# A comparative study of computation of Lyapunov spectra with different algorithms 

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#### Abstract

In this paper we make a detailed numerical comparison between three algorithms for the computation of the full Lyapunov spectrum as well as the associated eigenvectors of general dynamical systems. They are: (a) the standard method, (b) a differential formulation of the standard method, and (c) a new algorithm which does not require rescaling and reorthogonalization. We also bring out the relations among these methods. Moreover, we give a simplified formulation of the new algorithm when the dimensionality of the system is 4 . We find that there is reasonable agreement among the Lyapunov spectra obtained using the three algorithms in most cases. However the standard method seems to be the most efficient followed by the new method and the differential version of the standard method (in that order), as far as the CPU time for the computation of the Lyapunov spectra is concerned. The new method is hardly suitable for finding the eigenvectors, whereas the other procedures give nearly identical numerical results. ©2000 Elsevier Science B.V. All rights reserved.


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## 1. Introduction

Extreme sensitivity to initial conditions is the commonly accepted defining property of chaos in nonlinear systems. Lyapunov exponents which determine the exponential rates at which nearby trajectories diverge on an average, are the quantitative characteristics of a chaotic orbit. A dynamical system of dimension $n$ has $n$ Lyapunov exponents and $n$ principal directions or eigenvectors, corresponding to a set of nearby trajectories [1]. One of the standard and popular methods to compute the Lyapunov spectrum of a dynamical system involves a Gram-Schmidt Reorthonormalizaton (GSR) of the 'tangent vectors' [2,15,16]. A differential version of this method has been formulated which corresponds to a continuous GSR of the tangent vectors [3]. A modification of this method with the introduction of a stability

[^0]parameter makes it dynamically stable, applicable to systems with degenerate spectra, and reliable for computations [4]. Recently, a new algorithm for the computation of Lyapunov exponents has been proposed, which has been claimed to be valid even for evaluating partial Lyapunov spectra [5]. This is based on the 'QR' method for the decomposition of the tangent map (where $Q$ is an orthogonal matrix and $R$ is an upper triangular matrix) which has been studied by several authors [6]. It utilizes representations of orthogonal matrices applied to the tangent map, and does not require the GSR procedure. It has also been claimed that it has several advantages over the existing methods, as it involves a minimum number of equations. In this paper we have made a detailed comparison of the three algorithms as regards accuracy and efficiency, by computing the full Lyapunov spectra of some typical nonlinear systems with 2,3 and 4 variables. We also compare the performance of the standard method with its differential version, in computing the Lyapunov eigenvectors.

In Section 2, we outline the three methods with necessary details. We bring out the relation between the differential version of the standard method and the new procedure, by deriving the differential equations of the latter from those of the former. It is difficult to use the new method with a standard representation of orthogonal matrices when the number of dimensions of the system is greater than 3. In Section 3, we give a convenient representation for them for $n=4$, by making use of the well-known fact that $S O(4) \sim S O(3) \times S O(3)$ [7]. This simplifies the calculations considerably. In Section 4, we make a comparative study of the three algorithms for the computation of Lyapunov spectra by taking up some typical 2, 3 and 4 dimensional systems. We have considered both dissipative and Hamiltonian systems of some physical interest, for comparison. In Section 5, we compare the computation of the Lyapunov eigenvectors (which are local properties), using these algorithms. In Section 6, we make a few concluding remarks.

## 2. Computation of Lyapunov exponents

Consider an $n$-dimensional continuous-time dynamical system

$$
\begin{equation*}
\frac{\mathrm{d} \mathbf{Z}}{\mathrm{~d} t}=\mathbf{F}(\mathbf{Z}, t) \tag{1}
\end{equation*}
$$

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 $\mathbf{Z}(0)$, we have to find the long term evolution of the axes of an infinitesimal sphere of states around $\mathbf{Z}(0)$. For this, consider the tangent map given by the set of equations,

$$
\begin{equation*}
\frac{\mathrm{d} \delta \mathbf{Z}}{\mathrm{~d} t}=\mathbf{J} \delta \mathbf{Z} \tag{2}
\end{equation*}
$$

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

$$
\begin{equation*}
J_{i j}=\frac{\partial F_{i}}{\partial Z_{j}} . \tag{3}
\end{equation*}
$$

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

$$
\begin{equation*}
\delta \mathbf{Z}(\mathrm{t})=\mathbf{M}(\mathbf{Z}(t), t) \delta \mathbf{Z}(0), \tag{4}
\end{equation*}
$$

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

$$
\begin{equation*}
\frac{\mathrm{d} \mathbf{M}}{\mathrm{~d} t}=\mathbf{J} \mathbf{M} . \tag{5}
\end{equation*}
$$

In the following, we give a brief description of the procedures for computing the $n$ Lyapunov exponents of the system using (a) the standard method, (b) the differential version of the standard method and (c) the new method
based on the 'QR' decomposition of $M$, which dispenses with the tangent vectors $\delta \mathbf{Z}$, and in a sense, computes the exponents directly.

### 2.1. Standard method

Let $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n}$ be the $n$ Lyapunov exponents of the system in a decreasing sequence, $\lambda_{1} \geq \lambda_{2} \geq \cdots \geq \lambda_{n}$. In the standard method $[2,15,16]$ one first chooses $n$ orthogonal tangent vectors as initial conditions for Eq. (2). The standard choice is $\hat{\mathbf{e}}_{1}(0)=(1,0,0, \ldots) ; \hat{\mathbf{e}}_{2}(0)=(0,1,0,0, \ldots)$, etc. Eq. (2) is then solved up to time $\tau$ for each of the initial conditions yielding vectors $\mathbf{v}_{1}(\tau), \mathbf{v}_{2}(\tau), \ldots, \mathbf{v}_{n}(\tau)$. These vectors are orthonormalized using a GSR procedure to yield

$$
\begin{equation*}
\hat{\mathbf{e}}_{1}(\tau)=\frac{\mathbf{v}_{1}}{\left\|\mathbf{v}_{1}\right\|}, \quad \hat{\mathbf{e}}_{2}(\tau)=\frac{\mathbf{v}_{2}-\left(\mathbf{v}_{2}, \hat{\mathbf{e}}_{1}(\tau)\right) \hat{\mathbf{e}}_{1}(\tau)}{\left\|\mathbf{v}_{2}-\left(\mathbf{v}_{2}, \hat{\mathbf{e}}_{1}(\tau)\right) \hat{\mathbf{e}}_{1}(\tau)\right\|} \tag{6}
\end{equation*}
$$

