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Alternative algorithm for the computation of Lyapunov spectra of dynamical systems

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Recently a new method for the computation of Lyapunov exponents that does not require rescaling and reorthogonalization was proposed [Rangarajan, Habib, and Ryne, Phys. Rev. Lett. **80**, 3747 (1998)]. In this paper we make a detailed numerical comparison of the new method and a standard algorithm, as regards accuracy and efficiency, by applying them to some typical two-, three-, and four-dimensional systems. We find that in most cases there is reasonable agreement between the Lyapunov spectra obtained using the two algorithms. The CPU times required for computation are also comparable. However, in certain strongly chaotic cases, the new method was found to be either inefficient (taking a lot of CPU time for computation) or inaccurate. [S1063-651X(99)50907-0]

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I. INTRODUCTION

Consider an n-dimensional continuous-time dynamical system

$$\frac{d\mathbf{Z}}{dt}=\mathbf{F}(\mathbf{Z},t), \tag{1}$$

where $\mathbf{Z}$ and $\mathbf{F}$ are n-dimensional vector fields. To determine the n Lyapunov exponents of the system, corresponding to some initial condition $\mathbf{Z}(\mathbf{0})$, we have to find the long term evolution of the axes of an infinitesimal sphere of states around $\mathbf{Z}(\mathbf{0})$. For this, consider the tangent map given by the set of equations

$$\frac{d\,\delta\mathbf{Z}}{dt}=\mathbf{DF}\cdot\delta\mathbf{Z}, \tag{2}$$

where $\mathbf{DF}$ is the $n\times n$ Jacobian matrix with

$$DF_{ij}=\frac{\partial F_i}{\partial Z_j}. \tag{3}$$

One of the standard methods used to determine the full Lyapunov spectrum due to Benettin *et al.* and Shimada and Nagashima [1] uses the Gram-Schmidt reorthonormalization (GSR) procedure. An explicit source code for computations based on this procedure is given by Wolf *et al.* [2]. In this method we have to integrate $n(n+1)$ coupled equations, as there are n equations for the fiducial trajectory in Eq. (1) and n copies of the n tangent map equations in Eq. (2). We refer to this method as the standard method in the following.

Recently, Rangarajan, Habib, and Ryne proposed a new algorithm for the computation of Lyapunov exponents [3] based on the QR method [1] for the decomposition of the tangent map. This does not require the GSR procedure. We summarize the essentials of this method below. The reader can refer to [3] for details.

A solution of Eq. (2) can be formally written as

$$\delta\mathbf{Z}(t)=\mathbf{M}(\mathbf{Z}(t),t)\,\delta\mathbf{Z}(0), \tag{4}$$

where $\mathbf{M}(\mathbf{Z}(t),t)$ is the tangent map matrix whose evolution equation is easily seen to be

$$\frac{d\mathbf{M}}{dt}=\mathbf{DF}\cdot\mathbf{M}. \tag{5}$$

The idea of the new method is to evaluate the Lyapunov exponents without using the vectors $\delta\mathbf{Z}$ directly and consequently without using the associated reorthogonalization and rescaling. For this one uses the fact that $\mathbf{M}$ can be written as $\mathbf{M}=QR$, a product of an orthogonal $n\times n$ matrix Q and an upper triangular matrix R with positive diagonal entries [4]. Then it can be easily shown that

$$\tilde{Q}\dot{Q}+\dot{R}R^{-1}=\tilde{Q}\mathbf{DF}Q\equiv S, \tag{6}$$

where the overdot denotes a time derivative. The Lyapunov exponents λ_i are equal to σ_i/t in the limit $t\to\infty$ where $\sigma_i=\ln(R_{ii})$ [5]. $\dot{R}R^{-1}$ is also an upper triangular matrix and it is easily shown that the evolution equations for σ_i are controlled by the diagonal elements of S:

$$\dot{\sigma}_i=S_{ii},\quad i=1,\ldots,n. \tag{7}$$

Now Q, which is an $n\times n$ orthogonal matrix, is essentially the diagonalizing matrix for the tangent map flow and is parametrized by $n(n-1)/2$ angles (θ's). $\tilde{Q}\dot{Q}$ is an antisymmetric matrix and the evolution equations for these angles can be obtained from the subdiagonal elements of S in Eq. (6). For $n<4$, we can work with any explicit representation for Q. For $n=4$, we employ a representation for Q based on the well known fact that $SO(4)\sim SO(3)\times SO(3)$ [6]. This simplifies the calculations and numerical computations considerably. Hence, we have to solve $n(n+3)/2$ coupled equations to find the Lyapunov exponents in this method, as there are n equations for the fiducial trajectory in Eq. (1), n equations for the exponents in Eq. (7), and $n(n-1)/2$ equations for the angles.

