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Global vector-field reconstruction of nonlinear dynamical systems from a time series with SVD method and validation with Lyapunov exponents

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A method for the global vector-field reconstruction of nonlinear dynamical systems from a time series is studied in this paper. It employs a complete set of polynomials and singular value decomposition (SVD) to estimate a standard function which is central to the algorithm. Lyapunov exponents and dimension, calculated from the differential equations of a standard system, are used for the validation of the reconstruction. The algorithm is proven to be practical by applying it to a Rössler system.

Keywords: global vector-field reconstruction, Lyapunov exponents, model validation
PACC: 0545, 0520

1. Introduction

The theory of nonlinear dynamical systems has been studied for many years, but it is only in the past four decades, with the advent of modern computers, that it has become an important topic for mathematicians and physicist and has attracted increasing attention. One of its interesting sub- topics, namely the global vector-field reconstruction of nonlinear systems from a time series, is becoming more and more practical and powerful in relation to the analysis of experimental systems. In this field, there exist a number of methods for system reconstruction and validation, which have been tested by model systems and applied to some experimental systems.[1−3] Gouesbet proposed a method which uses the derivatives of a time series to span the phase space, then describes the flow in phase space with a standard system involving a standard function which is estimated by polynomials, and finally integrates the differential equations of the standard system to display the reconstructed system.[4−7] His group successfully reconstructed some classical models and experimental systems with this method.[8−11] In the present paper, following the methodology of Gouesbet,[7] we use a complete set of polynomials with a singular value decomposition (SVD) method for the estimation of the standard function. This method is simpler and easier to implement, but the original method depends on a driving vector of reconstruction when the system is too complex. In the case of complex systems, it is indeed required to carefully choose the parameters driving the reconstruction.

The validation of a reconstructed system is of same importance as the reconstruction itself. During the 1990s, the topological characterization has been used as a means for validation[8] but, because a topological description of an object only retains reductionistic topological aspects, this technique evaluates the reconstruction rather in quality than in quantity. Furthermore, it is essentially limited to three-dimensional phase spaces. However, the Lyapunov exponents (LEs) and Lyapunov dimensions (LDs) or other dimensions[4−6] are useful quantitative tools for validation. If a reconstruction is successful, not only must the reconstructed system and the original system be topologically compatible, but also they must exhibit equal or near equal values of LEs and LDs, because these parameters characterize the sensitivity to initial conditions of an attractor.

A positive Lyapunov exponent is the signature of the existence of chaos in an attractor. But the estimation of an entire Lyapunov exponent spectrum is

known to be a nontrivial task, because it is a typically ill-conditioned problem.[12] There are however some reliable and practical methods for the calculation of Lyapunov exponents if the differential equations of the system are known.[13–16] Unfortunately, in most cases, we do not know the differential equations of the systems under study. We only possess one (or more) observable time series from the systems. Therefore, developing methods for calculating the Lyapunov exponents from a time series became very important to assess the existence of deterministic chaos in a system. Wolf and Swift [17] presented an algorithm allowing one to estimate the non-negative largest Lyapunov exponent of a time series by tracking the evolution of a set of vectors in the embedding space. Sano and Sawada [18] and Eckmann *et al* [19] proposed a Jacobian algorithm which estimates a local flow operator from the evolution of spatially neighbouring points to quantify the mean divergence of nearby orbits of the attractor. Rosenstein *et al* [20] presented an improved method of Sano and Sawada [18] by pointing out and overcoming the drawbacks of the existing methods which are unreliable for small data sets, computationally intensive and relatively difficult to implement. But we found that his method also suffers from the same drawbacks. In recent years, a new algorithm with moving box was published for the analysis of time series.[21]

Most of the methods for estimating LEs from a time series, as mentioned above, are based on a phase space embedding with a time delay technique. In this paper, however, the phase space is embedded by using derivatives of time series. A specific method for estimating the entire spectrum of LEs, in connection with a validation of a global vector-field reconstruction, is then investigated. When the standard system is integrated, local Lyapunov exponents defined by the contracting or expanding rates of the orthogonal basis vectors in phase space are simultaneously calculated at each time step. When the reconstruction is successfully achieved, the obtained (mean) Lyapunov exponents are reliable.

The paper is organized as follows. Section 2 provides details on the reconstruction technique including the description of the basis of polynomials, the estimation of the standard function and the integration of the standard system. Section 3 describes the method for calculating the Lyapunov spectrum and the validation of reconstructions with LEs. Section 4 draws conclusions.