and so on. The norms in the denominators, denoted by $N_{1}(1), N_{2}(1), \ldots, N_{n}(1)$, are stored for the computation of Lyapunov exponents. The procedure is repeated for a subsequent time $\tau$ of integration using $\hat{\mathbf{e}}_{i}(\tau)$ as initial conditions for Eq. (2). The resulting vectors $\mathbf{v}_{i}(2 \tau)$, are again orthonormalized using a GSR procedure to yield orthonormal tangent vectors $\hat{\mathbf{e}}_{i}(2 \tau), \quad i=1, \ldots, n$ and the norms $N_{1}(2), N_{2}(2), \ldots, N_{n}(2)$. After $r$ iterations, we get the orthonomal set of vectors $\hat{\mathbf{e}}_{i}(r \tau), i=1, \ldots, n$ at time $t=r \tau$. The Lyapunov exponents are

$$
\begin{equation*}
\lambda_{i}=\lim _{r \rightarrow \infty} \frac{\sum_{m=1}^{r} \log N_{i}(m)}{r \tau} \tag{7}
\end{equation*}
$$

This is due to the following reason. Since GSR never affects the direction of the first vector in a system, this vector tends to seek out the direction in the tangent space, which is most rapidly growing and its norm is proportional to $\mathrm{e}^{\lambda_{1} t}$ for large $t$. The second vector has its component along the direction of the first vector removed and its norm would be proportional to $\mathrm{e}^{\lambda_{2} t}$ for large $t$ and so on.

It is to be noted that we have to integrate $n(n+1)$ coupled equations in this method, as there are $n$ equations for the fiducial trajectory in (1) and $n$ copies of the tangent map equations in (2).

### 2.2. Differential version of the standard method

In this method [3], the orthonormal set of vectors $\hat{\mathbf{e}}_{i}(t)$ are obtained by solving differential equations set up for them, instead of resorting to the GSR at discrete steps. Rather, GSR is incorporated in the procedure itself. It can be shown that

$$
\begin{equation*}
\frac{\mathrm{d}}{\mathrm{~d} t} \hat{\mathbf{e}}_{i}(t)=\mathbf{G} \hat{\mathbf{e}}_{i}-G_{i i} \hat{\mathbf{e}}_{i}-\sum_{j=1}^{i-1}\left(G_{i j}+G_{j i}\right) \hat{\mathbf{e}}_{j} \tag{8}
\end{equation*}
$$

where $\mathbf{G}=\mathbf{J}$ is the Jacobian matrix introduced in Eq. (2) and

$$
\begin{equation*}
G_{i j}=\left(\hat{\mathbf{e}}_{i}(t), \mathbf{J}(\mathbf{Z}(t)) \hat{\mathbf{e}}_{j}(t)\right) \tag{9}
\end{equation*}
$$

that is, $G_{i j}$ are the matrix elements of the Jacobian in the basis $\hat{\mathbf{e}}_{i}(t)$. Now let $\hat{\mathbf{e}}_{i}(0)$ evolve to $\mathbf{e}_{i}(t)$ :

$$
\begin{equation*}
\mathbf{e}_{i}(t)=\mathbf{M}(\mathbf{Z}(t), t) \hat{\mathbf{e}}_{i}(0) \tag{10}
\end{equation*}
$$

In fact, $\hat{\mathbf{e}}_{i}(t)$ is the orthonormalized set corresponding to $\mathbf{e}_{i}(t) i=1, \ldots, n$. Define

$$
\begin{equation*}
d_{i j}=\left(\mathbf{e}_{i}(t), \hat{\mathbf{e}}_{j}(t)\right) \tag{11}
\end{equation*}
$$

The GSR procedure ensures that $\mathrm{d}_{i j}$ is a lower triangular matrix

$$
\begin{equation*}
d_{i j}=0, \quad i<j \tag{12}
\end{equation*}
$$

It can be shown that

$$
\begin{equation*}
\dot{d}_{i i}=G_{i i} d_{i i}, \quad i=1, \ldots, n \tag{13}
\end{equation*}
$$

and that,

$$
\begin{equation*}
d_{i i}=\mathrm{e}^{\lambda_{i} t} \tag{14}
\end{equation*}
$$

for large $t$. That is,

$$
\begin{equation*}
\lambda_{i}=\lim _{t \rightarrow \infty} \frac{1}{t} \log d_{i i} \tag{15}
\end{equation*}
$$

The Lyapunov exponents are computed by solving the coupled Eqs. (1), (8) and (13), in this method. As there are $n^{2}$ equations for the $n$ components each of the orthonormal vectors $\hat{\mathbf{e}}_{i}(t)$ in Eq. (8), $n$ equations for $d_{i i}$ in Eq. (13), apart from the $n$ equations for the fiducial trajectory in (1), we have to integrate $n(n+2)$ coupled equations in this method.

In practice, this procedure is not numerically 'stable', as the set $\hat{\mathbf{e}}_{i}(t)$ may not remain orthonormal under the time evolution. In particular, $\Delta_{i j}$ defined by $\Delta_{i j}=\left(\hat{\mathbf{e}}_{i}(t), \hat{\mathbf{e}}_{j}(t)\right)-\delta_{i j}, 1 \leq i, j \leq n$ may not all vanish. Moreover, the method is not applicable to systems with degenerate exponents. These are remedied by a modification of the method, using a stability parameter $\beta[4]$. We replace $G_{i i}$ by $G_{i i}+\beta\left(\left(\hat{\mathbf{e}}_{i}, \hat{\mathbf{e}}_{i}\right)-1\right)$ and $G_{i j}$ by $G_{i j}+\beta\left(\hat{\mathbf{e}}_{i}, \hat{\mathbf{e}}_{j}\right), i \neq j$ in Eqs. (8) and (13). Though it has been shown that the method is strongly stable when $\beta>-\lambda_{n}$, where $\lambda_{n}$ is the lowest exponent, it is found in certain problems, that $\beta$ has to be significantly larger than $-\lambda_{n}$ in practice. Moreover, it may be pointed out that this method requires prior knowledge of the lowest Lyapunov exponent $\lambda_{n}$ for the computation of the complete spectrum $\lambda_{i}$. If an arbitrarily high value is assigned to $\beta$, one ends up with an arithmetic overflow problem during computations.

