Periodic Orbits, Lyapunov Vectors, and Singular Vectors in the Lorenz System

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ABSTRACT

Some theoretical issues related to the problem of quantifying local predictability of atmospheric flow and the generation of perturbations for ensemble forecasts are investigated in the Lorenz system. A periodic orbit analysis and the study of the properties of the associated tangent linear equations are performed.

In this study a set of vectors are found that satisfy Oseledec theorem and reduce to Floquet eigenvectors in the particular case of a periodic orbit. These vectors, called Lyapunov vectors, can be considered the generalization to aperiodic orbits of the normal modes of the instability problem and are not necessarily mutually orthogonal.

The relation between singular vectors and Lyapunov vectors is clarified, and transient or asymptotic error growth properties are investigated. The mechanism responsible for super-Lyapunov growth is shown to be related to the nonorthogonality of Lyapunov vectors.

The leading Lyapunov vectors, as defined here, as well as the asymptotic final singular vectors, are tangent to the attractor, while the leading initial singular vectors, in general, point away from it. Perturbations that are *on the attractor* and maximize growth should be considered in meteorological applications such as ensemble forecasting and adaptive observations. These perturbations can be found in the subspace of the leading Lyapunov vectors.

1. Introduction

Recent improvements in the skill of weather prediction models have been supported by the parallel development of applied predictability theory. It has long been recognized that the a priori reliability of a forecast is an extremely variable function of the initial state, related to the local divergence of trajectories. A key question is how to quantify, locally in phase space, the flow's predictability. Furthermore, not all perturbations grow at the same rate, at least during an initial transient phase. The natural approach to the problem of estimating the average divergence consists in forecasting the skill from the spread of an ensemble of initial perturbations. Since a true Monte Carlo approach requires large ensembles and hence is impractical, the selection of perturbations to be used in small-ensemble forecasts has become an extremely important and debated issue in numerical weather prediction (Szunyogh et al. 1997; Molteni et al. 1996). The goals of ensemble prediction are improving the final forecast and estimating its reliability (Houtekamer and Derome 1995).

Ensemble prediction systems developed at the major operational forecasting centers are founded basically upon two different approaches. The first one, adopted among others at ECMWF (Molteni and Palmer 1993; Mureau et al. 1993), relies upon the construction of the most rapidly growing perturbations over the optimization time, as described by the singular vectors of the error matrix, corresponding to the largest singular values. The second one, implemented at NMC (now the National Centers for Environmental Prediction) and known as the ''bred grown modes'' method (Toth and Kalnay 1993) is aimed, in principle, at determining the perturbations that grow fastest asymptotically, the leading Lyapunov vectors.

It is well known that, for a stationary solution, singular vectors describe amplifying disturbances that, over the optimization time, can exceed normal-mode growth if the eigenvectors are not orthogonal (Farrell 1988, 1990; Lacarra and Talagrand 1988). The theoretical foundations necessary to apply these concepts to a chaotic system, such as we currently envisage an atmospheric model to be, are not well established.

It is the main goal of the present work to give a suitable definition of Lyapunov vectors that can be considered the generalization to aperiodic orbits of normal modes. These are not expected, in general, to be mutually orthogonal.

Growth rates larger than predicted by the first Lyapunov exponent have been documented in the literature, but the underlying mechanism is controversial (Trevisan and Legnani 1995; Nicolis et al. 1995). Nonorthogonality of the vectors associated with asymptotic growth rates given by the Lyapunov exponents has been in-

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voked as a possible mechanism for super-Lyapunov growth. However, the methods used to compute Lyapunov exponents are based on definitions of mutually orthogonal vectors, commonly referred to as Lyapunov vectors (Lorenz 1965; Benettin et al. 1976, 1980; Shimada and Nagashima 1979).

In the present study, starting from the relationship between Floquet eigenvectors and singular vectors, with varying optimization times, a theoretical explanation for the time-dependent behavior of phase space average error growth is provided.

After applying these concepts to periodic orbits in the Lorenz (1963) model, we extend the analysis to aperiodic orbits, giving a definition of Lyapunov vectors that coincides with that of Floquet eigenvectors in the periodic case.

In the Lorenz model, these vectors have nonzero projection on one another. It is shown that transient super-Lyapunov growth is accounted for by their nonorthogonality.

The relation of these vectors to the local attractor structure is also examined.

2. The Lorenz system: Periodic orbit analysis

In the present section we summarize some of the properties and results concerning periodic orbits of the Lorenz system. Periodic orbits are dense on a forced–dissipative system's attractor; that is, an unstable periodic orbit of arbitrarily large period can always be found arbitrarily close to any aperiodic orbit (Lichtenberg and Lieberman 1983). Furthermore, it has been shown that for hyperbolic systems, that is, for systems where the local, linear exponents of error evolution are either negative or positive and uniformly bounded away from zero, physically relevant invariant measures on the attractor can be computed as averages over a selected sequence of periodic orbits. The rapid convergence of the expression for these averages ensures good accuracy even for a small number of such orbits (Cvitanović 1991). Eckhardt and Ott (1994) applied this method to the Lorenz system, at the standard parameter values, to compute, among other quantities, the average Lyapunov exponent. Convergence to a very accurate estimate for the first Lyapunov exponent of the flow, computed from very long integrations, is obtained from orbits recurrent after a small number of iterations of the Poincaré map. Therefore, the study of the stability of periodic orbits is a tool to unfold the structure of the whole attractor.

Periodic solutions of the Lorenz (1963) system:

$$\begin{aligned}\dot{X} &= -\sigma X + \sigma Y\\ \dot{Y} &= -XZ + rX - Y\\ \dot{Z} &= XY - bZ,\end{aligned} \tag{1}$$

where $r = 28$, $b = 8/3$, and $\sigma = 10$ can be found, given a sufficiently accurate first guess of the orbit and its period, using a Newton–Raphson scheme on the residual of the return map (Ghil and Tavantzis 1983).