2. Global vector-field reconstruction of systems

2.1. Standard system

The aim of a global vector-field reconstruction is to establish the differential equations reproducing the dynamics of the studied system from a time series. In this section we just briefly outline the methodology of Gouesbet. For more details see Refs.[4–11] and the review paper Ref.[1].

From a scalar time series $\{x_i\}$ of an observable of the system under study, we can obtain successive derivatives of the observable, for instance by using a finite difference scheme,[22] and determine a vectorial time series $\{X_i, Y_i, Z_i, \ldots\}$ for the reconstruction of phase space according to

$$X_i = x_i, \quad Y_i = \dot{x}_i, \quad Z_i = \ddot{x}_i, \ldots \tag{1}$$

The number of variables to be used (components of the vectorial time series) is the embedding dimension. There are several methods to determine the embedding dimension, reviewed in Ref.[1]. Let us only state here that, if a global vector-field reconstruction is successful by using d_{E} variables, then d_{E} is a correct embedding dimension. In the sequel, we assume d_{E}=3 which is sufficient to our purpose. Following the approach introduced in Ref.[4], we then introduce the differential equations of motion under the form of a standard system as

$$\dot{X} = Y, \tag{2}$$

$$\dot{Y} = Z, \tag{3}$$

$$\dot{Z} = F(X, Y, Z), \tag{4}$$

where $F(X,Y,Z)$ is called the standard function. A successful global vector-field reconstruction then requires to evaluate a good enough approximation to the standard function. As in Ref.[7] we use multivariate polynomials but we implement the approximation technique in a different way.

2.2. Estimation of the standard function with polynomials

In contrast with Ref.[7], we use a SVD method [23] to determine the best coefficients of the expansion of the standard function over a set of multivariate monomials. The standard function expansion may be written as (for arbitrary embedding dimension)

$$F(x_1, x_2, \ldots, x_m) = \sum_{n=1}^{N_{\mathrm{P}}} A_n x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_m^{\alpha_m}, \tag{5}$$

where m is the embedding dimension, x_1, x_2, $x_3, \ldots, x_m$ are derivative coordinates spanning the phase space, and α_1, α_2, $\alpha_3, \ldots, \alpha_m$ are their power indices, respectively. Also $N_{\rm P}$ is the number of monomials retained in the expansion and A_n are the constant coefficients to be evaluated. Obviously, each subscript n of A_n corresponds to only one set of indices α_1, α_2, $\alpha_3, \ldots, \alpha_m$. We define the polynomial range $M_{\rm P}$ as the number of integer values, starting from 0, which may be accepted by each power index. For instance, if $M_{\rm P}$=2, then we have to deal with monomials containing x_i^0 and x_i^1 (i=1, 2, ..., m). When the embedding dimension m and the polynomial range $M_{\rm P}$ are given, then the total number of monomials is determined, namely, $N_{\rm P} = M_{\rm P}^m$. The index list α_1, α_2, $\alpha_3, \ldots, \alpha_m$ can then be considered as a m bit $M_{\rm P}$-decimal number (like binary or hexadecimal number). For instance, for m=2, $M_{\rm P}$=2, we have four monomials with indices 00, 01, 10, 11 which are binary representations of 0, 1, 2, 3. Therefore, for a given subscript n which is a decimal number, the associated index list α_1, α_2, $\alpha_3, \ldots, \alpha_m$ can be derived by the number transform:

$$\begin{aligned}
&\alpha_1 = \mathrm{Int}[(n-1)/M_{\rm P}^{m-1}],\\
&\alpha_2 = \mathrm{Int}\{[(n-1) - \alpha_1 M_{\rm P}^{m-1}]/M_{\rm P}^{m-2}\},\\
&\alpha_3 = \mathrm{Int}\{[(n-1) - \alpha_1 M_{\rm P}^{m-1} - \alpha_2 M_{\rm P}^{m-2}]/M_{\rm P}^{m-3}\},\\
&\quad \ldots\ldots\\
&\alpha_m = \mathrm{Int}[(n-1) - \alpha_1 M_{\rm P}^{m-1} - \alpha_2 M_{\rm P}^{m-2} \ldots \alpha_{m-1} M_{\rm P}],
\end{aligned} \tag{6}$$