### 2.3. New method based on a ' $Q R$ ' decomposition of $M$

The new algorithm [5] is based on a ' QR ' decomposition of $M$, where $Q$ is an orthogonal matrix and $R$ is an upper triangular matrix. This results in a set of coupled differential equations for the Lyapunov exponents along with the various angles parametrizing the orthogonal matrices. In this subsection, we derive these equations from the differential version of the standard method considered in the previous subsection.

Consider the tangent map matrix M. From Eq. (10),

$$
\begin{equation*}
M_{i j}=\left(\hat{\mathbf{e}}_{i}(0), \mathbf{M} \hat{\mathbf{e}}_{j}(0)\right)=\left(\hat{\mathbf{e}}_{i}(0), \mathbf{e}_{j}(t)\right) \tag{16}
\end{equation*}
$$

As $\hat{\mathbf{e}}_{j}(t)$ form an orthonormal set of vectors, we have from Eq. (11),

$$
\begin{equation*}
\mathbf{e}_{j}(t)=\sum \hat{\mathbf{e}}_{k}(t) d_{j k} \tag{17}
\end{equation*}
$$

Hence,

$$
\begin{equation*}
M_{i j}=\sum_{k}\left(\hat{\mathbf{e}}_{i}(0), \hat{\mathbf{e}}_{k}(t)\right) d_{j k} \tag{18}
\end{equation*}
$$

Define the matrices $Q$ and $R$ by

$$
\begin{equation*}
Q_{i j}=\left(\hat{\mathbf{e}}_{i}(0), \hat{\mathbf{e}}_{j}(t)\right)=\left(\hat{\mathbf{e}}_{j}(t)\right)_{i} \tag{19}
\end{equation*}
$$

and

$$
\begin{equation*}
R_{i j}=d_{j i} \tag{20}
\end{equation*}
$$

Hence,

$$
\begin{equation*}
M=Q R \tag{21}
\end{equation*}
$$

Clearly the columns of $Q$ are the orthonormal vectors $\hat{\mathbf{e}}_{j}(t)$, and $Q$ an orthogonal matrix. As $d$ is a lower triangular matrix, $R$ an upper triangular matrix.

Now $G_{i j}$ and $J_{i j}$ are the matrix elements of the Jacobian in the orthonormal bases $\hat{\mathbf{e}}_{i}(t)$ and $\hat{\mathbf{e}}_{i}(0)$, respectively, and related by a rotation transformation represented by $Q$.

Introducing complete sets of states at the appropriate places, we have

$$
\begin{equation*}
G_{i j}=\left(\hat{\mathbf{e}}_{i}(t), \mathbf{J} \hat{\mathbf{e}}_{j}(t)\right)=\sum_{k, l}\left(\hat{\mathbf{e}}_{i}(t), \hat{\mathbf{e}}_{k}(0)\right)\left(\hat{\mathbf{e}}_{k}(0), \mathbf{J} \hat{\mathbf{e}}_{l}(0)\right)\left(\hat{\mathbf{e}}_{l}(0), \hat{\mathbf{e}}_{j}(t)\right)=\sum_{k, l} \tilde{Q}_{i k} J_{k l} Q_{l j}=(\tilde{Q} J Q)_{i j} \tag{22}
\end{equation*}
$$

Taking the scalar product of Eq. (8) with $\hat{\mathbf{e}}_{j}(0)$ and making appropriate changes of indices, we have

$$
\begin{align*}
\frac{\mathrm{d}}{\mathrm{~d} t} Q_{j k} & =\frac{\mathrm{d}}{\mathrm{~d} t}\left(\hat{\mathbf{e}}_{j}(0), \hat{\mathbf{e}}_{k}(t)\right)=\left(\hat{\mathbf{e}}_{j}(0), \mathbf{J} \hat{\mathbf{e}}_{k}(t)\right)-G_{k k}\left(\hat{\mathbf{e}}_{j}(0), \hat{\mathbf{e}}_{k}(t)\right)-\sum_{l=1}^{k-1}\left(G_{k l}+G_{l k}\right)\left(\hat{\mathbf{e}}_{j}(0), \hat{\mathbf{e}}_{l}(t)\right) \\
& =\left(\hat{\mathbf{e}}_{j}(0), \mathbf{J} \hat{\mathbf{e}}_{k}(t)\right)-G_{k k} Q_{j k}-\sum_{l=1}^{k-1}\left(G_{k l}+G_{l k}\right) Q_{j l} \tag{23}
\end{align*}
$$

As all the quantities are real,

$$
\begin{equation*}
\tilde{Q}_{i j}=Q_{j i}=\left(\hat{\mathbf{e}}_{j}(0), \hat{\mathbf{e}}_{i}(t)\right)=\left(\hat{\mathbf{e}}_{i}(t), \hat{\mathbf{e}}_{j}(0)\right) \tag{24}
\end{equation*}
$$

Multiplying Eq. (23) by $Q_{i j}$ on the right and using the fact that

$$
\begin{equation*}
\tilde{Q}_{i j}\left(\hat{\mathbf{e}}_{j}(0), \mathbf{J} \hat{\mathbf{e}}_{k}(t)\right)=\sum_{j}\left(\hat{\mathbf{e}}_{i}(t), \hat{\mathbf{e}}_{j}(0)\right)\left(\hat{\mathbf{e}}_{j}(0), \mathbf{J} \hat{\mathbf{e}}_{k}(t)\right)=\left(\hat{\mathbf{e}}_{i}(t), \mathbf{J} \hat{\mathbf{e}}_{k}(t)\right)=G_{i k} \tag{25}
\end{equation*}
$$