It might be thought that the new method has advantages over the standard methods, as a minimal number of variables

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is used and rescaling and reorthogonalization are also eliminated. However, in this method the evolution equations for the angles and Lyapunov exponents are highly nonlinear, involving sines and cosines of the angles, whereas the standard method uses the linearized equations for $\delta\mathbf{Z}$ directly. Hence, there is a need to compare the efficiency and accuracy of this method with a standard method. That is the subject of the present investigation. Here, we consider some typical nonlinear systems of physical interest with $n=2$, 3, and 4. The driven Van der Pol oscillator is taken as an example of a two-dimensional system, whereas the standard Lorenz system is chosen for $n=3$. For $n=4$, we consider the coupled quartic oscillators and anisotropic Kepler problem as examples of conservative Hamiltonian systems and Rössler hyperchaos system as an example of a dissipative system. In all these cases, the full Lyapunov spectrum is computed using both methods. The time of integration is chosen to ensure reasonable convergence of the Lyapunov exponents.

II. COMPARISON OF THE TWO METHODS

In this section, we take up the following systems for a detailed comparison of the two methods.

(i) Driven Van der Pol oscillator ($n=2$).

$$\frac{d}{dt}\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} z_2 \\ -d(1-z_1^2)z_2 - z_1 + b\cos\omega t, \end{pmatrix}, \tag{8}$$

where b and d are parameters and ω is the driven frequency. In our numerical work we have chosen $d=-5.0$, $b=5.0$, and $\omega=2.47$ as the parameter values.

(ii) Lorenz system ($n=3$).

$$\frac{d}{dt}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} \sigma(z_2-z_1) \\ z_1(\rho-z_3)-z_2 \\ z_1z_2-\beta z_3 \end{pmatrix}. \tag{9}$$

This system is too well known to require any further discussion. For computations we set $\sigma=10.0$, $\rho=28.0$, and $\beta=8/3$.

(iii) Coupled quartic oscillators ($n=4$). This is a conservative system and the Hamiltonian is given by

$$H=\frac{z_3^2}{2}+\frac{z_4^2}{2}+z_1^4+z_2^4+\alpha z_1^2z_2^2, \tag{10}$$

where z_1 and z_2 are the canonical coordinates, z_3 and z_4 are the corresponding momenta, and α is a parameter. The equations of motion are readily obtained from the Hamiltonian. This system is known to be integrable for $\alpha=0$, 2 and 6.

(iv) Anisotropic Kepler problem ($n=4$). The Hamiltonian of this system is given by

$$H=\frac{p_\rho^2}{2}+\gamma\frac{p_z^2}{2}-\frac{e^2}{\sqrt{\rho^2+z^2}}, \tag{11}$$

where γ is a number.

The Hamiltonian given above describes the motion of an electron in the Coloumb field in an anisotropic crystal, where its effective mass along the x-y plane and z direction are different. $\gamma=1$ corresponds to the isotropic case and is integrable. When $\gamma\neq1$, the system is nonintegrable. Because of the singularity at $\rho=z=0$, the Hamiltonian in the above form is hardly suitable for numerical integration. For this we choose $z_1=\sqrt{\rho+z}$ and $z_2=\sqrt{\rho-z}$ as the canonical variables. We can find the corresponding canonical momenta z_3 and z_4 in terms of p_ρ and p_z. We also use a reparametrized time variable τ defined by $dt=d\tau(z_1^2+z_2^2)$.

The original Hamiltonian with old variables and energy E corresponds to the following Hamiltonian with $H'=2$ in terms of the new variables [7]:

$$H'=2=\frac{1}{2}(z_3^2+z_4^2)-E(z_1^2+z_2^2)+(\gamma-1)\frac{(z_1z_3-z_2z_4)^2}{2(z_1^2+z_2^2)}. \tag{12}$$

The equations of motion can be easily obtained from the above Hamiltonian. We have chosen $\gamma=0.61$ for computational purposes.