Consider now the stability problem and linearize (1) about a closed orbit to obtain the evolution equations for infinitesimal perturbations $\mathbf{x}(t)$,

$$\dot{\mathbf{x}} = \mathsf{J}(\mathbf{X}(t))\mathbf{x} \tag{2}$$

where $\mathsf{J}(\mathbf{X}(t))$ is the Jacobian, periodic with period T, $\mathbf{X}(t)$ being a closed orbit solution with $\mathbf{X} = (X, Y, Z)$.

In view of Floquet's theorem, a fundamental solution matrix is of the form $\mathsf{Q}(t) = \mathsf{P}(t)e^{\mathsf{R}t}$ (Hartman 1982), where Q, P, and R are matrices and $\mathsf{P}(t)$ is periodic with period T. The eigenvalues of the constant matrix $e^{\mathsf{R}T}$ are $\Lambda_i = e^{\lambda_i T}$, where λ_i are the characteristic exponents of the closed orbit.

For the Lorenz system (1),

$$\mathsf{J}(\mathbf{X}(t)) = \begin{pmatrix} -\sigma & \sigma & 0\\ r - Z(t) & -1 & -X(t)\\ Y(t) & X(t) & -b \end{pmatrix}. \tag{3}$$

Integrating between t_0 and $t_0 + \tau$ one obtains

$$\mathbf{x}(t_0 + \tau) = \mathsf{A}(\mathbf{X}(t_0), \tau)\mathbf{x}(t_0), \tag{4}$$

where A depends upon the values of $\mathbf{X}$ between t_0 and $t_0 + \tau$.

After one period T, the error matrix $\mathsf{A}(\mathbf{X}(t_0), T)$ has real and distinct eigenvalues, $\Lambda_i = e^{\lambda_i T}$, independent of $\mathbf{X}(t_0)$ with $\lambda_1 > 0$, $\lambda_2 = 0$, and $\lambda_3 < 0$. The sum of the characteristic exponents is

$$\sum_{i=1}^{3} \lambda_i = -(\sigma + b + 1).$$

The eigenvectors $\mathbf{e}_i(\mathbf{X}(t))$ are periodic and the eigenvector corresponding to the zero exponent is tangent to the flow. We identify local Lyapunov vectors with unitary vectors in the direction of the Floquet eigenvectors $\mathbf{e}_i$.

Local Lyapunov exponents for the orbit are given by

$$\lambda(\mathbf{e}_i) = \frac{d}{dt}\log\|\mathbf{x}_i\|, \tag{5}$$

where $\mathbf{x}_i$ are infinitesimal perturbations in the direction of the Lyapunov vectors.

The average over one period of the local Lyapunov exponents $\lambda(\mathbf{e}_i)$ is given by the characteristic exponents, λ_i.

3. Singular vectors: Basic formalism

In the present section we review and develop the stability analysis applied to the case of a fixed point or periodic solution.

In order to keep the notation simple, in this section we drop any dependence of the matrices on their arguments, keeping in mind that for a periodic orbit A is a function not only of τ, as for a fixed point, but also of $\mathbf{X}(t_0)$ [see (4)]; the eigenvectors $\mathbf{e}_i$ are a function of $\mathbf{X}(t_0)$ as well, and the eigenvalues of $\mathsf{A}(\mathbf{X}(t_0), T)$ are of the form $\Lambda_i = e^{\lambda_i T}$, where $\Lambda_i(T)$ are independent of $\mathbf{X}(t_0)$. For integer multiples, n, of the orbit's period the eigenvectors do not change, whereas the eigenvalues become $\Lambda_i = e^{n\lambda_i T}$.

The transient evolution of infinitesimal perturbations toward their asymptotic directions, given by the eigenvectors of $\mathbf{A}$, is described in terms of its singular vectors (Lorenz 1965, 1984; Yoden and Nomura 1993).

Setting

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Gamma}\mathbf{V}, \tag{6}$$

where $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices and $\boldsymbol{\Gamma}$ is diagonal with elements Γ_i, we have

$$\mathbf{A}\mathbf{A}^{\mathrm{T}}\mathbf{U} = \mathbf{U}\boldsymbol{\Gamma}^2 \tag{7}$$

$$\mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{V}^{\mathrm{T}} = \mathbf{V}^{\mathrm{T}}\boldsymbol{\Gamma}^2, \tag{8}$$

where $(\ )^{\mathrm{T}}$ denotes a transpose.

The initial and final singular vectors are the rows of $\mathbf{V}$ and columns of $\mathbf{U}$, respectively, and satisfy

$$\mathbf{A}\mathbf{V}^{\mathrm{T}} = \mathbf{U}\boldsymbol{\Gamma}. \tag{9}$$

As shown by Lorenz (1965) a sphere is transformed, under $\mathbf{A}$, into an ellipsoid. The eigenvectors $\mathbf{U}_i$ of $\mathbf{A}\mathbf{A}^{\mathrm{T}}$ are an orthonormal set that gives the direction of this ellipsoid's semiaxes, while their length is Γ_i.

Relations between the eigenvalues Γ_i^2 of $\mathbf{H} = \mathbf{A}^{\mathrm{T}}\mathbf{A}$ and the eigenvalues Λ_i and eigenvectors $\mathbf{e}_i$ of $\mathbf{A}$ can be obtained. Writing $\mathbf{A}$ in terms of the diagonal matrix $\boldsymbol{\Lambda}$ with elements Λ_i and the matrix $\mathbf{E}$ whose columns are the eigenvectors $\mathbf{e}_i$,

$$\mathbf{A} = \mathbf{E}\boldsymbol{\Lambda}\mathbf{E}^{-1}, \tag{10}$$

we can express $\mathbf{H}$ in terms of these quantities.