we find

$$
\begin{align*}
\left(\tilde{Q} \frac{\mathrm{~d}}{\mathrm{~d} t} Q\right)_{i k} & =\tilde{Q}_{i j} \frac{\mathrm{~d}}{\mathrm{~d} t} Q_{j k}=G_{i k}-G_{k k} \sum_{j} \tilde{Q}_{i j} Q_{j k}-\sum_{j} \sum_{l=1}^{k-1}\left(G_{k l}+G_{l k}\right) \tilde{Q}_{i j} Q_{j l} \\
& =G_{i k}-G_{k k} \delta_{i k}-\sum_{l=1}^{k-1}\left(G_{k l}+G_{l k}\right) \delta_{i l} \tag{26}
\end{align*}
$$

as $Q$ is an orthonormal matrix.
Again, $\tilde{Q}(\mathrm{~d} / \mathrm{d} t) Q$ is an antisymmetric matrix as $Q$ is orthogonal and it is sufficient to consider $i>k$. In this case, the last term vanishes and we obtain,

$$
\begin{equation*}
\left(\tilde{Q} \frac{\mathrm{~d}}{\mathrm{~d} t} Q\right)_{i k}=G_{i k}=(\tilde{Q} J Q)_{i k}, \quad i>k \tag{27}
\end{equation*}
$$

$Q$ is an orthogonal matrix is characterized by $n(n-1) / 2$ angles and we obtain differential equations for these angles. From Eqs. (13) and (14), the differential equations for the Lyapunov exponents are

$$
\begin{equation*}
\frac{\mathrm{d}}{\mathrm{~d} t}\left(\lambda_{i} t\right)=G_{i i}=(\tilde{Q} J Q)_{i i} \tag{28}
\end{equation*}
$$

In this method, we have essentially traded the orthonormal vectors $\hat{\mathbf{e}}_{i}(t)$ for the orthogonal matrix $Q$ parametrized by the $n(n-1) / 2$ angles. We have to solve the coupled equations (1), (27) and (28) in this procedure to obtain the Lyapunov exponents. We have to integrate $n+(n(n-1) / 2)+n=n(n+3) / 2$ coupled equations in this method.

## 3. A convenient representation for $Q$ and simplification of $\tilde{Q} \dot{Q}$ for $\boldsymbol{n}=4$

In [5], the explicit representation of the orthogonal matrix $Q$ used is the one in which it is represented as a product of $n(n-1) / 2$ orthogonal matrices, each of which corresponds to a simple rotation in the $(i-j)$ th plane $(i<j)$. Thus $Q$

$$
Q=O^{(12)} O^{(13)} O^{(14)} \cdots O^{(1 n)} O^{(23)} \cdots O^{(n-2, n-1)} O^{(n-1, n)}
$$

where

$$
O_{k l}^{(i j)}= \begin{cases}1 & \text { if } k=l \neq i, j  \tag{29}\\ \cos \theta_{i j} & \text { if } k=l=i \text { or } j \\ \sin \theta_{i j} & \text { if } k=i, l=j \\ -\sin \theta_{i j} & \text { if } k=j, l=i \\ 0 & \text { otherwise }\end{cases}
$$

In terms of the group generators, $O^{(i j)}$ can be written as

$$
\begin{equation*}
O^{(i j)}=e^{\theta_{i j}\left(t_{i j}\right)} \tag{30}
\end{equation*}
$$

where the generator $t_{i j}$ is represented by

$$
\begin{equation*}
\left(t_{i j}\right)_{k l}=\delta_{i k} \delta_{j l}-\delta_{i l} \delta_{j k} \tag{31}
\end{equation*}
$$

The generators satisfy the commutation relations,

$$
\begin{equation*}
\left[t_{i j}, t_{m n}\right]=\delta_{i n} t_{j m}+\delta_{j m} t_{i n}-\delta_{i m} t_{j n}-\delta_{j n} t_{i m} \tag{32}
\end{equation*}
$$

The above representation for $Q$ is conceptually simple and works very well for $n=2$ and 3 [5]. However, for $n>3$, it is hardly suitable for practical computations of Lyapunov exponents. This is because the expressions for $\tilde{Q} \dot{Q}$ and $\tilde{Q} \mathbf{J} Q$ are very lengthy and unmanageable even for $n=4$.

In the present work, we employ a representation for $Q$, which simplifies the calculations and numerical computations for $n=4$. This is based on the well-known fact that $S O(4) \sim S O(3) \times S O(3)$ [7]. From the generators $t_{i j}$ we construct the following combinations:

$$
\begin{array}{ll}
M_{1}=\frac{1}{2}\left(t_{23}+t_{14}\right), \quad N_{1}=\frac{1}{2}\left(t_{23}-t_{14}\right) ; \quad M_{2}=\frac{1}{2}\left(t_{31}+t_{24}\right), \quad N_{2}=\frac{1}{2}\left(t_{31}-t_{24}\right) \\
M_{3}=\frac{1}{2}\left(t_{12}+t_{34}\right), \quad N_{3}=\frac{1}{2}\left(t_{12}-t_{34}\right) \tag{33}
\end{array}
$$

Then it is easily verified that $M_{i}$ and $N_{i}$ generate two mutually commuting $S O$ (3) algebras

$$
\begin{equation*}
\left[M_{i}, M_{j}\right]=-\epsilon_{i j k} M_{k}, \quad\left[N_{i}, N_{j}\right]=-\epsilon_{i j k} N_{k}, \quad\left[M_{i}, N_{j}\right]=0 \tag{34}
\end{equation*}
$$

We write $Q$ as

$$
\begin{equation*}
Q=Q_{I I} Q_{I} \tag{35}
\end{equation*}
$$

where

$$
\begin{equation*}
Q_{I I}=O^{(6)} O^{(5)} O^{(4)}=\mathrm{e}^{\theta_{6} N_{3}} \mathrm{e}^{\theta_{5} N_{2}} \mathrm{e}^{\theta_{4} N_{1}} \tag{36}
\end{equation*}
$$

and

$$
\begin{equation*}
Q_{I}=O^{(3)} O^{(2)} O^{(1)}=\mathrm{e}^{\theta_{3} M_{3}} \mathrm{e}^{\theta_{2} N_{2}} \mathrm{e}^{\theta_{1} M_{1}} \tag{37}
\end{equation*}
$$

