OPTIMAL CONDITIONS FOR THE NUMERICAL CALCULATION OF THE LARGEST LYAPUNOV EXPONENT FOR SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

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A general indicator of the presence of chaos in a dynamical system is the largest Lyapunov exponent. This quantity provides a measure of the mean exponential rate of divergence of nearby orbits. In this paper, we show that the so-called two-particle method introduced by Benettin et al. could lead to spurious estimations of the largest Lyapunov exponent. As a comparator method, the maximum Lyapunov exponent is computed from the solution of the variational equations of the system. We show that the incorrect estimation of the largest Lyapunov exponent is based on the setting of the renormalization time and the initial distance between trajectories. Unlike previously published works, we here present three criteria that could help to determine correctly these parameters so that the maximum Lyapunov exponent is close to the expected value. The results have been tested with four well known dynamical systems: Ueda, Duffing, Rössler and Lorenz.

Keywords: Chaotic Dynamics; Lyapunov Exponents; Runge-Kutta Methods

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1. Introduction

Lyapunov exponents tell us whether or not two points in the phase space of a dynamical system, that are initially very close together, stay close in the subsequent motion. In other words, they measure the average rate of divergence or convergence of nearby orbits. The exponential divergence of orbits, in a practical sense, implies the lost of predictability of the system, so any system with at least one positive Lyapunov exponent is defined as chaotic.

A formal definition can be given by considering the dynamical system

$$\dot{x} = F(x),$$

where $\dot{x}$ represents the temporal derivative of $x$ with solution $f^t(x)$. Also consider two initial conditions in phase space $x_0$ and $x_0 + \delta x_0$, where $\delta x_0$ is a
small perturbation of \( x_0 \). After time \( t \), the solution for the pair of conditions is given by \( f^t(x_0) \) and \( f^t(x_0 + \delta x_0) \). Denoting \( U_t = f^t(x_0 + \delta x_0) - f^t(x_0) \), and \( U_0 = f^0(x_0 + \delta x_0) - f^0(x_0) = \delta x_0 \) (see Fig. 1), the largest Lyapunov exponent \( \lambda_{\text{max}} \) is given by

\[
\lambda_{\text{max}} = \lim_{t \to \infty} \frac{1}{t} \ln \left| \frac{|U_t|}{|U_0|} \right|
\]

As can be noted, there exist as many Lyapunov exponents as phase space dimensions (the so-called Lyapunov characteristic exponents). However, the asymptotic rate of expansion of the largest axis, which corresponds to the most unstable direction of the flow, will obliterate the effect of the other exponents over time making the largest Lyapunov exponent (henceforth LLE) the relevant parameter to determine the degree of chaoticity of the system.

Since the seminal works of Wolf et al., Benettin et al. and Contopoulos et al., new methods have been proposed to compute Lyapunov exponents in the literature (see e.g. Refs. 5, 6, 7, 8, 9), some of them for data series and some others for differential equations.

Our main interest in this paper is to propose a solution to the problem of incorrect estimation of LLE when the Benettin et al. method (henceforth two-particle method) is used. To do so, we define some criteria that could help to determine optimal parameters of renormalization time and initial distance between trajectories. Additionally, as a reference criterion we will compare the results with the...
Contopoulos method (henceforth variational method)\footnote{In all that follows $D_q$ represents the partial derivative with respect to $q$} which can be implemented easily and gives very accurate results.

The importance of the two-particle method lies in the fact that in spite of its lack of accuracy, it is a powerful and efficient tool when the system of equations is very cumbersome as in the case of geodesic motion of test particles in General Relativity (see for instance Ref. \cite{10} or when the linear approximations are not valid, e.g. when we are close to a singularity. Moreover, due to the fact that this is an easy to implement method and in some cases the only alternative, in many research fields has been extensively used (see for instance Ref. \cite{11} and references therein), a fact that deserves serious attention, taking into account that this method often produces wrong results.

The paper is organized as follow, in section 2 we introduce the variational method which will serve as the reference method. In section 3 the two-particle method is introduced. Next, in section 4 we present some examples of the incorrect estimation of the LLE for some particular and well known dynamical systems: Ueda, Rössler, Duffing and Lorenz. In section 5 we propose some criteria for the accurate determination of the largest Lyapunov exponent. Finally in section 6 the conclusions are presented.