The relation between the determinants of $\mathbf{A}$ and $\mathbf{H}$, $\det(\mathbf{H}) = \det(\mathbf{A})\det(\mathbf{A}^{\mathrm{T}})$, in terms of the respective eigenvalues gives

$$\prod_{i=1}^{N} \Gamma_i^2 = \prod_{i=1}^{N} \Lambda_i^2 \tag{11}$$

in N dimensions.

In two dimensions, the determinant and the trace of $\mathbf{H}$ are sufficient to determine the two roots Γ_i of the characteristic equation. The trace of $\mathbf{H}$ is given by

$$\sum_{i=1}^{2} \Gamma_i^2 = \sum_{i=1}^{2} \Lambda_i^2 + \Delta^2, \tag{12a}$$

where

$$\Delta^2 = \frac{(\mathbf{e}_1 \cdot \mathbf{e}_2)^2}{1 - (\mathbf{e}_1 \cdot \mathbf{e}_2)^2}(\Lambda_1 - \Lambda_2)^2. \tag{12b}$$

From (11) and (12) we obtain

$$\Gamma_{1,2}^2 = \frac{\Lambda_1^2 + \Lambda_2^2}{2} + \frac{\Delta^2}{2} \pm \frac{1}{2}\sqrt{(\Lambda_1^2 - \Lambda_2^2)^2 + \Delta^4 + 2\Delta^2(\Lambda_1^2 + \Lambda_2^2)}. \tag{13}$$

When the eigenvectors are orthogonal, $\Delta^2 = 0$ and the axes of the ellipsoid are equal in length to Λ_i; otherwise, we have $\Delta^2 > 0$, which implies that, for the major axis, $\Gamma_1 > \Lambda_1$.

Analogously, the root-mean-square error (RMS) is given by the Lorenz index (Lorenz 1965):

$$\mathrm{RMS} = \sqrt{\frac{1}{N}\sum_{i=1}^{N} \Gamma_i^2} \geq \sqrt{\frac{1}{N}\sum_{i=1}^{N} \Lambda_i^2}, \tag{14}$$

where the equal sign is valid only if the eigenvectors are orthogonal, in view of the Δ^2 term in (12).

It should be stressed that (13) and (14) describe transient error growth. In the asymptotic limit the following relations hold:

$$\lim_{t\to\infty} \Gamma_1 = \frac{\Lambda_1}{\sqrt{1 - (\mathbf{e}_1 \cdot \mathbf{e}_2)^2}} \tag{15a}$$

$$\lim_{t\to\infty} \mathrm{RMS} = \frac{\Lambda_1}{\sqrt{2(1 - (\mathbf{e}_1 \cdot \mathbf{e}_2)^2)}}, \tag{15b}$$

where $\Lambda_1 = e^{\lambda_1 t}$ and time is an integer multiple of the period in the periodic orbit case.

The associated asymptotic growth rates are in both cases equal to λ_1. We notice that only if $\Delta^2 > 0$ can growth rates, at some stage, be larger than λ_1.

In previous works, similar behavior has been observed for some chaotic systems, where phase space average growth rates are larger than predicted by the first global Lyapunov exponent. Some results are reviewed in section 5. It has been suggested that this so-called super-Lyapunov growth is due to a mechanism similar to nonmodal growth, being related to the nonorthogonality of eigenvectors. One of the objectives of the present work is to investigate this mechanism in the Lorenz system, with the aid of stability analysis of unstable periodic orbits.

Based on expressions analogous to (12) and (14), Nicolis et al. (1995) concluded that RMS growth rates larger than those given by the largest Lyapunov are obtained under conditions that they considered too restrictive to be realized. Before we apply it to the periodic orbits of the Lorenz system and arrive at firm conclusions about the envisaged mechanism, we have to extend the analysis to the three-dimensional case.

In three dimensions, after some algebra we obtain the following expression for the sum of the squares of the axis lengths, given by the trace of $\mathbf{A}^{\mathrm{T}}\mathbf{A}$:

$$\sum_{i=1}^{3} \Gamma_i^2 = \sum_{i=1}^{3} \Lambda_i^2 + \Delta^2, \tag{16}$$

where

$$\Delta^2 = \frac{1}{[\mathbf{e}_1 \cdot (\mathbf{e}_2 \wedge \mathbf{e}_3)]^2}\{(\Lambda_1 - \Lambda_2)^2(\mathbf{e}_1 \cdot \mathbf{e}_2)[(\mathbf{e}_1 \cdot \mathbf{e}_2) - (\mathbf{e}_1 \cdot \mathbf{e}_2)(\mathbf{e}_2 \cdot \mathbf{e}_3)(\mathbf{e}_1 \cdot \mathbf{e}_3)] + (\Lambda_1 - \Lambda_3)^2(\mathbf{e}_1 \cdot \mathbf{e}_3) \times [(\mathbf{e}_1 \cdot \mathbf{e}_3) - (\mathbf{e}_1 \cdot \mathbf{e}_2)(\mathbf{e}_2 \cdot \mathbf{e}_3)(\mathbf{e}_1 \cdot \mathbf{e}_3)] + (\Lambda_2 - \Lambda_3)^2(\mathbf{e}_2 \cdot \mathbf{e}_3)[(\mathbf{e}_2 \cdot \mathbf{e}_3) - (\mathbf{e}_1 \cdot \mathbf{e}_2)(\mathbf{e}_2 \cdot \mathbf{e}_3)(\mathbf{e}_1 \cdot \mathbf{e}_3)]\} \quad (17)$$

and $(\mathbf{e}_i \wedge \mathbf{e}_j)$ denotes the vector product. Because of the identity

$$[\mathbf{e}_1 \cdot (\mathbf{e}_2 \wedge \mathbf{e}_3)]^2 = 1 - (\mathbf{e}_1 \cdot \mathbf{e}_2)^2 - (\mathbf{e}_1 \cdot \mathbf{e}_3)^2 - (\mathbf{e}_2 \cdot \mathbf{e}_3)^2 + 2(\mathbf{e}_1 \cdot \mathbf{e}_2)(\mathbf{e}_1 \cdot \mathbf{e}_3)(\mathbf{e}_2 \cdot \mathbf{e}_3), \quad (18)$$

we know that $\Delta^2 \geq 0$. Nonorthogonality of the eigenvectors again implies a strict inequality. It is also possible to find a characteristic equation for the three-dimensional case in terms of the eigenvalues and eigenvectors of A, but its roots Γ_i cannot be cast in as simple a form as (13).