Using

$$
\begin{equation*}
\mathrm{e}^{X} Y \mathrm{e}^{-X}=Y+[X, Y]+\frac{1}{2!}[X,[X, Y]]+\cdots \tag{38}
\end{equation*}
$$

for any matrices $X, Y$ and the commutation relations in Eq. (32), it can be easily verified that

$$
\begin{align*}
\tilde{Q} \dot{Q}= & \tilde{Q}_{I} \dot{Q}_{I}+\tilde{Q}_{I I} \dot{Q}_{I I}=\left[\dot{\theta}_{1}+\dot{\theta}_{3} \sin \theta_{2}\right] M_{1}+\left[\dot{\theta}_{2} \cos \theta_{1}+\dot{\theta}_{3} \sin \theta_{1} \cos \theta_{2}\right] M_{2} \\
& +\left[\dot{\theta}_{2} \sin \theta_{2}+\dot{\theta}_{3} \cos \theta_{1} \cos \theta_{2}\right] M_{3}+\left[\dot{\theta}_{4}+\dot{\theta}_{6} \sin \theta_{5}\right] N_{1}+\left[\dot{\theta}_{5} \cos \theta_{4}-\dot{\theta}_{6} \sin \theta_{4} \cos \theta_{5}\right] N_{2} \\
& +\left[\dot{\theta}_{5} \sin \theta_{5}+\dot{\theta}_{6} \cos \theta_{4} \cos \theta_{5}\right] N_{3} . \tag{39}
\end{align*}
$$

The explicit form of the matrices $M_{i}$ and $N_{i}$ can be found using Eqs. (31) and (33) and are written in terms of $2 \times 2$ blocks as given below

$$
\begin{align*}
& M_{1}=\frac{1}{2}\left[\begin{array}{ccc}
0 & \vdots & \sigma_{1} \\
\cdots & \ldots & \cdots \\
-\sigma_{1} & \vdots & 0
\end{array}\right], \quad M_{2}=\frac{1}{2}\left[\begin{array}{ccc}
0 & \vdots & -\sigma_{3} \\
\cdots & \ldots & \cdots \\
\sigma_{3} & \vdots & 0
\end{array}\right], \quad M_{3}=\frac{1}{2}\left[\begin{array}{cc}
\mathrm{i} \sigma_{2} & \vdots \\
\cdots & \cdots \\
\cdots \\
0 & \vdots \\
\mathrm{i} \sigma_{2}
\end{array}\right], \\
& N_{1}=\frac{1}{2}\left[\begin{array}{ccc}
0 & \vdots & -\mathrm{i} \sigma_{2} \\
\cdots & \ldots & \ldots \\
-\mathrm{i} \sigma_{2} & \vdots & 0
\end{array}\right], \quad N_{2}=\frac{1}{2}\left[\begin{array}{ccc}
0 & \vdots & -I \\
\cdots & \cdots & \cdots \\
I & \vdots & 0
\end{array}\right], \quad N_{3}=\frac{1}{2}\left[\begin{array}{ccc}
\mathrm{i} \sigma_{2} & \vdots & 0 \\
\cdots & \cdots & \cdots \\
0 & \vdots & -\mathrm{i} \sigma_{2}
\end{array}\right] . \tag{40}
\end{align*}
$$

Here I is the $2 \times 2$ identity matrix and $\sigma_{1}, \sigma_{2}, \sigma_{3}$ are the Pauli matrices:

$$
I=\left[\begin{array}{ll}
1 & 0  \tag{41}\\
0 & 1
\end{array}\right], \quad \sigma_{1}=\left[\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right], \quad \sigma_{2}=\left[\begin{array}{cc}
0 & -\mathrm{i} \\
\mathrm{i} & 0
\end{array}\right], \quad \sigma_{3}=\left[\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right] .
$$

Then we find that

$$
\tilde{Q} \dot{Q}=\left(\begin{array}{cccc}
0 & -f_{1}(\theta, \dot{\theta}) & -f_{2}(\theta, \dot{\theta}) & -f_{3}(\theta, \dot{\theta})  \tag{42}\\
f_{1}(\theta, \dot{\theta}) & 0 & -f_{4}(\theta, \dot{\theta}) & -f_{5}(\theta, \dot{\theta}) \\
f_{2}(\theta, \dot{\theta}) & f_{4}(\theta, \dot{\theta}) & 0 & -f_{6}(\theta, \dot{\theta}) \\
f_{3}(\theta, \dot{\theta}) & f_{5}(\theta, \dot{\theta}) & f_{6}(\theta, \dot{\theta}) & 0
\end{array}\right)
$$

where

$$
\begin{align*}
& f_{1}=-\frac{1}{2}\left(\dot{\theta}_{2} \sin \theta_{1}+\dot{\theta}_{3} \cos \theta_{1} \cos \theta_{2}+\dot{\theta}_{5} \sin \theta_{4}+\dot{\theta}_{6} \cos \theta_{4} \cos \theta_{5}\right), \\
& f_{2}=\frac{1}{2}\left(\dot{\theta}_{2} \cos \theta_{1}-\dot{\theta}_{3} \sin \theta_{1} \cos \theta_{2}+\dot{\theta}_{5} \cos \theta_{4}-\dot{\theta}_{6} \sin \theta_{4} \cos \theta_{5}\right), \\
& f_{3}=-\frac{1}{2}\left(\dot{\theta}_{1}+\dot{\theta}_{3} \sin \theta_{2}-\dot{\theta}_{4}-\dot{\theta}_{6} \sin \theta_{5}\right), \\
& f_{4}=-\frac{1}{2}\left(\dot{\theta}_{1}+\dot{\theta}_{3} \sin \theta_{2}+\dot{\theta}_{4}+\dot{\theta}_{6} \sin \theta_{5}\right), \\
& f_{5}=\frac{1}{2}\left(-\dot{\theta}_{2} \cos \theta_{1}+\dot{\theta}_{3} \sin \theta_{1} \cos \theta_{2}+\dot{\theta}_{5} \cos \theta_{4}-\dot{\theta}_{6} \sin \theta_{4} \cos \theta_{5}\right), \\
& f_{6}=-\frac{1}{2}\left(\dot{\theta}_{2} \sin \theta_{1}+\dot{\theta}_{3} \cos \theta_{1} \cos \theta_{2}-\dot{\theta}_{5} \sin \theta_{4}-\dot{\theta}_{6} \cos \theta_{4} \cos \theta_{5}\right) . \tag{43}
\end{align*}
$$

