. Computed in this way $\mathbf{A}_n(:, i)$ then has to be normalized. We see that the ith column of $\mathbf{A}(t_n)$ is influenced only by the submatrix $\mathbf{R}^{\mathcal{F}}(1:i, 1:i)$ that remains well-conditioned until i is sufficiently small. It means that even if $\mathbf{R}^{\mathcal{F}}$ has some small diagonal elements, errors that they can produce are not spread along the whole spectrum, but influence only minor covariant vectors from its right part.

When the trajectory passes close to tangencies of invariant manifolds of an attractor, $\mathbf{A}(t_n)$ becomes ill-conditioned, i.e., small values can appear on its diagonal. Because $\mathbf{A}(t_n)$ is used to compute $\mathbf{A}(t_{n-1})$, small values can accumulate and vanish

due to the numerical underflow. Then the zeros will be preserved in the course of iterations even if the trajectory goes far from the tangency points. This false indication of an exact tangency can be cured by adding a small amount of noise to the diagonal elements.

5.5 Comparison of the Methods

Computation of covariant vectors requires saving of intermediate matrices. We estimate the amount of the required memory for the "worst" case when the whole set of m covariant vectors is computed. Let K_{AB} be the number of trajectory points where we are going to compute covariant vectors, i.e., the number of steps in the stage AB in Fig. 4. It is reasonable to assume that this value depends on m, $K_{AB} = K_{AB}(m)$, where m is the dimension of the phase space. Denote the number of steps in the transient stage BC by K_{BC}. The convergence of columns of matrices to their asymptotic form during the transient stage is exponential with rates equal to differences between corresponding Lyapunov exponents (Wolfe and Samelson 2007). For extensive chaotic systems these differences are proportional to $1/m$; thus, the convergence time is proportional to m. Altogether, the length of the transient stage can be estimated as $K_{BC} = k_{BC}m$, where k_{BC} is an empirical constant, which depends on the particular system under consideration.

For the LU method, Sect. 5.2, and for the method of orthogonal complement, Sect. 5.3, the estimates are identical. Namely, we need K_{AB} matrices $\mathbf{\Phi}^-$, each of the size m^2, and $K_{AB} + K_{BC}$ trajectory vectors of the size m; see Fig. 4(a). Hence, the total amount of memory (in bytes) is $B_{LU} = (m^2(K_{AB}(m) + k_{BC}) + mK_{AB}(m))b$, where b is the number of bytes required to store one real number. For large m we have

$$B_{LU} \approx m^2 K_{AB}(m)b. \tag{66}$$

For example if the dimension is $m = 100$ and we want to compute $K_{AB} = 1000$ covariant vectors using double precision numbers, i.e., $b = 8$, we need $B_{LU} \approx 76$ megabytes.

For the method of backward iterations, Sect. 5.4, we need to save $K_{AB} + K_{BC}$ triangular matrices $\mathbf{R}^{\mathcal{F}}$, each of the size $(m^2 + m)/2$, and K_{AB} matrices $\mathbf{\Phi}^-$ of the size m^2, see Fig. 4(b). The total amount of memory can be estimated as $B_{BI} = (m^2(3K_{AB}(m) + k_{BC}m) + m(K_{AB}(m) + k_{BC}m))b/2$. Keeping only the leading terms for large m we obtain

$$B_{BI} \approx m^2(3K_{AB}(m) + k_{BC}m)b/2. \tag{67}$$

For the same numerical values as in the example for LU method and at $k_{BC} = 1$ we obtain, though higher, but close estimate: $B_{BI} \approx 118$ megabytes. Note, however, that the amount of memory for the transient stage grows with m as $k_{BC}m^3b/2$ for the backward iterations method, while for two other methods it grows as $k_{BC}m^2b$. Hence, the efficient application of the backward iterations requires closer attention to the minimization of the transient stage length, otherwise, one can easily exhaust the available memory.