(v) Rössler hyperchaos system ($n=4$). This is a dissipative system and an extension of the three-dimensional Rössler attractor [8,9]. It is described by the equations

$$\frac{d}{dt}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix} = \begin{pmatrix} -(z_2+z_3) \\ z_1+az_2+z_4 \\ b+z_1z_3 \\ cz_4-dz_3 \end{pmatrix}, \tag{13}$$

where a, b, c, and d are parameters whose values are taken to be 0.25, 3.0, 0.05, and 0.5, respectively, for our computations.

For all the systems, we have used a variable step-size Runge-Kutta routine (RKQC) for integration with an error tolerance $\epsilon\sim10^{-6}$–10^{-8}. All the computations were performed on a DEC Alpha based workstation running OpenVMS. We also noted the CPU time taken for each case with either of the algorithms. This is the actual time taken by the CPU to accomplish a specific process (independent of the other processes running in the system). The details of the comparison between the two methods are summarized in Table I.

It may be noticed that the two methods yield essentially the same Lyapunov spectrum. For any dynamical system, one of the Lyapunov exponents has to be zero (corresponding to the difference vector δz lying along the trajectory itself). For the Lorenz system, the Rössler hyperchaos system (both dissipative), and the coupled quartic oscillators, this condition is satisfied by both algorithms. For the driven Van der Pol oscillator and the anisotropic Kepler problem, both methods fail the test. This aspect needs to be studied further. For the coupled quartic oscillators, all the exponents should be zero corresponding to the integrable case of $\alpha=6$. This is indeed satisfied by both algorithms. In Fig. 1 we give plots of Lyapunov exponents as functions of time for a typical case. Again, there is little difference between the two algorithms as far as the convergence of the Lyapunov exponents is concerned.

However, for the system of coupled quartic oscillators, the CPU time is abnormally high for the new method, corresponding to the nonintegrable case of $\alpha=8$. This is true for both small and large energies. For large energies ($\sim25\,000$), since the energy varied by ~15 when we used

TABLE I. Comparison of the two methods for some systems with $n=2$, 3, and 4. The values given in parentheses correspond to the standard method.

System	Initial condition	Lyapunov spectrum, sum (s), and CPU time (t) in sec
Driven		0.0981 (0.0987)
van der Pol	$z_1=-1.0$	-6.8400 (-6.8411)
Oscillator	$z_2=1.0$	$s=-6.7419$ (-6.7424)
($n=2$)		$t=519.22$ (825.56)
		0.9056 (0.9051)
Lorenz	$z_1=0.0$	0.0000 (0.0000)
system	$z_2=1.0$	-14.5723 (-14.5718)
($n=3$)	$z_3=0.0$	$s=-13.6667$ (-13.6667)
		$t=2394.30$ (1668.68)
		0.1360 (0.1332)
Anisotropic	$z_1=1.0$	0.0831 (0.0832)
Kepler	$z_2=2.0$	-0.0833 (-0.0833)
problem	$z_3=1.0$	-0.1357 (-0.1331)
($n=4$)	$z_4=0.5$	$s=-0.0000$ (-0.0000)
		$t=350.18$ (201.04)
		0.1128 (0.1121)
	$z_1=-20.0$	0.0214 (0.0196)
Rössler	$z_2=0.0$	-0.0000 (-0.0000)
hyperchaos	$z_3=0.0$	-24.7527 (-25.1886)
($n=4$)	$z_4=15.0$	$s=-24.6185$ (-25.0568)
		$t=1527.58$ (5594.99)
		0.0001 (0.0001)
	$z_1=0.8$	0.0001 (0.0001)
Coupled	$z_2=0.5$	-0.0001 (-0.0001)
quartic oscr.	$z_3=1.0$	-0.0001 (-0.0001)
($n=4$, $\alpha=6$)	$z_4=1.3$	$s=0.0000$ (0.0000)
		$t=803.49$ (492.09)
		0.1806 (0.1738)
	$z_1=0.8$	0.0001 (0.0001)
Coupled	$z_2=0.5$	-0.0001 (-0.0001)
quartic oscr.	$z_3=1.0$	-0.1806 (-0.1738)
($n=4$, $\alpha=8$)	$z_4=1.3$	$s=0.0000$ (0.0000)
		$t=39012.77$ (855.64)

the RKQC routine, we also used a symplectic procedure that eliminates secular variations in the energy. With this routine, the CPU times were nearly the same for both methods. However, the new method yields poor results for the Lyapunov spectrum. For instance, corresponding to the initial condition $z_1=7.0$, $z_2=7.0$, $z_3=5.0$, and $z_4=4.0$, the Lyapunov spectra computed using the new and the standard methods are (1.5506, 0.3254, -0.3261, -1.5499) and (1.5205, 0.0001, -0.0001, -1.5205), respectively.