where Int( ) is the integer function. For example, if m=6, $M_{\rm P}$=5, n=13, then the index list is $\alpha_1, \ldots, \alpha_6$=0, 0, 0, 0, 2, 2. That means the 13th term in the polynomial expansion (5) is $A_{13}\ x_5^2\ x_6^2$. This method for indexing the monomials is an improvement with respect to the more complicated one used in Ref.[7]. Finally, by applying (5) to points of the flow in phase space, the coefficients A_n of a standard function can be estimated by solving linear algebra equations with a SVD method. In fact, the SVD includes the least squares optimum algorithm, and it is especially suitable for this kind of problem. The aforementioned linear equations read as

$$\left(\sum_{n=1}^{N_{\rm P}} A_n x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_m^{\alpha_m} \right)_i = (\dot{x}_m)_i, \quad (i = 1, N_{\rm q}), \tag{7}$$

where $N_{\rm q}$ is the number of points used for fitting the function ($N_{\rm q} \geq N_{\rm P}$). We can utilize all the points of the available vectorial time series or only a sample of them. In the last case, it may be necessary to sample enough points $N_{\rm s}$ during one pseudo-period of the attractor. Otherwise, the lost information may lead to a failure of the reconstruction. To select a best model, we may use an estimation error which is defined by

$$Err = \frac{1}{N_{\rm q}} \sum_{i=1}^{N_q} \left| \frac{F(x_1, x_2, \ldots, x_m) - \dot{x}_m}{\dot{x}_m} \right|_i . \tag{8}$$

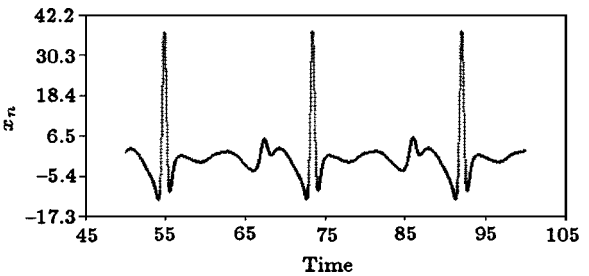

Fig.1. Comparison of fitted curve and original data points.

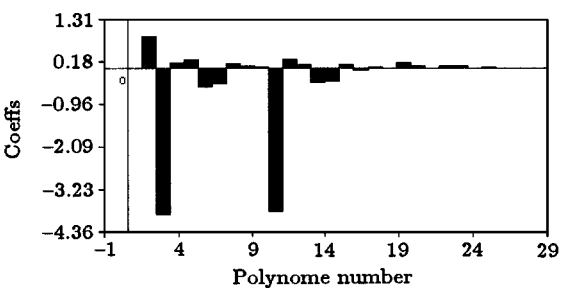

Fig.2. Spectrum of polynomial coefficients.

As an example, the observable x of the Rössler system and its derivatives are employed as original data for a global vector-field reconstruction. With the parameters m=3, $M_{\rm P}$=3, $N_{\rm s}$=1, $N_{\rm p}$=27, $N_{\rm q}$=25000, we obtain $Err = 7.1 \times 10^{-2}$. Figure 1 displays a satisfactory comparison between the reconstructed and the original data (for the sake of clarity only 5000 from the total 25000 points are plotted). Figure 2 displays the coefficient spectrum of the reconstructed polynomials.

2.3. System reconstruction

When the standard function F is obtained, we have to integrate the equations of the standard system (2)–(4). Usually, it is not a difficult task if we possess a good enough estimation of the standard function. A fourth-order Runge–Kutta integrator is then employed with a time step δt which is small enough to guarantee the numerical stability and accuracy. This

same time step is used to evaluate standard coordinates (derivatives) with a second-order centred finite difference scheme. Under these circumstance, the reconstruction quality depends on a driving vector defined by Gouesbet [6] as (δt, N_q, N_s, N_P). We can try with different driving vectors to determine an optimal one by using the criterion of estimation error Err (8).