4. Lyapunov stability

The Floquet eigenvalues and eigenvectors completely describe the asymptotic behavior of perturbations to a periodic orbit. If the orbit is aperiodic or—the orbit being periodic—if the time interval is not equal to a multiple of the period, the eigenvalues and eigenvectors of the stability matrix lose their significance. In the Lorenz system, the Lyapunov spectrum is nondegenerate and the Floquet multipliers are real, whereas the eigenvalues of the stability matrix are complex for arbitrary time intervals.

The existence of Lyapunov exponents and vectors characterizing the stability of aperiodic orbits has been proven by Oseledec (1968) for a large class of dynamical systems and has been used as a working hypothesis in numerical studies of various systems including the Lorenz model (Shimada and Nagashima 1979; Lorenz 1984).

The result is that, for almost every initial point $\mathbf{X}(t)$, there exists a set of vectors, $\mathbf{e}_i$, $1 < i < N$ such that

$$\lambda_i = \lim_{\tau\to\infty} \frac{1}{\tau} \log\|\mathsf{A}(\mathbf{t}, \tau)\mathbf{e_i}(\mathbf{t})\|, \quad (19)$$

which means that the limit on the rhs of (19) exists and equals a number λ_i, $1 < i < N$. The numbers λ_i are the Lyapunov exponents and are global properties of the attractor. We will assume that these values are distinct, which is generally the case.

The vectors $\mathbf{e}_i$ in (19) are not unique. We will adopt as a definition of Lyapunov vectors the particular choice of the vectors $\mathbf{e}_i$ that satisfy Oseledec theorem (19) and reduce to the Floquet eigenvectors in the case of a periodic orbit. This definition is based on (20) and (21), given below. Therefore we use the same symbol, $\mathbf{e}_i$, to denote Lyapunov vectors and Floquet eigenvectors. Local Lyapunov exponents, associated to the vectors $\mathbf{e}_i$, can be defined as in (5).

If $\mathbf{X}(t)$ belongs to a periodic orbit, the Floquet eigenvectors not only satisfy (19), but have the desired properties of being independent of the definition of the norm. They are functions of position along the orbit that are invariant by the tangent flow.

Furthermore, since aperiodic orbits can be approximated arbitrarily closely by periodic orbits, it is plausible to assume that the Lyapunov vectors as well as the local Lyapunov exponents of the aperiodic orbit can be approximated with arbitrary accuracy by those of the nearby periodic orbit.

Singular vectors do not have the same properties of Lyapunov vectors and the example of a periodic orbit will clarify differences and mutual relationships. If the optimization time τ equals an integer number n of periods, both initial and final sets of singular vectors converge for n going to infinity and the logarithms of the singular values approach the orbit's Floquet exponents. However, the orthonormal set of initial vectors is transformed into the final set and, except for the particular case when the Floquet eigenvectors are mutually orthogonal, the initial and final sets do not coincide. As a consequence, the vector that has grown at the rate given approximately by λ_i during a given, arbitrarily large, number of periods does not coincide with the vector that will grow at the same rate during future iterations.

These simple considerations illustrate the difficulties that have led to conflicting definitions of Lyapunov vectors. Some authors, in fact, define Lyapunov vectors as the initial set of singular vectors in the limit of infinite time (Goldhirsch et al. 1987; Yoden and Nomura 1993), other authors as the final set (Lorenz 1965, 1984; Shimada and Nagashima 1979). Legras and Vautard (1996) call the former forward and the latter backward Lyapunov vectors. The particular definition has no consequences upon the estimate of global Lyapunov exponents but is crucial for correctly defining local exponents and associated vectors.

We will build upon results relative to periodic orbits to extend the analysis to the case of aperiodic trajectories and find a method to compute Lyapunov vectors in the general case when they are not mutually orthogonal.

The final singular vectors, columns of U, constitute an orthonormal set and, in the limit of infinite time, become independent of the initial perturbed point. For a periodic orbit, the Lyapunov vectors $\mathbf{e}_i$ are the Floquet eigenvectors; setting $t_1 = t_0 + \tau$, $\tau = nT$, and $\mathbf{e}_i = \mathbf{e}_i(t_0) = \mathbf{e}_i(t_1)$, the following relations hold:

$$\mathbf{u}_i^\infty(t_1) = \lim_{(t_1-t_0)\to\infty} \mathbf{u}_i\,(t_0,\, t_1) = \frac{\mathbf{e}_i - \sum_{k<i} (\mathbf{e}_i\cdot\mathbf{e}_k)\mathbf{e}_k}{\|\mathbf{e}_i - \sum_{k<i} (\mathbf{e}_i\cdot\mathbf{e}_k)\mathbf{e}_k\|},$$

$$1 < i < N. \tag{20}$$

Analogously, the initial singular vectors, columns of $\mathbf{V}^{\mathrm{T}}$ are related to $\mathbf{e}_i$ by

$$\mathbf{v}_i^{\mathrm{T}\infty}(t_0) = \lim_{(t_1-t_0)\to\infty} \mathbf{v}_i^{\mathrm{T}}\,(t_0,\, t_1) = \frac{\mathbf{e}_i - \sum_{k>i} (\mathbf{e}_i\cdot\mathbf{e}_k)\mathbf{e}_k}{\|\mathbf{e}_i - \sum_{k>i} (\mathbf{e}_i\cdot\mathbf{e}_k)\mathbf{e}_k\|},$$

$$1 < i < N. \tag{21}$$

The result given by (20) and (21) states that, in the limit of infinite optimization time, the initial singular vectors are obtained by orthogonalizing the $\mathbf{e}_i$ starting from the last one, while the initial vectors are obtained by orthogonalizing the $\mathbf{e}_i$ starting from the first one.