We also compared the new method with another procedure for computing Lyapunov spectra with continuous Gram-Schmidt orthonormalization [10]. Here the number of equations that need to be integrated to obtain the complete spectrum is $n(n+2)$, as compared to $n(n+1)$ equations in the standard method and $n(n+3)/2$ equations in the new method, where n is the order of the system. The CPU time for this method, corresponding to the initial conditions given in Table I for $\alpha=8$, is 7658.57 s, as compared to 39 012.77

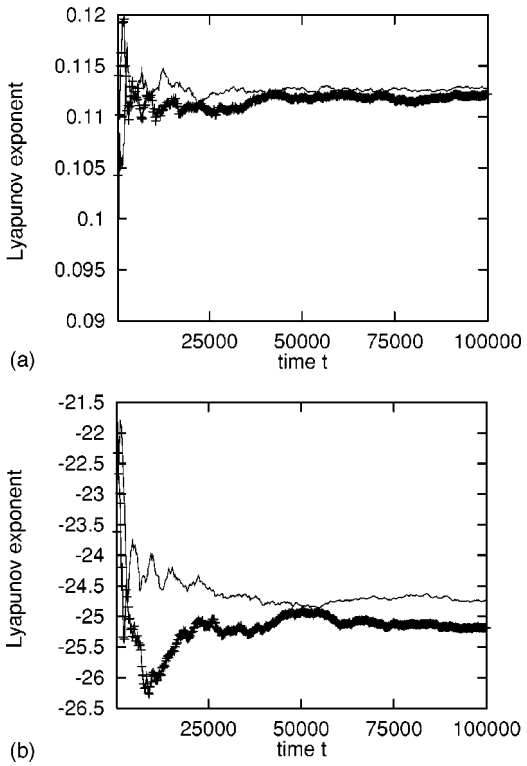

FIG. 1. Plots of the Lyapunov exponent for the Rössler hyperchaos system. (a) Highest exponent λ_1, (b) lowest exponent λ_4. The thick and thin lines correspond to the new and standard algorithms, respectively.

with the new method (with hardly any difference in the Lyapunov spectrum).

In the standard method, as well as in Ref. [10], after solving for the fiducial trajectory, the equations for the tangent flow are linearized equations. In the new method, these equations are replaced by the equations for the angles determining the principal axes or the bases associated with the Lyapunov spectrum and the Lyapunov exponents. These equations involving sines and cosines of the angles are highly nonlinear. For dissipative systems this nonlinearity does not pose a problem. However, in many cases, this nonlinearity renders the new method less efficient, and can even lead to inaccuracies in strongly chaotic situations.

III. CONCLUSIONS

In a recently proposed new method for the computation of Lyapunov exponents, the Lyapunov exponents are calculated directly, so to say, by utilizing representations of orthogonal matrices applied to the tangent map. Since it does not require renormalization or reorthogonalization and requires a lesser number of equations, it has been claimed that it has several advantages over existing methods. To test this claim, we have computed the full Lyapunov spectrum of some typical nonlinear systems with two, three, and four variables and made a detailed comparison with the results obtained using a standard algorithm. For dissipative systems, there is reasonable agreement between the spectra obtained using the two algorithms. The CPU time taken for the computation is also comparable. However, in certain strongly chaotic situations, the new algorithm could lead to inaccuracies in the

Lyapunov spectrum, when one uses fixed step-size integrator routines, however small the step size may be. This could be remedied by a variable step-size routine with a reasonable value of error tolerance. But this makes the new method far less efficient (taking abnormally long times for computation), compared to the standard algorithm. This could be attributed to the highly nonlinear nature of the evolution equations for the tangent map inherent in this method. However, the proposed new method is still useful as an alternate algorithm for the computation of Lyapunov spectra.

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