Using Eq. (39), we find that the equations for $\dot{\theta}_{i}$, split neatly into two sets

$$
\left(\begin{array}{ccc}
-1 & 0 & -\sin \theta_{2}  \tag{44}\\
0 & -\sin \theta_{1} & -\cos \theta_{1} \cos \theta_{2} \\
0 & \cos \theta_{1} & -\sin \theta_{1} \cos \theta_{2}
\end{array}\right) \quad\left(\begin{array}{c}
\dot{\theta}_{1} \\
\dot{\theta}_{2} \\
\dot{\theta}_{3}
\end{array}\right)=\left(\begin{array}{c}
G_{32}+G_{41} \\
G_{21}+G_{43} \\
G_{31}-G_{42}
\end{array}\right)
$$

and

$$
\left(\begin{array}{ccc}
-1 & 0 & -\sin \theta_{5}  \tag{45}\\
0 & -\sin \theta_{4} & -\cos \theta_{4} \cos \theta_{5} \\
0 & \cos \theta_{4} & -\sin \theta_{4} \cos \theta_{5}
\end{array}\right) \quad\left(\begin{array}{c}
\dot{\theta}_{4} \\
\dot{\theta}_{5} \\
\dot{\theta}_{6}
\end{array}\right)=\left(\begin{array}{c}
G_{32}-G_{41} \\
G_{21}-G_{43} \\
G_{31}+G_{42}
\end{array}\right)
$$

We also have

$$
\begin{equation*}
\frac{\mathrm{d}}{\mathrm{~d} t}\left(\lambda_{i} t\right)=G_{i i}, \quad i=1, \ldots, 4 \tag{46}
\end{equation*}
$$

from Eq. (28). Hence, to find the Lyapunov exponents of a dynamical system with four variables, we have to solve the evolution equations for the system given by Eq. (1) and the tangent map equations given by Eqs. (44)-(46), after finding $G \equiv \tilde{Q} \mathbf{J} Q$.

Any $4 \times 4$ matrix $\mathbf{J}$ can be written as

$$
\begin{equation*}
\mathbf{J}=\sum_{i=1}^{16} a_{i} X_{i} \tag{47}
\end{equation*}
$$

where the 16 matrices $X_{i}$ are defined in terms of $2 \times 2$ blocks as

$$
\begin{align*}
& X_{1}=\left[\begin{array}{ll}
I & 0 \\
0 & I
\end{array}\right], \quad X_{2}=\left[\begin{array}{cc}
-I & 0 \\
0 & I
\end{array}\right], \quad X_{3}=\left[\begin{array}{cc}
\sigma_{3} & 0 \\
0 & \sigma_{3}
\end{array}\right], \quad X_{4}=\left[\begin{array}{cc}
-\sigma_{3} & 0 \\
0 & \sigma_{3}
\end{array}\right], \\
& X_{5}=\left[\begin{array}{cc}
\sigma_{1} & 0 \\
0 & \sigma_{1}
\end{array}\right], \quad X_{6}=\left[\begin{array}{cc}
-\sigma_{1} & 0 \\
0 & \sigma_{1}
\end{array}\right], \quad X_{7}=\left[\begin{array}{cc}
\mathrm{i} \sigma_{2} & 0 \\
0 & \mathrm{i} \sigma_{2}
\end{array}\right], \quad X_{8}=\left[\begin{array}{cc}
\mathrm{i} \sigma_{2} & 0 \\
0 & -\mathrm{i} \sigma_{2}
\end{array}\right], \\
& X_{9}=\left[\begin{array}{ll}
0 & I \\
I & 0
\end{array}\right], \quad X_{10}=\left[\begin{array}{cc}
0 & I \\
-I & 0
\end{array}\right], \quad X_{11}=\left[\begin{array}{cc}
0 & \sigma_{3} \\
\sigma_{3} & 0
\end{array}\right], \quad X_{12}=\left[\begin{array}{cc}
0 & \sigma_{3} \\
-\sigma_{3} & 0
\end{array}\right], \quad X_{13}=\left[\begin{array}{cc}
0 & \sigma_{1} \\
\sigma_{1} & 0
\end{array}\right], \\
& X_{14}=\left[\begin{array}{cc}
0 & \sigma_{1} \\
-\sigma_{1} & 0
\end{array}\right], \quad X_{15}=\left[\begin{array}{cc}
0 & -\mathrm{i} \sigma_{2} \\
-\mathrm{i} \sigma_{2} & 0
\end{array}\right], \quad X_{16}=\left[\begin{array}{cc}
0 & -\mathrm{i} \sigma_{2} \\
\mathrm{i} \sigma_{2} & 0
\end{array}\right] . \tag{48}
\end{align*}
$$

It is easy to find commutators [ $X_{i}, M_{j}$ ] and [ $X_{i}, N_{j}$ ] from Eqs. (40) and (48). Then, using Eqs. (35)-(38), we can obtain

$$
\begin{equation*}
G=\tilde{Q} \mathbf{J} Q \tag{49}
\end{equation*}
$$

## 4. A comparative study of the three algorithms for the computation of Lyapunov spectra

The standard algorithm involves an explicit GSR for finding the orthonormal set $\hat{\mathbf{e}}_{i}(t)$ and the Lyapunov spectrum. The differential version considered in Section 2.2 amounts to computing the spectrum with continuous GSR. Here explicit GSR is avoided as it is incorporated in the method. However, the differential equations for $\hat{\mathbf{e}}_{i}(t)$ in this method are nonlinear, as they involve $\left(\hat{\mathbf{e}}_{i}(t), \mathbf{J} \mathbf{e}_{j}(t)\right)$ in the RHS, in contrast to the standard method which uses the linearized equations for $\delta Z$ directly. In the new method, one deals directly with the orthogonal matrix relating $\hat{\mathbf{e}}_{i}(t)$
and $\hat{\mathbf{e}}_{i}(0)$. It uses a minimal number of variables and rescaling and reorthogonalization are eliminated. However, in this method, the evolution equations for the angles and Lyapunov exponents are highly nonlinear involving sines and cosines of the angles. Hence it is not clear 'a priori' which method is 'superior' and there is a need to compare the efficiency and accuracy of the three methods. That is the subject matter 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 the Rössler hyperchaos system as an example of a dissipative system. We give the differential equations for these dynamical systems in the following.