2. Variational Method

Let us consider the dynamical system \footnote{In all that follows $D_q$ represents the partial derivative with respect to $q$}, with general solution $f^t(x)$ and initial condition $x(t = 0) = x_0 = f^0(x_0)$. The particular solution is given by $x(t) = f^t(x_0)$, so that $\dot{x}(t) = f^t(x_0) = F(f^t(x_0))$. Differentiating the last expression with respect to $x_0$ we get

$$D_{x_0} f^t(x_0) = D_{x_0} F(f^t(x_0)) = D_x F(f^t(x_0)) D_{x_0} f^t(x_0)$$

(3)

denoting $D_{x_0} f^t(x_0) = \phi^t(x_0)$, equation (3) becomes

$$\dot{\phi}^t(x_0) = D_x F(f^t(x_0)) \phi^t(x_0)$$

(4)

which is the variational equation, with initial condition $\phi^0(x_0) = I$, where $I$ is the identity matrix.

From the expression for the divergence between nearby orbits, we may write

$$\mathcal{U}_t = f^t(x_0 + \delta x_0) - f^t(x_0) = D_{x_0} f^t(x_0) \cdot \mathcal{U}_0$$

(5)

with

$$\mathcal{U}_0 = f^0(x_0 + \delta x_0) - f^0(x_0) = \delta x_0$$

(6)

substituting (5) and (6) into definition (2), the LLE takes the form

$$\lambda_{\text{max}} = \lim_{t \to \infty} \lim_{\delta x_0 \to 0} \frac{1}{t} \ln \frac{|\phi^t(x_0) \cdot \delta x_0|}{|\delta x_0|},$$

(7)
In order to guarantee that the vector $U_0$ have a component in the maximal growth direction, it is very useful to choose an ensemble of $n$ trajectories with different initial orientations, i.e.,

$$
\lambda_{\text{max}} = \lim_{t \to \infty} \lim_{\delta x_0 \to 0} \frac{1}{n} \sum_{i=1}^{n} \frac{1}{t} \ln \frac{|\phi^t(x_0) \cdot \delta x_0|}{|\delta x_{0i}|}.
$$

(8)

In essence, in the variational method the LLE is calculated after solving simultaneously the variational equation (4) and the original system (1), with initial conditions $x(0) = x_0$ and $\phi^0(x_0) = I$.12

3. Two-particle Method

The two-particle method is based on Oseledec’s theorem.13 In this method we need to consider two trajectories: a reference orbit and a shadow orbit. The reference orbit is solution to the dynamical system (1), with initial condition $x(t = 0) = x_0 = f^0(x_0)$, while the shadow orbit is solution to the initial condition $x(t = 0) = x_0 + \delta x_0 = f^0(x_0 + \delta x_0)$. After time $\tau$, the distance between the two trajectories is calculated as

$$
d_1 = f^\tau(x_0 + \delta x_0) - f^\tau(x_0).
$$

(9)

Then, the point $f^\tau(x_0 + \delta x_0)$ approaches to the reference orbit along the separation vector $d_1$, down to the initial distance $\delta x_0$, so that the shadow orbit starts at the same distance for the next iteration (see Fig. 2). If this renormalization is made at fixed time intervals $\tau$, then we can write

$$
d_i = f^{i\tau}(x_0 + \delta x_0) - f^{i\tau}(x_0).
$$

(10)

Fig. 2. Periodic renormalization of the distance for the determination of the LLE in the two-particle method.
From definition (2) an exponent can be calculated for each iteration

$$\lambda_1 = \frac{1}{\tau} \ln \frac{|d_1|}{|\delta x_0|}, \lambda_2 = \frac{1}{\tau} \ln \frac{|d_2|}{|\delta x_0|}, \ldots, \lambda_i = \frac{1}{\tau} \ln \frac{|d_i|}{|\delta x_0|}, \ldots, \lambda_n = \frac{1}{\tau} \ln \frac{|d_n|}{|\delta x_0|},$$

(11)

such that the LLE is calculated as the average

$$\lambda_{\text{max}} = \lim_{n \to \infty} \lim_{\delta x_0 \to 0} \frac{1}{n \tau} \sum_{i=1}^{n} \ln \frac{|d_i|}{|\delta x_0|}.$$  

(12)

4. Incorrect estimation of the Lyapunov exponents

Both the variational method and the two-particle method, have been widely used in the literature and there is no reason to expect that the results obtained by each method should be different. Yet some authors have pointed out that in many cases the results of both methods are not even similar (see for instance Ref. 11). To illustrate this, we shall consider four of the most studied dynamical systems: the Ueda system\textsuperscript{14} Rössler system\textsuperscript{15} Duffing system\textsuperscript{16} and Lorenz system\textsuperscript{17} In table 1 we present the systems considered above together with their respective parameters and expected LLE. In Fig. we numerically calculate the LLE using the two-particle method with different orders of the explicit Runge-Kutta method\textsuperscript{c} by setting arbitrary values of the renormalization time $\tau$, and the initial distance between trajectories $\delta x_0$, for each system\textsuperscript{d}