The Rössler system was selected to exemplify our new implementation of algorithm, because it is a well studied and relatively simple system. It is specifically defined by the following equations:

$$\dot{x} = -y - z, \tag{9}$$

$$\dot{y} = x + ay, \tag{10}$$

$$\dot{z} = b + z(x - c), \tag{11}$$

with the parameters a=0.398, b=2.0, c=4.0 for the chaotic behaviour displayed in Fig.3. Its standard system can be easily derived from the original equations by transforming the original coordinates (x, y, z) to the new ones (X, Y, Z).[5] If the observable x and its derivatives are used to span the phase space, then

$$X = x, \tag{12}$$

$$Y = -y - z, \tag{13}$$

$$Z = -b - x - ay + z(c - x). \tag{14}$$

The exact standard system under the form (2)–(4) is then obtained with the standard function as

$$\begin{aligned} F(X, Y, Z) =& ab - cX + X^2 - aXY + XZ \\ &+ (ac - 1)Y + (a - c)Z \\ &- \frac{Y}{a + c - X}(X + b - aY + Z). \end{aligned} \tag{15}$$

This exact standard system has a singularity at $x = a + c$, leading to numerical difficulties when the integration is performed. As an alternative, we obtain the exact phase-portrait of the standard system by transforming the coordinates of the integrated original system with the aid of (10)–(12) leading to Fig.4.

Now, we treat the Rössler system as an unknown system, and try to reconstruct an equivalent system from a time series issued from it. The only available information is the time series $\{x_i\}$ obtained by integrating the original system. We reconstruct the system in two different ways.

First, we integrate only the last equation (4) of the standard system, i.e. the one which expresses the standard function. Other variables are calculated with known derivatives. Figure 5 is the reconstructed system with driving vector (10^{-2}, 45000, 1, 51). It has almost the same map as the exact one, that means the standard function is accurate enough at the original points. Second, we integrate all equations of standard system (1)–(3) just with a given initial point, and so on. With the same driving vector, the reconstructed system is shown in Fig.6. Although the reconstructed system still possesses two attractors, the second attractor becomes more weak, that results in more smooth trajectories between the two attractors. We can find some evidence from Fig.1 to explain this: there are periodical peaks of the third derivative, which correspond to steep trajectories near the second attractor in the original system. No matter how accurate is the estimation of standard function with polynomials, after all, we lose some information, especially at the points of steep trajectories. Another reason may be the intrinsic character of the dynamical system. If the system is sensitive to initial conditions, we can only reconstruct the main characteristics of the original system with different portraits in the phase space. The validation will be discussed later with LEs in Section 3.2.

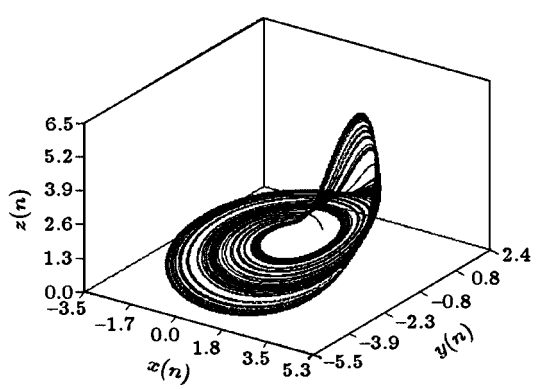

Fig.3. Original Rössler system.

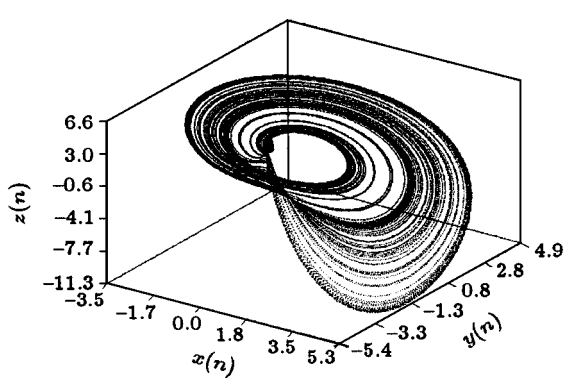

Fig.4. Exact standard system.

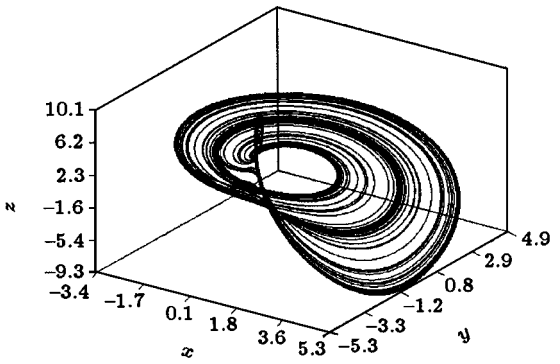

Fig.5. Reconstructed system (a).