In principle, all methods may suffer from a shortage of memory. One possible way to handle this problem is to save intermediate data to binary files. The disadvantage of this approach is deceleration of computations due to the slowness of file operations. Alternatively, see Ginelli et al. (2007), instead of keeping all necessary matrices moving forward in time, one can periodically (and sufficiently seldom to fit in the available memory) save snapshots of the procedure for Lyapunov exponents (i.e., the trajectory points of the basic system together with corresponding matrices $\boldsymbol{\Phi}^-$). Then, moving backward, one periodically uses these snapshots to recompute forward steps and obtain missing data. Of course, this approach also slows down the computations, now due to the recomputations. To choose the preferable way one has to compare the average time for writing to file and subsequent reading of one matrix with the time needed to recompute it. The result of the comparison depends on the particular computer system. Note also that, using the method of backward iterations, one can reduce the memory consumption if only the angles between covariant vectors are needed. As we already mentioned in Sect. 5.2, the triangle matrices $\mathbf{A}^-$ are suitable for finding the angles, and hence, in this case one does not need to save matrices $\boldsymbol{\Phi}^-$.

Let us estimate the computation speed of the methods presented (the straightforward intersection of the Oseledec subspaces is not taken into account). If all the methods have enough memory to avoid either using files or performing recomputing, the backward iterations are the fastest. Local methods of LU factorization and orthogonal complement loose the race on the backward stage B-A, see Fig. 4. Each iteration is simultaneously a time step and also a computation of the covariant vectors. The time steps for local methods are performed via the procedure for Lyapunov exponents and also some time is required to compute the covariant vectors.

6 Examples

6.1 System with Constant Jacobian Matrix

Consider a system with a constant Jacobian matrix

$$\mathbf{J} = \begin{pmatrix} 1 & -2 & 0 \\ 0 & -1 & 0 \\ 0 & 2 & -3 \end{pmatrix}. \tag{68}$$

Since $\mathbf{J}$ is time-independent and has real eigenvalues, the Lyapunov exponents for this system simply coincide with the magnitude of its eigenvalues, $\lambda_{1,2,3} = 1, -1, -3$. The corresponding eigenvectors are simultaneously the covariant Lyapunov vectors, and the eigenvectors of $(-\mathbf{J}^\mathrm{T})$ are the adjoint covariant vectors:

$$\boldsymbol{\Gamma} = \begin{pmatrix} 1 & \sqrt{1/3} & 0 \\ 0 & \sqrt{1/3} & 0 \\ 0 & \sqrt{1/3} & 1 \end{pmatrix}, \qquad \boldsymbol{\Theta} = \begin{pmatrix} \sqrt{1/2} & 0 & 0 \\ -\sqrt{1/2} & 1 & -\sqrt{1/2} \\ 0 & 0 & \sqrt{1/2} \end{pmatrix}. \tag{69}$$

$\mathbf{D} = \mathbf{\Theta}^T\mathbf{\Gamma} = \mathrm{diag}[\sqrt{1/2}, \sqrt{1/3}, \sqrt{1/2}]$. The propagator reads

$$\mathcal{F}(t_1, t_2) = \mathbf{\Gamma}\mathbf{L}\mathbf{\Gamma}^{-1} = \begin{pmatrix} e^\tau & e^{-\tau}(1 - e^{2\tau}) & 0 \\ 0 & e^{-\tau} & 0 \\ 0 & e^{-3\tau}(e^{2\tau} - 1) & e^{-3\tau} \end{pmatrix}, \tag{70}$$

where $\tau = t_2 - t_1$, and $\mathbf{L} = \mathrm{diag}[e^{\lambda_1 \tau}, e^{\lambda_2 \tau}, e^{\lambda_3 \tau}]$. Forward and backward Lyapunov vectors can be computed as eigenvectors of far-future and far-past operators, respectively, directly from Eqs. (13) and (14) (finding the limits one has to keep constant norms of vectors):

$$\mathbf{\Phi}^- = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{1/2} & -\sqrt{1/2} \\ 0 & \sqrt{1/2} & \sqrt{1/2} \end{pmatrix}, \qquad \mathbf{\Phi}^+ = \begin{pmatrix} \sqrt{1/2} & \sqrt{1/2} & 0 \\ -\sqrt{1/2} & \sqrt{1/2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{71}$$