| System | Equations | Parameters | Expected $\lambda$ |
|--------|-----------|------------|--------------------|
| Ueda   | $\dot{x} = ay$ | $a = 0.15$ | 0.11 Ref. [18] |
|        | $\dot{y} = x$ | $b = 0.20$ | 0.09 Ref. [2] |
|        | $\dot{z} = c + z(x - c)$ | $c = 10.0$ |
| Rössler| $\dot{x} = -y - z$ | $\dot{y} = x + ay$ | $\dot{z} = b + z(x - c)$ |
|        | $\dot{y} = x + ay$ | $b = 0.20$ | |
|        | $\dot{z} = c + z(x - c)$ | $c = 10.0$ |
| Lorenz | $\dot{x} = \sigma(y - x)$ | $\sigma = 16.0$ | |
|        | $\dot{y} = x(R - z) - y$ | $R = 45.92$ | 1.50 Ref. [2] |
|        | $\dot{z} = xy - bz$ | $b = 4.0$ |
| Duffing| $\dot{x} = y(1 - y^2) - \alpha x + A \cos(\omega z)$ | $\alpha = 0.25$ | |
|        | $\dot{y} = x$ | $\omega = 1.0$ | 0.115 Ref. [19] |
|        | $\dot{z} = 1$ | $A = 0.3$ |

\textsuperscript{c}Henceforth RK-\textit{n} denotes \textit{n}-th Runge-Kutta order.

\textsuperscript{d}In all that follows we exclude the 4th Runge-Kutta order. The only reason to do so, is that in most of the cases the numerically calculated value is far apart from the set of values obtained with the higher R-K orders, this behavior force us to increase the range in the vertical axis making the figures unclear for the reader.
This behavior is not particular for the set of parameters or integration methods used, rather it is a common tendency as pointed out by Tancredi et al.\cite{11} On the other hand, when the variational method is used, the LLE in all cases are practically the same as presented in table \ref{table1} (Rössler 0.088, Ueda 0.108, Lorenz 1.49 and Duffing 0.115).

![Graphs](a) (b) (c) (d)

Fig. 3. LLE calculated with the two-particle method for the systems a) Rössler ($\tau = 50, \delta x_0 = 10^{-2}$), b) Duffing ($\tau = 1, \delta x_0 = 10^{-6}$), c) Lorenz ($\tau = 10, \delta x_0 = 10^{-6}$) and d) Ueda ($\tau = 4, \delta x_0 = 10^{-6}$), using different orders of the explicit Runge-Kutta method. The respective parameters have been set as in table \ref{table1}.

The possible causes of unreliable estimates of LLE with the two-particle method, have been previously explored by Holman and Murray\cite{20} and Tancredi et al.\cite{11} The analysis by Holman and Murray leads to the conclusion that the two-particle technique has an accompanying threshold time scale that depends on the rescaling parameters $\delta x_0$ and $\tau$. In other words, after the $i$-th renormalization the distance between trajectories $d_i$ is given approximately by

$$d_i = \delta x_0 (1 + \alpha \tau^n) \exp(\lambda_{\text{max}} \tau),$$

where $\alpha$ and $n$ are constants associated to the initial power-law transient separation, so that in practice, the numerically calculated LLE is given by

$$\lambda_{\text{max}} + \frac{\ln(1 + \alpha \tau^n)}{\tau},$$

(14)
which should affect mainly the quasi-regular trajectories (i.e. when $\lambda_{\text{max}} \ll \ln(1 + \alpha \tau^n)/\tau$).

The explanation given by Holman and Murray has been refuted by Tancredi et al. who show that $\alpha$ in Eqs. (13) and (14) is not actually a constant as they assumed, and that the rescaling technique should also lead to a wrong estimate of the LLE when the variational method is used. Furthermore, Tancredi et al. found a good agreement in the final values of the LLE for different initial distances up to certain $\delta x_0$. With this result, they conclude that there seems to be an optimal value of $\delta x_0$ and that the false estimates of the LLE in the two-particle method rely on the accumulation of round-off errors during the computation of the distance between trajectories $d_i$ in the course of successive renormalizations.

In order to validate (or refute) the premises stated by Tancredi et al. and given that the round-off errors should depend on the number of renormalizations, which are indicated by the parameter $\tau$, we start numerically calculating the LLE using the two-particle method with different orders of the explicit Runge-Kutta method for different values of the initial distance between trajectories $\delta x_0$, keeping fixed values of the renormalization time $\tau$. The results for the Ueda and Lorenz systems are presented in Figs. 4 and 5 respectively.

From Fig. 4 it can be seen that when the LLE does not depend on the integration method (red lines), the calculated LLE (which is roughly the expected one) apparently does not depend on the renormalization time $\tau$ nor the initial distance between trajectories $\delta x_0$. A different behavior is observed for the Lorenz system Fig. 5, in this case even when the LLE does not depend on the integration method (red lines), for a larger renormalization time $\tau$ there is a tendency to a different LLE depending on the initial separation $\delta x_0$.