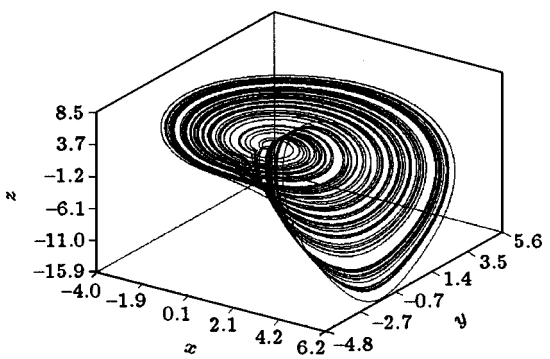

Fig.6. Reconstructed system (b).

3. Validation with Lyapunov exponents

3.1. Algorithm for Lyapunov exponents

Extreme sensitivity to initial conditions is commonly accepted as one of the most important properties of a nonlinear system. This property is quantified by Lyapunov exponents. A m-dimensional dynamical system has m principal direction in which the nearby trajectories diverge or converge in phase space. The Lyapunov exponents are the average exponential rates of the divergence or convergence of nearby trajectories. Any system containing at least one positive Lyapunov exponent is defined as chaotic.

As discussed in Section 1, there exist several methods for calculating the LEs of known and unknown systems, respectively. We selected a classic method [15] from the group for known systems because our standard system has explicit equations. Consider a m-dimensional continuous-time dynamic system

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = F(t, Z), \tag{16}$$

where Z and F are m-dimensional vector fields. To determine the Lyapunov exponents, we must trace the long-term evolution of an infinitesimal m-sphere of states in phase space from the initial conditions $Z(0)$. To analyse the propagation of small deviation from initial condition, we linearize Eq.(16) and get

$$\frac{\mathrm{d}\delta Z}{\mathrm{d}t} = J\delta Z, \tag{17}$$

where δZ is the tangent vector, and J is a $m \times m$ Jacobian matrix with $J_{i,j} = \partial F_i/\partial z_j$. For our standard system (1)–(3), for example, the Jacobian matrix of a three-dimensional system is

$$J = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ \partial F/\partial X & \partial F/\partial Y & \partial F/\partial Z \end{pmatrix}.$$

A solution of (17) can be obtained by numerical integration:

$$\delta Z^{n+1} = (I + \delta t J)\delta Z^n, \tag{18}$$

where I is unit matrix. To integrate Eq.(18), a m-dimensional orthogonal tangent vector must be chosen as initial condition of δZ. The standard choice is

$$e_1 = (1, 0, 0, 0, \ldots, 0),$$

$$e_2 = (0, 1, 0, 0, \ldots, 0),$$

$$\ldots\ldots$$

$$e_m = (0, 0, 0, 0, \ldots, 1).$$

After one time step, the yielded vectors become $v_1,\ v_2,\ \ldots, v_m$. These vectors are orthonormalized using a GSR (Gram–Schimdt reorthonormalization) procedure [13,24] to get new base vectors,

$$\begin{aligned}
\hat{e}_1 =& v_1/||v_1||, \\
\hat{e}_2 =& [v_2 - (v_2, \hat{e}_1)\hat{e}_1]/||v_2 - (v_2, \hat{e}_1)\hat{e}_1||, \\
& \ldots\ldots \\
\hat{e}_m =& [v_m - (v_m\hat{e}_1)\hat{e}_1 - (v_m\hat{e}_2)\hat{e}_2 - \cdots] \\
& /||v_m - (v_m, \hat{e}_1)\hat{e}_1 - (v_m, \hat{e}_2)\hat{e}_2 - \cdots||.
\end{aligned}$$

This procedure is performed at each time step and the norms $L_1, L_2, \ldots, L_m$ in the denominators are stored for calculating the LEs. The orthonormalized vectors are used as new conditions for next iteration. The Lyapunov exponents can be computed from its definition that the norms are proportional to $\mathrm{e}^{\lambda t}$ in the long run if there exists an attractor as

$$|\delta Z^{n+1}| = \mathrm{e}^{\lambda\delta t}|\delta Z^n|. \tag{19}$$

Substituting the vectors $e_1, e_2, \ldots, e_m$ to (19) respectively, we obtain the LEs of different direction. After N step integration at time $N\delta t$, the average Lyapunov exponents are

$$\lambda_i = \frac{1}{N\delta t}\sum_{n=1}^{N}\ln(L_i), \quad (i = 1, 2, \ldots, m). \tag{20}$$