The first k final singular vectors span the same subspace as the first k Lyapunov vectors, whereas the last $N - k + 1$ initial singular vectors span the same subspace as the last $N - k + 1$ Lyapunov vectors. The vectors $\mathbf{e}_i$ can therefore be constructed by intersecting the initial and final families of sets.

When the flow is not periodic, it is still possible to define the family of vectors $\mathbf{e}_i$ by the intersection of the asymptotic initial and final singular vectors referred to the same point. We will apply this method to compute the vectors $\mathbf{e}_i$ for aperiodic orbits in the Lorenz system and show that they can consistently be defined as local Lyapunov vectors.

During the revision process, the authors became aware that the vectors $\mathbf{e}_i$ were independently used by Legras and Vautard (1996), who suggested their application in ensemble prediction. In their study the vectors $\mathbf{e}_i$ are referred to as characteristic vectors.

5. Transient growth and Lyapunov exponents

The average stability properties of a system can be studied by averaging the growth rate of perturbations over an ensemble of initial perturbed states sampled on the attractor according to its natural density.

Evidence supporting the hypothesis that the motion on the attractor of the Lorenz system is ergodic is found in the literature (Lichtenberg and Lieberman 1983). Time average and ensemble average of the first local Lyapunov exponent computed from a long integration of the Lorenz system converge to the same estimate, and the ensemble average is independent of the time interval (Trevisan 1993). This result is a consequence of the property of local Lyapunov vectors being uniquely defined functions of the state vector, $\mathbf{X}(t)$.

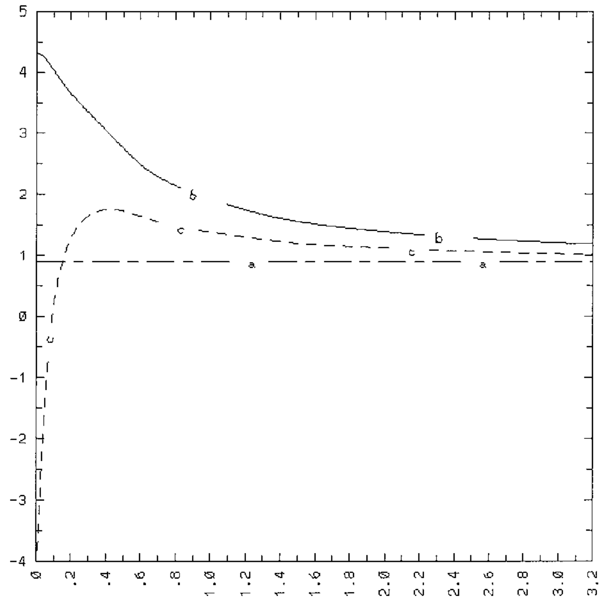

FIG. 1. (a: long–short dash) Global Lyapunov exponent, $\overline{\lambda}_1$; (b: solid) ensemble average growth rate of the most unstable perturbation, $\langle \tau^{-1} \log\Gamma_1(t_k,\, \tau)\rangle$ as a function of optimization time τ; (c: short dash) ensemble average growth rate of the rms error, $\langle \tau^{-1} \log\sqrt{(1/N) \Sigma_{i=1}^N \Gamma_i^2(t_k,\, \tau)}\rangle$. Averages are over the whole attractor phase space. See text for details of computation.

Ensemble average growth rates associated with the singular vectors are instead characterized by transient behavior, documented for some simple systems which include the Lorenz model (Trevisan 1993; Krishnamurty 1993; Trevisan and Legnani 1995; Nicolis et al. 1995).

For subsequent reference, Fig. 1 summarizes previous results (Trevisan and Legnani 1995); the figure shows ensemble average growth rates computed from a long integration of (1) for the most unstable perturbation, $\langle \tau^{-1} \log\Gamma_1(t_k,\, \tau)\rangle$ and for the rms error,

$$\langle \tau^{-1} \log \sqrt{(1/N)\ \Sigma_{i=1}^N\ \Gamma_i^2(t_k,\, \tau)}\rangle,$$

that is, the growth rate associated with the Lorenz index as functions of the optimization time τ. The operator $\langle * \rangle$ indicates average over an ensemble of initial conditions $\mathbf{X}(t_k)$, equally spaced in time along the orbit.

As opposed to Lyapunov exponents, whose ensemble average is constant in time, average growth rates of singular vectors have a time-dependent behavior. Singular vectors are, in fact, functions not only of the initial perturbed state but also of the time of integration, τ. As a consequence of this time dependence, phase–space ensemble averages of growth rates, defined above, are still functions of τ.

Transient error growth is thus related to the evolution of perturbations and in particular of singular vectors toward their asymptotes.