Note that in accordance with Eq. (43) the first backward vector $\{1, 0, 0\}$ and the last forward Lyapunov vector $\{0, 0, 1\}$ coincide with the first and the last covariant vectors, i.e., with eigenvectors of $\mathbf{J}$. One can also check that the logarithms of eigenvalues of the limit operators, i.e., the Lyapunov exponents, indeed coincides with the magnitude of the eigenvalues of $\mathbf{J}$. The matrix $\mathbf{P}$, as defined by Eq. (47), reads

$$\mathbf{P} = \begin{pmatrix} \sqrt{1/2} & -1/2 & 1/2 \\ \sqrt{1/2} & 1/2 & -1/2 \\ 0 & \sqrt{1/2} & \sqrt{1/2} \end{pmatrix}. \tag{72}$$

To compute covariant vectors via the LU method, we have to find the matrix $\mathbf{A}^-$. As follows from Eq. (55), the first column of this matrix is always $\{1, 0, 0\}$ while for the other elements we have $a_{12}^-/\sqrt{2} - a_{22}^-/2 = 0$, $a_{13}^-/\sqrt{2} - a_{23}^-/2 + a_{33}^-/2 = 0$, and $a_{13}^-/\sqrt{2} + a_{23}^-/2 - a_{33}^-/2 = 0$. For the matrix $\mathbf{B}^+$, needed to compute the adjoint covariant vectors, we construct equations according to Eq. (56) using $\mathbf{P}^T$: $b_{12}/\sqrt{2} + b_{22}/\sqrt{2} = 0$, $b_{13}/\sqrt{2} + b_{23}/\sqrt{2} = 0$, $-b_{13}/2 + b_{23}/2 + b_{33}/\sqrt{2} = 0$. Both of these equation sets have to be solved with the additional requirement of unit column norms:

$$\mathbf{A}^- = \begin{pmatrix} 1 & \sqrt{1/3} & 0 \\ 0 & \sqrt{2/3} & \sqrt{1/2} \\ 0 & 0 & \sqrt{1/2} \end{pmatrix}, \qquad \mathbf{B}^+ = \begin{pmatrix} 1 & -\sqrt{1/2} & 1/2 \\ 0 & \sqrt{1/2} & -1/2 \\ 0 & 0 & \sqrt{1/2} \end{pmatrix}. \tag{73}$$

One can check that Eqs. (43) and (44) are fulfilled, i.e., $\mathbf{\Gamma} = \mathbf{\Phi}^-\mathbf{A}^-$ and $\mathbf{\Theta} = \mathbf{\Phi}^+\mathbf{B}^+$.

The method of Wolfe and Samelson does essentially the same job. Computing $\mathbf{A}^-$ we have to multiply submatrices of $\mathbf{P}$ by the transposed submatrices and construct equations; see Eq. (63). Similarly one can get $\mathbf{B}^+$ and verify that the results coincide with Eq. (73).

For the method of Ginelli et al. we find $\mathbf{R}^{\mathcal{F}}(t_1, t_2) = [\mathbf{\Phi}^-]^T\mathcal{F}(t_1, t_2)\mathbf{\Phi}^-$; see Eq. (31). Since the iterations (64) converge in backward time, consider $\mathbf{R}^{\mathcal{F}}(t_1, t_2)^{-1}$:

$$\mathbf{R}^{\mathcal{F}}(t_1, t_2)^{-1} = \begin{pmatrix} e^{-\tau} & (e^\tau - e^{-\tau})/\sqrt{2} & (e^{-\tau} - e^\tau)/\sqrt{2} \\ 0 & e^\tau & e^{3\tau} - e^\tau \\ 0 & 0 & e^{3\tau} \end{pmatrix}. \tag{74}$$

Fig. 5 Attractor of the
generalized Hénon map
Eq. (75). *Dark (red) colors*
indicate closeness to homoclinic
tangencies (Color figure online)
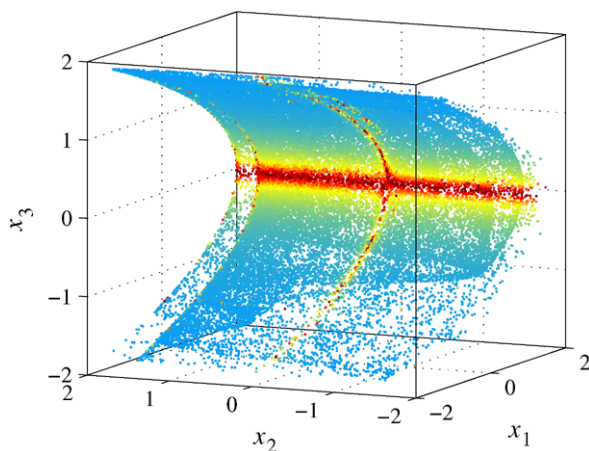
As follows from Eq. (64), at $\tau \to \infty$ the column norms of $\mathbf{R}^{\mathcal{F}}(t_1, t_2)^{-1}$ have to grow as $e^{-\lambda_i \tau}$. Indeed, it can be checked that the column norms of this matrix are asymptotically dominated by the terms $e^{-\tau}$, e^{τ}, and $e^{3\tau}$, respectively. If we normalize columns to the unit, the elements of this matrix converge to $\mathbf{A}^-$, see Eq. (73), i.e., we again obtain the covariant vectors.