Since the GSR never affects the direction of the first vector, then the first vector tends to seek the direction in which its norm grows most rapidly, so the first LE will be the largest one. The Lyapunov dimension is defined by Kaplan and York [18] as

$$d_{\mathrm{f}} = j + \frac{1}{|\lambda_{j+1}|}\sum_{i=1}^{j}\lambda_i, \tag{21}$$

where j is defined by the condition

$$\sum_{i=1}^{j}\lambda_i > 0 \quad \text{and} \quad \sum_{i=1}^{j+1}\lambda_i < 0.$$

This definition implies that the calculation of Lyapunov dimension needs all the positive and most of the negative Lyapunov exponents. However, for most algorithms designed for computing the LEs from a time series, it is very difficult or even impossible to estimate all Lyapunov exponents. With our method, if the standard system is integrated, the Jacobian matrix J is also obtained by computing the partial derivatives of the standard function. Theoretically, it has no problem calculating all the Lyapunov exponents from the time series.

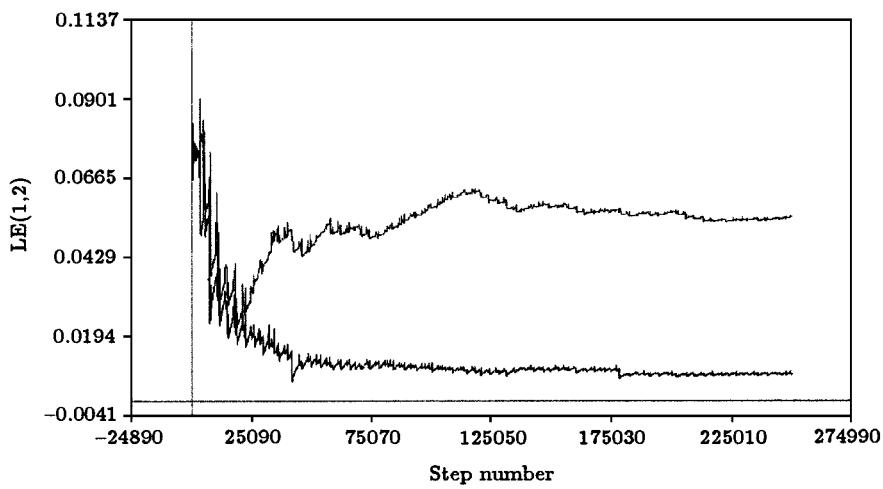

Fig.7. 1st, 2nd LEs with integration step of original Rössler system.

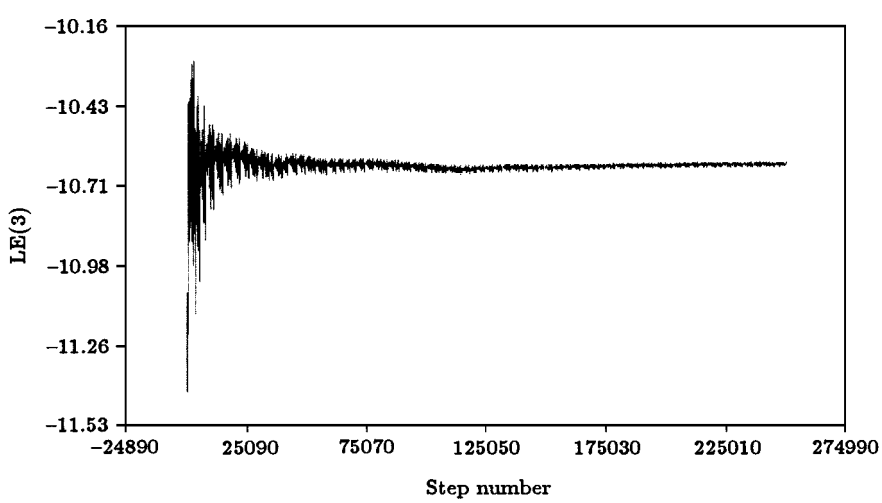

Fig.8. Third LE with integration step of original Rössler system.