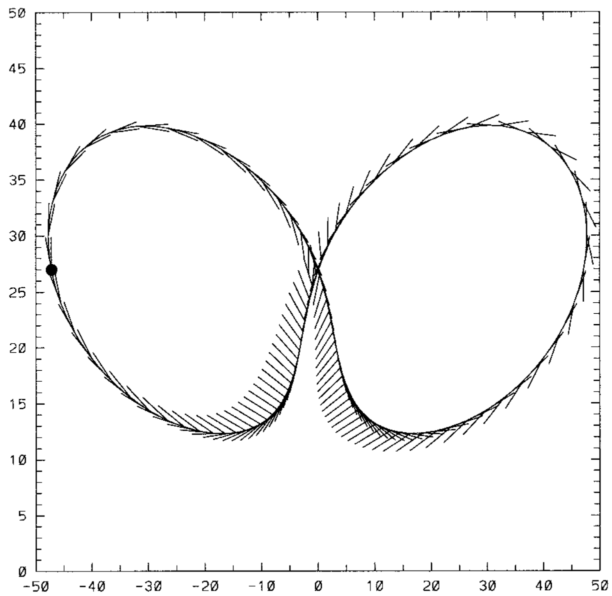

FIG. 2. Periodic orbit $\bar{j}$ and first and second Lyapunov vectors, projected on the plane $x = y$. The second Lyapunov vector, corresponding to the exponent $\lambda_2 = 0$, is tangent to the flow. The orbit's period is $T = 1.558$.

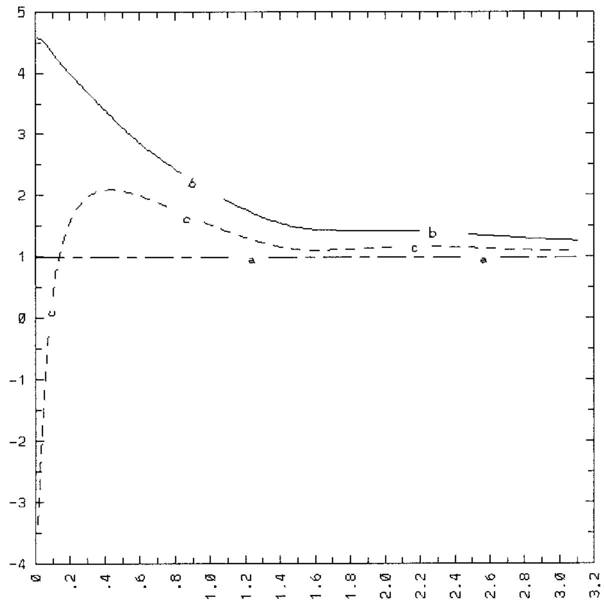

FIG. 3. As in Fig. 1 but averages are computed over the periodic orbit $\bar{j}$ shown in Fig. 2.

6. Numerical results

a. Periodic orbits

Periodic orbits in the Lorenz system are labeled according to the number of turns around one or the other of the fixed points. We refer to Eckhardt and Ott (1994) for details on the symbolic coding of periodic orbits. In their notation, two consecutive turns around the same fixed points are indicated by the symbol n (no jump), and two consecutive turns, the first around one and the second around the other of the fixed points, are indicated by j (jump). The orbit with smallest period takes one turn around each of the fixed points and is coded $\bar{j}$. The Lorenz system is invariant under reflection R in the Z axis, $R(X, Y, Z) = (-X, -Y, Z)$. The orbit corresponding to the coding $\bar{j}$ is symmetric under rotation. If an orbit is not symmetric, as, for example, the one corresponding to the coding $\overline{nj}$, the orbit $R(\mathbf{X}(t))$ with the same coding satisfies the invariance of the equations.

After a periodic orbit, $\mathbf{X}(t)$, $\mathbf{X}(t + T) = \mathbf{X}(t)$ has been located, and Eq. (2) is integrated along the orbit starting from an orthonormal set of initial perturbation vectors to obtain the error matrix $\mathsf{A}(\mathbf{X}(t), \tau)$ (Lorenz 1965). The Floquet eigenvectors $\mathbf{e}_i$ of $\mathsf{A}(\mathbf{X}(t_0), T)$ are computed for an arbitrary $\mathbf{X}(t_0)$ along the orbit. The local Floquet eigenvectors are then computed for the whole orbit from

$$\mathbf{e}_i(t) = \mathbf{e}_i(t_0 + \tau) = \frac{\mathsf{A}(\mathbf{X}(t_0), \tau)\mathbf{e}_i(t_0)}{\|\mathsf{A}(\mathbf{X}(t_0), \tau)\mathbf{e}_i(t_0)\|}.$$

Estimates of the local Lyapunov exponents are then given by

$$\frac{1}{\Delta t} \log\|A(\mathbf{X}(t), \Delta t)\mathbf{e}_i(t)\|,$$

with Δt small.

We also compute the singular values $\Gamma_i(t, \tau)$ and matrices of initial and final singular vectors, $\mathsf{U}(t, \tau)$ and $\mathsf{V}^{\mathrm{T}}(t, \tau)$, for a set of initial states $\mathbf{X}(t)$, equally spaced in time along the periodic orbit, $\mathbf{X}(t) \equiv \mathbf{X}(t_k)$, $t_k = \Delta t$, $2\Delta t, \cdots, T$, and for $0 < \tau < 2T$.

The periodic orbit $\bar{j}$ and its first and second Lyapunov vectors are shown in Fig. 2, in a projection on the plane $X = Y$. Whereas the second Lyapunov vector is, as expected, tangent to the flow, the first Lyapunov vector is not orthogonal to the flow: the vectors have nonzero projection on one another.

The average Lyapunov exponents for this orbit are $\lambda_1 = 0.99$, $\lambda_2 = 0.00$, and $\lambda_3 = -14.66$; these values are very close to the global Lyapunov exponents, $\bar{\lambda}_1 = 0.90$, $\bar{\lambda}_2 = 0.00$, and $\bar{\lambda}_3 = -14.61$ (Trevisan 1993). The sum of the exponents is in good agreement with the value of the divergence of the vector field, $-(\sigma + b + 1) = -(13 + 2/3)$.