1. Driven van der Pol oscillator $(n=2)$ :

$$
\begin{equation*}
\frac{\mathrm{d}}{\mathrm{~d} t}\binom{z_{1}}{z_{2}}=\binom{z_{2}}{-d\left(1-z_{1}^{2}\right) z_{2}-z_{1}+b \cos \omega t} \tag{50}
\end{equation*}
$$

where $b$ and $d$ are parameters and $\omega$ is the driving frequency. In our numerical work we have chosen $d=$ $-5.0, b=5.0$ and $\omega=2.47$ as the parameter values.
2. Lorenz system $(n=3)$ :

$$
\frac{\mathrm{d}}{\mathrm{~d} t}\left(\begin{array}{c}
z_{1}  \tag{51}\\
z_{2} \\
z_{3}
\end{array}\right)=\left(\begin{array}{c}
\sigma\left(z_{2}-z_{1}\right) \\
z_{1}\left(\rho-z_{3}\right)-z_{2} \\
z_{1} z_{2}-\beta z_{3}
\end{array}\right)
$$

This system is too well-known to require any further discussion. For computations we set $\sigma=10.0, \rho=28.0$ and $\beta=\frac{8}{3}$.
3. Coupled quartic oscillators $(n=4)$ : This is a conservative system and the Hamiltonian is given by

$$
\begin{equation*}
H=\frac{z_{3}^{2}}{2}+\frac{z_{4}^{2}}{2}+z_{1}^{4}+z_{2}^{4}+\alpha z_{1}^{2} z_{2}^{2} \tag{52}
\end{equation*}
$$

where $z_{1}$ and $z_{2}$ are the canonical coordinates, $z_{3}$ and $z_{4}$ the corresponding momenta and $\alpha$ a parameter. The Hamiltonian in Eq. (53) finds applications in high energy physics [8], to mention just one example. The equations of motion are

$$
\frac{\mathrm{d}}{\mathrm{~d} t}\left(\begin{array}{c}
z_{1}  \tag{53}\\
z_{2} \\
z_{3} \\
z_{4}
\end{array}\right)=\left(\begin{array}{c}
z_{3} \\
z_{4} \\
-\left(4 z_{1}^{3}+2 \alpha z_{1} z_{2}^{2}\right) \\
-\left(4 z_{2}^{3}+2 \alpha z_{1}^{2} z_{2}\right)
\end{array}\right)
$$

This system is known to be integrable for $\alpha=0,2$ and 6 [9].
4. Anisotropic Kepler problem $(n=4)$ : The Hamiltonian of this system is given by

$$
\begin{equation*}
H=\frac{p_{\rho}^{2}}{2}+\gamma \frac{p_{z}^{2}}{2}-\frac{e^{2}}{\sqrt{\rho^{2}+z^{2}}} \tag{54}
\end{equation*}
$$

where $\gamma$ 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 [10]. $\gamma=1$ corresponds to the isotropic case and is integrable. When $\gamma \neq 1$, 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 $p_{\rho}$ and $p_{z}$. We also use a re-parametrized time variable $\tau$ defined by $\mathrm{d} t=\mathrm{d} \tau\left(z_{1}^{2}+z_{2}^{2}\right)$.

The original Hamiltonian with the old variables and energy $E$ corresponds to the following Hamiltonian with $H^{\prime}=2$ in terms of the new variables [11]:

$$
\begin{equation*}
H^{\prime}=2=\frac{1}{2}\left(z_{3}^{2}+z_{4}^{2}\right)-E\left(z_{1}^{2}+z_{2}^{2}\right)+(\gamma-1) \frac{\left(z_{1} z_{3}-z_{2} z_{4}\right)^{2}}{2\left(z_{1}^{2}+z_{2}^{2}\right)} \tag{55}
\end{equation*}
$$

The equations of motion resulting from this are

$$
\frac{\mathrm{d}}{\mathrm{~d} t}\left(\begin{array}{c}
z_{1}  \tag{56}\\
z_{2} \\
z_{3} \\
z_{4}
\end{array}\right)=\left(\begin{array}{c}
z_{3}+(\gamma-1) z_{1} \frac{\left(z_{1} z_{3}-z_{2} z_{4}\right)}{\left(z_{1}^{2}+z_{2}^{2}\right)} \\
z_{4}-(\gamma-1) z_{2} \frac{\left(z_{1} z_{3}-z_{2} z_{4}\right)}{\left(z_{1}^{2}+z_{2}^{2}\right)} \\
2 E z_{1}-(\gamma-1) \frac{\left(z_{3}^{2} z_{1} z_{2}^{2}+z_{2} z_{3} z_{4}\left(z_{1}^{2}-z_{2}^{2}\right)-z_{2}^{2} z_{1} z_{4}^{2}\right)}{\left(z_{1}^{2}+z_{2}^{2}\right)} \\
2 E z_{2}-(\gamma-1) \frac{\left(z_{4}^{2} z_{2} z_{1}^{2}-z_{1} z_{3} z_{4}\left(z_{1}^{2}-z_{2}^{2}\right)-z_{1}^{2} z_{2} z_{3}^{2}\right)}{\left(z_{1}^{2}+z_{2}^{2}\right)}
\end{array}\right) .
$$

We have chosen $\gamma=0.61$ for computational purposes.
5. Rössler hyperchaos system ( $n=4$ ): This is a dissipative system and an extension of the three dimensional Rössler attractor [12]. It is described by the equations

$$
\frac{\mathrm{d}}{\mathrm{~d} t}\left(\begin{array}{l}
z_{1}  \tag{57}\\
z_{2} \\
z_{3} \\
z_{4}
\end{array}\right)=\left(\begin{array}{c}
-\left(z_{2}+z_{3}\right) \\
z_{1}+a z_{2}+z_{4} \\
b+z_{1} z_{3} \\
c z_{4}-d z_{3}
\end{array}\right)
$$