To test the computational program, we firstly calculated the Lyapunov exponents of the original Rössler systems with the constants a=0.15, b=0.20, c=10.0 for comparison. Figures 7 and 8 show the evolution of three exponents with iteration steps. Obviously, the LEs converge to constants with the time, and the algorithm is stable. The average exponents are listed in Table 1 with the values from Ref.[18] and Ref.[21]. It must be noted that Wolf used log2 to evaluate the LEs in Ref.[18], while we revalued them in Table 1 with natural logarithms. Our first LE is smaller, the second is greater than those given in Ref.[18] and Ref.[21], but the Lyapunov dimension $d_{\rm f}$ is nearly equal. Usage of a different kind of phase space for the calculation may be the main explanation of the different results. In our opinion, the Rössler system has two attractors, and it should have two positive LEs, and keep the total amount of LEs negative, because the system is global deterministic and stable, but is locally unstable.

3.2. Validation of reconstruction by LEs and LD

There are several techniques for validating a reconstructed system, such as topologic map, synchronization, diagram of bifurcation, etc. But here, we employ the LEs and LD. With the exact standard system and the algorithm for computing Lyapunov exponents, we can validate the reconstructed systems by identifying if it has the same dynamical characters of the original system.

Table 1. LEs of Rössler system with a=0.15, b=0.20, c=10.0.

	λ_1	λ_2	λ_3	$d_{\rm f}$
Ref.[18]	0.0901	0.00	–9.773	2.009
Ref.[21]	0.0853	–	–	–
Our results	0.05767	0.00895	–10.640	2.006

The Rössler system is employed again as the test case. The LEs and LDs of the original system, exact standard system and reconstructed systems are calculated and listed in Table 2. As we expected, the LEs and LD values of all these systems are nearly equivalent, the number of positive LEs also keeps the same value. So we can use the LEs and LD to validate the system reconstruction.

The first two LEs of the exact standard system are greater than those of the original system, but the third negative LE and LD have very small differences from the original ones. Despite of the differences, we have reason to believe that the exact standard system is equivalent to the original system. That means that it is possible to reconstruct the original system from a time series, because the exact standard system, in fact, is the theoretical reconstructed system.

Table 2. LEs of Rössler system with a=0.389, b=2.0, c=4.0.

	Driving vector	λ_1	λ_2	λ_3	$d_{\rm f}$
Original system	$\delta_{\rm t}=10^{-2}$	0.0457	0.0015	–3.3234	2.0142
Exact standard system	$N_{\rm q}$=150000	0.0821	0.0023	–3.3987	2.0248
Reconstructed (a)	$\delta_{\rm t}=2\times10^{-3}$, $N_{\rm P}$=27	0.1174	0.0192	–3.7688	2.0362
Reconstructed (b)	$N_{\rm q}$=222600, $N_{\rm s}$=1	0.0866	0.0139	–3.6030	2.0278

The LEs of the reconstructed system are also greater than that of the original system, but the sign of LEs, and the sum of LEs and the LD remain near to the values of the original system. The LEs of reconstructed system (a) (Fig.5) are greater than the LEs of the exact standard system. However, the LEs of reconstructed system (b) (Fig.6) are near to that of the original system and the exact standard system. There may be two reasons for this. First, the exact standard system causes the original attractor to become stronger (more sensitive) because of the derivative techniques; system (a) is integrated using the known derivatives (Y, Z) and only the last equation is integrated. Second, although the reconstructed system (b) is based on the same derivatives with which the exact standard system is embedded, it is impossible to avoid the smoothing of the peaks of derivative $\dot{z}$ when they are fitted by polynomials; as we discussed in Section 2, these peaks correspond to the steep trajectories near the second attractors. Therefore, when the system is reconstructed from a given start point as in system (b), the standard function is no longer limited to the known derivatives (Y, Z); it tends to show smoother trajectories (see Fig.6) and smaller LEs.

The Lyapunov dimension, like the fractal dimension, can be used not only to diagnose the chaos, but also to provide some dynamical information for embedding. Normally, the LD is set as $d_{\rm f} = D + \delta$,

where $0 < \delta < 1$, D is an integer. Then the smallest dimension needed for embedding is $D+1$. All the LDs of the original, exact and reconstructed standard systems are nearly equal to 2. We can conclude that the reconstruction with derivatives does not change the dimension of attractors existing in the original Rössler system.

4. Conclusions

The methods we have presented for the global vector-field reconstruction and validation were applied successfully to the Rössler system. Reconstruction with derivatives can retain the topological character and keep close to the LE values of the original system. Therefore, it is not enough to validate the reconstructed system just by comparison of topological character; the Lyapunov exponents and dimension must be considered as important criteria. A good standard function $F(X, Y, Z)$ is the primary factor for a successful reconstruction. Other methods, such as wavelets, will be tried in our future work.

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