Figure 3 illustrates the time dependence of growth rates for the most unstable perturbation and for the rms error averaged over initial states $\mathbf{X}(t_k)$ on the periodic orbit $\bar{j}$. Figures 1 and 3 show a close similarity also during the transient phase: the average growth rate associated with the optimal perturbation for τ small is much larger than λ_1 and monotonically decreases. The average growth rate associated with the Lorenz index is negative for τ small when the negative exponent dominates (14) (see also Mukougawa et al. 1991) and is larger than λ_1 for a limited time interval. This behavior is common to all periodic orbits that we have analyzed

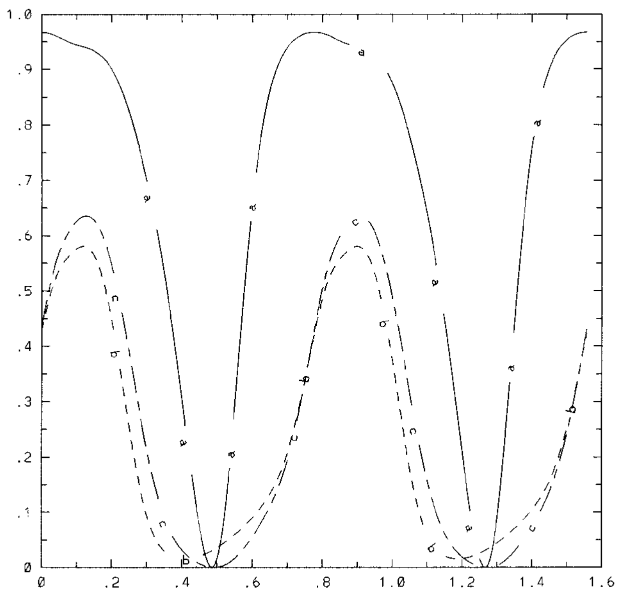

FIG. 4. Scalar products of Lyapunov vectors along the orbit $\bar{j}$. (a: solid) $(\mathbf{e}_1 \cdot \mathbf{e}_2)^2$; (b: short dash) $(\mathbf{e}_1 \cdot \mathbf{e}_3)^2$; (c: long–short dash) $(\mathbf{e}_2 \cdot \mathbf{e}_3)^2$ as a function of time. $\mathbf{X}(t)$ at $t = 0$ is the point of intersection of the orbit with the plane $z = 27$ marked with a dot in Fig. 2.

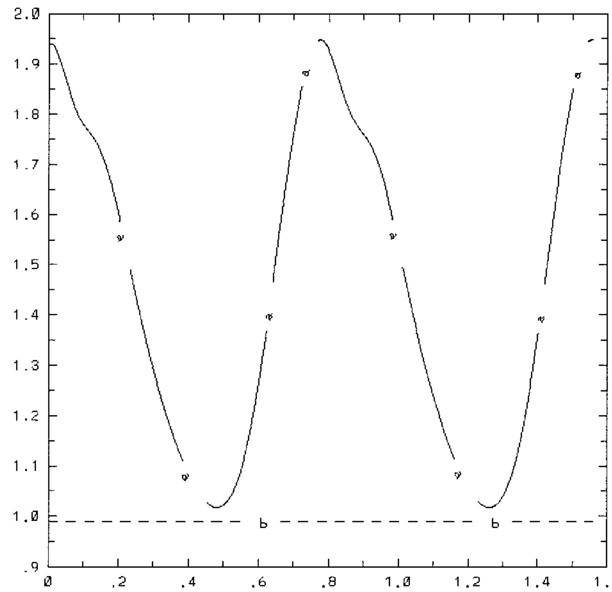

FIG. 5. (a: solid) growth rate of the rms error as a function of the initial time, along the orbit $\bar{j}$, computed for a fixed optimization time $\tau = T$: $\tau^{-1} \log\sqrt{(1/N)\ \Sigma_{i=1}^{N} \Gamma_i^2(t, T)}$; (b: short dash) first Lyapunov exponent of the orbit, λ_1. As in Fig. 4 but $t = 0$ corresponds to the intersection of the orbit with the plane $z = 27$.

and is thus representative of the behavior over the whole attractor.

In order to demonstrate that super-Lyapunov growth is related to the nonorthogonality of eigenvectors, the scalar products $(\mathbf{e}_i \cdot \mathbf{e}_j)$ were computed along the orbit and are shown in Fig. 4 for the orbit $\bar{j}$.

In Fig. 5 the growth rate associated with the rms error is shown as a function of t_k, for $\tau = T$. The first Lyapunov exponent for $\tau = T$, λ_1 is independent of $\mathbf{X}(t_k)$ and is also shown.

The growth rate of the rms error for $\tau = T$, shown in Fig. 5, is related to the scalar products of the Lyapunov vectors by the exact expression (16). Although at $\tau = T$ the average growth rate is not much larger than the first Lyapunov exponent, as shown in Fig. 3, the large variability of the RMS growth rate reflects the large variability of the scalar products as functions of the initial state: when the eigenvectors are approximately orthogonal, the RMS growth rate is close to λ_1.

Singular vectors, in the limit of large τ, were also computed. The following conclusions can be drawn about the asymptotic initial and final singular vectors. The first final singular vector tends to the first Lyapunov vector. The second final singular vector, in the same limit, lies in the plane of the first two Lyapunov vectors, but it is orthogonal to the first one, in agreement with (20); therefore, it is not tangent to the flow, a property of the Lyapunov vector corresponding to $\lambda_2 = 0$. Due to the nonorthogonality of the vectors $\mathbf{e}_i$, perturbations in the direction of the second (and third) final singular vector belong to the unstable manifold.