6.2 Generalized Hénon Map

As a second example we consider a generalized three-dimensional Hénon map (Baier and Klein 1990):

$$
\begin{aligned}
x_1^{n+1} &= a - \left[x_2^n\right]^2 - b x_3^n, \\
x_2^{n+1} &= x_1^n, \\
x_3^{n+1} &= x_2^n.
\end{aligned}
\tag{75}
$$

For $a = 1.76$ and $b = 0.1$ this system generates a hyperchaotic attractor with Lyapunov exponents $\lambda_1 = 0.225$, $\lambda_2 = 0.188$, and $\lambda_3 = -2.716$. Figure 5 shows the chaotic attractor, where the color of the points corresponds to $\det[\mathbf{P}(1:2, 1:2)]$ (see Sect. 5.2). Dark (red) colors indicate locations of the attractor where (almost) tangent CLVs occur and the submatrix $\mathbf{P}(1:j, 1:j)$ with $j = 2$ is (almost) singular.

7 Conclusion

We presented an extensive description of modern achievements of Lyapunov analysis. The Lyapunov exponents, the forward and backward Lyapunov vectors as well as covariant Lyapunov vectors were discussed in detail.

The systematic approach allowed us to reveal a symmetry in the structure of the tangent space and to introduce the concept of adjoint covariant vectors. There are tangent linear propagators that can be characterized by left and right singular vectors. When the propagators are considered on asymptotically growing time intervals

these singular vectors converge to backward and forward Lyapunov vectors. One can also define adjoint propagators that are associated with the same singular vectors, but have reciprocal singular values. The backward and forward Lyapunov vectors can be used as frameworks for two sets of Oseledec subspaces and for two adjoint Oseledec subspaces that are orthogonal to the Oseledec subspaces. The main feature of these subspaces is the covariance with the tangent dynamics: the propagator maps each Oseledec subspace onto the corresponding Oseledec subspace associated with the image point of the trajectory, and the adjoint propagator does the same with the adjoint subspaces. Within these subspaces one can find vectors with the same property of covariance. There are covariant Lyapunov vectors whose exponential growth under the action of the propagators is characterized by Lyapunov exponents, and there are also adjoint covariant Lyapunov vectors that grow under the action of adjoint propagators with Lyapunov exponents of opposite signs.

The adjoint covariant vectors are not independent characteristic vectors, because in principle one can always compute them using the original covariant Lyapunov vectors. Important are the norm-independent angles between corresponding covariant and adjoint vectors. They provide a compact representation of the information provided by covariant vectors. In particular, homoclinic tangencies between stable and unstable manifolds (characteristic for non-hyperbolic chaos) are indicated by orthogonality of corresponding original and adjoint vectors.

An important result of our detailed analysis is an efficient method for computing covariant Lyapunov vectors. The basic idea of the method is an optimized LU decomposition of the matrix $\mathbf{P}$ consisting of scalar products of forward and backward Lyapunov vectors. Our approach is very close to the method by Wolfe and Samelson (2007), but its advantages are a more transparent explanation, and the explicit formulation of the matrix $\mathbf{P}$ which is interesting by itself. Moreover our approach is slightly more efficient because we avoid some redundant computations.

Using the matrix $\mathbf{P}$, we present a method for detecting non-hyperbolicity of chaotic dynamics without explicit computation of the covariant vectors. In brief, the violation indicator is the singularity of a $j \times j$ submatrix of $\mathbf{P}$, where j is the number of positive Lyapunov exponents. The chaotic dynamics is non-hyperbolic if, moving along a trajectory, we encounter nearly singular submatrices.