Next we apply the same criteria for the other two systems (Duffing and Rössler) for a wide range of $\tau$ values, but in these cases we obtain no tendency towards an unique LLE. The results are presented in Fig. 6. To solve this question we invert the procedure, keeping fixed $\delta x_0$ and varying $\tau$. In this case (see Figs. 7 and 8) we observe a tendency towards unique LLE for certain $\tau$ values (red lines), which is not necessarily the expected LLE. From the plots we conclude that the more accurate result belong to the smaller $\delta x_0$, with corresponding smaller $\tau$.

5. Criteria for the accurate determination of the largest Lyapunov exponent

The results presented in the previous section can be explained as follows: The two-particle method could depend on three parameters, namely the number of renor-

*Ensuring a $\delta x_0$ below the machine precision.
Fig. 4. (color online) LLE calculated with the two-particle method for the Ueda system using different orders of the explicit Runge-Kutta method, keeping fixed values of the renormalization time $\tau$, for different values of the initial distance between trajectories $\delta x_0$. The respective parameters have been set as in Table 1. $\lambda_{exp}$ represents the expected LLE.

malizations $n$, the initial distance between trajectories $\delta x_0$, and the renormalization time $\tau$. When it is possible to guarantee a stable convergence of the LLE, we could ensure that $n$ is large enough to avoid any trouble with the number of terms chosen for the approximation, so the possible incorrect estimates of the LLE should rely on setting $\tau$ and $\delta x_0$.

As can be noted from Figs. 7 and 8 there should exist an optimal range of $\tau$ values. This is due to the fact that if we choose $\tau$ too small it is possible to induce significant round-off errors due to the large number of approximations performed; while choosing too large $\tau$ could cause saturation due to the fact that the chaotic region is generally bounded. Something similar occurs with the $\delta x_0$ parameter. From the LLE definition (2), the distance between trajectories should tend to zero, however from Figs. 4 and 5 we observe that for small enough $\delta x_0$ the calculated LLE depends on the integration method, while choosing a larger value of $\delta x_0$ could lead to approximation errors.

The analysis given above and the results of the previous section show us that each particular system can be affected strongly by one or other of the parameters, so let us to formulate some simple criteria in order to obtain reliable results of the numerically calculated LLE. This criteria can be stated as follows:
Fig. 5. (color online) LLE calculated with the two-particle method for the Lorenz system using different orders of the explicit Runge-Kutta method, keeping fixed values of the renormalization time $\tau$, for different values of the initial distance between trajectories $\delta x_0$. The respective parameters have been set as in Table 1. $\lambda_{\exp}$ represents the expected LLE.

Fig. 6. LLE calculated with the two-particle method for the Duffing system using different orders of the explicit Runge-Kutta method as indicated in the horizontal axis. The respective parameters have been set as in Table 1.

- The final value of the largest Lyapunov exponent among different runs with different integration techniques should be the same.
- By fixing $\tau$ and varying $\delta x_0$, the largest Lyapunov exponent corresponds to the set of values independent of the integration algorithm, with smaller $\delta x_0$. 
6. Conclusions

In the present paper we have shown that the two-particle method could lead to inconsistent results of the calculation of the largest Lyapunov exponent, particularly when using arbitrary values of the initial separation between trajectories and the renormalization time. With the aim to contribute to the solution of this interesting problem, we performed a numerical exploratory survey which let us propose three criteria that could help to determine confident estimates of the LLE. As shown in section 5, the proposed criteria do not depend of the kind of system under study, and the calculated largest Lyapunov exponent tends to the expected value, independently if it is mainly caused by round-off errors or by approximation inaccuracies.

- If it is impossible to determine a set of LLE independent of the integration method, we proceed to set a small $\delta x_0$ and vary $\tau$, the largest Lyapunov exponent corresponds to the set of identical values with smaller $\delta x_0$ and smaller $\tau$.

Under these conditions the obtained LLE are close to the expected ones, i.e. $\approx 0.12$ for the Ueda system, $\approx 1.44$ for the Lorenz system, $\approx 0.12$ for the Duffing system, $\approx 0.13$ for the Rössler system.
Fig. 8. (color online) LLE calculated with the two-particle method for the Rössler system using different orders of the explicit Runge-Kutta method as indicated in the horizontal axis. The respective parameters have been set as in table 1. $\lambda_{\text{exp}}$ represents the expected LLE.

Finally we would like to emphasize that to our knowledge, this is the first proposed procedure to determine optimal values of $\tau$ and $\delta$ in the calculation of the LLE with the method of Benettin et al.\cite{3}

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