The initial (asymptotic) third singular vector, according to (21), is in the stable direction $\mathbf{e}_3$. The first and second initial singular vector do not belong to the subspace spanned by $\mathbf{e}_1$ and $\mathbf{e}_2$. Since the attractor has Cantor set structure in any direction out of the plane spanned by the first two Lyapunov vectors—two being the integer part of the system dimension—the first two final singular vectors identify perturbations on the attractor while none of the initial singular vectors has such property.

b. Aperiodic orbits

In section 4 we have defined the vectors $\mathbf{e}_i$ as the Lyapunov vectors and discussed how they can be constructed by intersecting the subspaces spanned by the asymptotic initial and final singular vectors.

We test numerically this hypothesis in the Lorenz system against the knowledge that the Lyapunov vector corresponding to the zero exponent is tangent to the flow.

To this end, we compute the initial and final singular vectors referred to the same point along an aperiodic trajectory, for increasing optimization times, until convergence is obtained. We intersect the plane of the first two final singular vectors with the plane of the last two singular vectors to construct the vector $\mathbf{e}_2$ and take the scalar product with the tangent to the flow. The mean and standard deviation of the scalar product computed for 10 000 different points, sampled along a trajectory once every 100 time units, is shown in Table 1 as a function of the optimization time interval τ.

The results support our conclusions that (19)–(20)

TABLE 1. Mean and standard deviation of the scalar product, s, between the vector obtained intersecting the planes of the first two final and the last two initial singular vectors with the tangent to the flow, **t**, as a function of optimization time, τ. For sufficiently large τ, we obtain the vector $\mathbf{e}_2$; that is, the Lyapunov vector corresponding to the zero exponent and $s = \mathbf{t} \cdot \mathbf{e}_2$ converges to one.

τ	$\langle s \rangle$	Standard deviation of s
1	0.94	0.15
2	0.99	0.05
3	0.99	0.04
4	1.00	0.02
5	1.00	0.02
6	1.00	0.01
7	1.00	0.01
8	1.00	0.01
9	1.00	0.00
10	1.00	0.00

define a set of vectors with the required property of Lyapunov vectors, as discussed in section 4.

7. Summary and conclusions

The original motivation of this work was to investigate the relation between singular vectors and Lyapunov vectors, as well as the consequences for finite time error growth and in particular the mechanism responsible for super-Lyapunov growth.

To this end, we have exploited unstable periodic orbits of the Lorenz system as a tool for the study of Lyapunov stability and transient error growth. Based upon Floquet theory, we arrived at a number of conclusions applicable also to aperiodic orbits.

We have proposed a definition of Lyapunov vectors that satisfies the Oseledec theorem and is consistent with Floquet theory. These vectors coincide with Floquet eigenvectors in the specific case of a periodic orbit and can be considered their generalization to the aperiodic case. The main properties can be summarized as follows.

1) Lyapunov vectors (as Floquet eigenvectors) can be obtained by intersecting the orthonormal sets of initial and final asymptotic singular vectors. In fact, the initial and final sets of singular vectors in the limit of infinite optimization time converge to the sets obtained by orthonormalizing the Lyapunov vectors, starting from the first one and the last one, respectively.
2) In contrast to the eigenvalues and eigenvectors of the stability matrix, which are complex if computed for arbitrary time intervals, Floquet eigenvectors as well as Lyapunov vectors are real, because their spectrum in not degenerate.
3) Lyapunov vectors and Floquet eigenvectors are independent of the norm definition.
4) The local Lyapunov exponents are the local growth rates associated with Lyapunov vectors (Floquet eigenvectors, for periodic orbits). In fact, their average is given by the global Lyapunov exponents (the Floquet exponents of the orbit) for time going both to plus and minus infinity (plus or minus one period). The same does not hold for growth rates associated with singular vectors.
5) The Lyapunov vector (and Floquet eigenvector) corresponding to the zero exponent is tangent to the flow; this property has been exploited to give numerical evidence that our definition is consistent with the notion of Lyapunov stability.
6) Lyapunov vectors (Floquet eigenvectors) are not in general mutually orthogonal and, in fact, are found to have large projections on one another in the Lorenz system.
7) From 1) it follows that the leading Lyapunov vectors (and the asymptotic final singular vectors) are tangent to the attractor, whereas, in the generic case of nonorthogonality of Lyapunov vectors, the initial singular vectors point in directions with Cantor set structure of the attractor. In the Lorenz system, it can be verified that the plane of the first two Lyapunov vectors, two being the integer part of the system's dimension, is tangent to the surface where a continuum of analogs can be found.

As an application, the mechanism responsible for super-Lyapunov growth has been clarified. Growth rates of random perturbations and perturbations in the direction of singular vectors are mathematically related to local Lyapunov exponents via the scalar products of the Lyapunov vectors. Accordingly, super-Lyapunov growth in the Lorenz system is accounted for by the nonorthogonality of the Lyapunov vectors. In short, Lyapunov vectors play the same role as normal modes in the stability of steady solutions and, because of their nonorthogonality, perturbations may grow very fast in a limited period of time.

A few remarks can be made on the implications of the present findings and open questions regarding meteorological applications.

Evidence of super-Lyapunov growth of the *average* error has not been found in GCMs (Savijarvi 1995; Simmons et al. 1995). However, we would expect to see large amplifications in those *individual* cases where Lyapunov vectors have large projections on one another and for particular perturbations. An example of this is found in Szunyogh et al. (1997), who compared the growth rate of finite time optimal perturbations with the local Lyapunov exponent in a low-resolution GCM.

In ensemble forecasting, because of the large number of degrees of freedom of numerical prediction models, there may be a number of initial singular vectors that grow very quickly during an initial short transient but that, pointing in directions where the attractor is not continuous, may be incompatible with the dynamics. Instead, the relevant perturbations are those that grow particularly fast during an initial transient period, yet, being confined to the subspace of the leading Lyapunov vectors, are on the attractor.

The generation of such perturbations should be tested against other current methods used in ensemble forecasting and adaptive observations.

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