In presence of degenerate Lyapunov exponents all types of Lyapunov vector are not unique. We provide an analysis of this case. As for the forward and backward Lyapunov vectors, the standard algorithms can be used without modifications. Selection of an orthogonal initial matrix eliminates the ambiguity. Starting from different seed matrices, we can obtain different sets of vectors, but any one of them is appropriate. Moreover, in practical computations the degeneracy of the Lyapunov exponents manifests itself very weakly, especially for systems of high dimension. Typically, due to numerical errors all computed exponents are distinct, and one cannot identify degenerated exponents just by examining the computed spectrum. The same is true for the covariant vectors. Theoretically the degeneracy of the Lyapunov exponents can result in multiple sets of covariant vectors, but in practice the computations can be organized in a such way that one always obtains a unique appropriate solution, regardless of the degeneracy.

Appendix: Pseudocode for the LU Method

Input: `nclv`, number of computed covariant Lyapunov vectors; `nstore`, number of trajectory points where the covariant vectors are computed; `m`, dimension of the tangent space; `dt`, time interval between orthogonalizations (normally, a multiple of time discretization step); `nspend_att`, `nspend_fwd`, `nspend_bkw`, steps to converge to the attractor, forward and backward vectors, respectively.

Subroutines: `solve_bas()`, solving of the basic system; `solve_lin_fwd()`, `solve_lin_trp()`, action of forward and transposed propagators, respectively (see Sect. 3); `null_vect()`, computing a null vector (in the case of multiple solutions, an arbitrary null vector can be taken); `orthog()`, QR-orthogonalization (matrix **R** is abandoned); `transpose()`, transpose of a matrix; `random()`, generate random matrix or vector; `A.B`, multiplication of matrices `A` and `B`.

Result: `Gamma`, array of `nstore` matrices `m` by `nclv`, whose columns are the covariant Lyapunov vectors

```
BEGIN clv_lu
  // *** ARRIVE AT THE ATTRACTOR ***
  CREATE u[1:m]=random(1,m)
  u=solve_bas(u,dt*nspend_att)
  // *** PRELIMINARY STAGE ***
  CREATE Q[1:m][1:nclv]=random(1,m,1,nclv)
  Q=orthog(Q)
  FOR i=1 TO nspend_fwd
    Q=solve_lin_fwd(Q,u,dt)
    Q=orthog(Q)
    u=solve_bas(u,dt)
  NEXT i
  // *** STAGE A-B ***
  CREATE PhiMns[1:nstore][1:m][1:nclv]
  CREATE traj[1:nstore+nspend_bkw][1:m]
  FOR i=1 TO nstore
    Q=solve_lin_fwd(Q,u,dt)
    Q=orthog(Q)
    u=solve_bas(u,dt)
    traj[i]=u
    PhiMns[i]=Q
  NEXT i
  // *** STAGE B-C ***
  FOR i=1 TO nspend_bkw
    u=solve_bas(u,dt)
```

```
      traj[nstore+i]=u
    NEXT i
    // *** STAGE C-B ***
    // Now we use one column less
    RECREATE Q[1:m][1:nclv-1]=random(1,m,1,nclv-1)
    Q=orthog(Q)
    // We leave this cycle at the (nstore+1)-th trajectory
    // point!
    FOR i=nspend_bkw TO 2 STEP -1
      u=traj[nstore+i]
      Q=solve_lin_trp(Q,u,dt)
      Q=orthog(Q)
    NEXT i
    // *** STAGE B-A ***
    CREATE P[1:nclv-1][1:nclv]
    CREATE Gamma[1:nstore][1:m][1:nclv]
    CREATE a[1:nclv]
    // We come into this cycle being at the (nstore+1)-th
    // point and take traj[i+1], but not traj[i].
    FOR i=nstore TO 1 STEP -1
      u=traj[i+1]
      Q=solve_lin_trp(Q,u,dt)
      Q=orthog(Q)
      P=transpose(Q).PhiMns[i]
      Gamma[i][1:m][1]=PhiMns[i][1:m][1]
      FOR j=2 TO nclv
        a[1:j]=null_vect(P[1:j-1][1:j])
        Gamma[i][1:m][j]=PhiMns[i][1:m][1:j].a[1:j]
      NEXT j
    NEXT i
END
```

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