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.
In all these cases, the full Lyapunov spectrum is computed using the three methods. The time of integration is chosen to ensure reasonable convergence of the Lyapunov exponents. In most of the cases the time of integration was $t=100000$ (the exceptions are the anisotropic Kepler problem and the Rössler hyperchaos system using the differential version of the standard method due to the problem of numerical overflow). For all the systems, we have used a variable step-size Runge Kutta routine (RKQC) for integration, with an error tolerance, $\epsilon=10^{-6}-10^{-8}$. All the computations were performed on a DEC Alpha based workstation running OpenVMS. The CPU time taken for each system with each of the algorithms was noted. 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 1.
It may be noticed that all the methods yield essentially the same Lyapunov spectrum. For any autonomous dynamical system, one of the Lyapunov exponents has to be zero (corresponding to the difference vector $\delta z$ 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 all the algorithms. For the anisotropic Kepler problem all the methods fail the test. This aspect needs to be studied further. For Hamiltonian systems, for every eigenvalue $\lambda$, there is an eigenvalue $-\lambda$. This symmetry is respected by all the algorithms. For the coupled quartic oscillators, all the exponents should be zero corresponding to the integrable case of $\alpha=6$. This is indeed satisfied by all the algorithms. In Fig. 1 we give plots of Lyapunov exponents as functions of time, for a typical case. Again, there

Table 1
Comparison of the Lyapunov spectrum obtained by standard, differential and new methods and the computational time required to evaluate them with three different methods for some of the systems with $n=2,3$ and $4^{\text {a }}$

| System with initial condition | $t=10000$ |  |  | $t=100000$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Standard | Differential | New | Standard | Differential | New |
| Driven van der Pol oscillator ( $n=2$ ) |  |  |  |  |  |  |
| $z_{1}=-1.0$ | 0.0985 | 0.0980 | 0.0989 | 0.0987 | 0.0991 | 0.0981 |
| $z_{2}=1.0$ | $\begin{gathered} -6.8494 \\ (-6.7509) \end{gathered}$ | $\begin{aligned} & -6.8300 \\ & (-6.7321) \end{aligned}$ | $\begin{gathered} -6.8379 \\ (-6.7390) \end{gathered}$ | $\begin{gathered} -6.8411 \\ (-6.7424) \end{gathered}$ | $\begin{gathered} -6.8359 \\ (-6.7368) \end{gathered}$ | $\begin{gathered} -6.8400 \\ (-6.7419) \end{gathered}$ |
|  |  |  |  | [825.56] | [2224.31] | [519.22] |
| Lorenz system ( $n=3$ ) |  |  |  |  |  |  |
| $z_{1}=0.0$ | 0.9022 | 0.9040 | 0.9038 | 0.9051 | 0.9056 | 0.9056 |
| $z_{2}=1.0$ | 0.0003 | 0.0003 | 0.0001 | 0.0000 | 0.0000 | 0.0000 |
| $z_{3}=0.0$ | -14.5691 | -14.5710 | -14.5705 | -14.5718 | $-14.5723$ | -14.5723 |
|  | (-13.667) | $(-13.667)$ | $(-13.667)$ | (-13.667) | (-13.667) | (-13.667) |
|  |  |  |  | [1668.7] | [15492.7] | [2394.30] |
| Anisotropic Kepler problem ( $n=4$ ) |  |  |  |  |  |  |
| $z_{1}=1.0$ | 0.1386 | 0.1343 | 0.1434 | 0.1332 |  | 0.1360 |
| $z_{2}=2.0$ | 0.0834 | 0.0830 | 0.0860 | 0.0832 |  | 0.0831 |
| $z_{3}=1.0$ | -0.0845 | -0.0817 | -0.0864 | -0.0833 |  | -0.0833 |
| $z_{4}=0.5$ | -0.1375 | -0.1355 | -0.1429 | -0.1331 |  | -0.1357 |
|  | (0.0000) | (0.0000) | (0.0000) | (0.0000) |  | (0.0000) |
|  |  | [303.25] |  | [201.04] |  | [350.18] |
| Rössler hyperchaos ( $n=4$ ) |  |  |  |  |  |  |
| $z_{1}=-20.0$ | 0.1108 | 0.1080 | 0.1125 | 0.1121 |  | 0.1128 |
| $z_{2}=0.0$ | 0.0224 | 0.0218 | 0.0225 | 0.0196 |  | 0.0214 |
| $z_{3}=0.0$ | -0.0003 | -0.0003 | -0.0003 | -0.0000 |  | -0.0000 |
| $z_{4}=15.0$ | -25.9113 | -23.7753 | -23.9904 | -25.1886 |  | -24.7527 |
|  | (-25.778) | (-23.646) | (-23.862) | (-25.057) |  | (-24.619) |
|  |  | [4792.61] |  | [5595.99] |  | [1527.68] |
| Coupled quartic oscillator ( $n=4, \alpha=6$ ) |  |  |  |  |  |  |
| $z_{1}=0.8$ | 0.0009 | 0.0010 | 0.0010 | 0.0001 | 0.0001 | 0.0001 |
| $z_{2}=0.5$ | 0.0008 | 0.0008 | 0.0008 | 0.0001 | 0.0001 | 0.0001 |
| $z_{3}=1.0$ | -0.0008 | -0.0008 | -0.0008 | -0.0001 | -0.0001 | -0.0001 |
| $z_{4}=1.3$ | -0.0009 | -0.0010 | -0.0010 | -0.0001 | -0.0001 | -0.0001 |
|  | (0.0000) | (0.0000) | (0.0000) | (0.0000) | (0.0000) | (0.0000) |
|  |  |  |  | [492.09] | [5453.3] | [803.49] |
| Coupled quartic oscillator ( $n=4, \alpha=8)$ |  |  |  |  |  |  |
| $z_{1}=0.8$ | 0.1892 | 0.2096 | 0.1739 | 0.1738 | 0.1793 | 0.1806 |
| $z_{2}=0.5$ | 0.0011 | 0.0011 | 0.0010 | 0.0001 | 0.0001 | 0.0001 |
| $z_{3}=1.0$ | -0.0011 | -0.0011 | -0.0013 | -0.0001 | -0.0001 | -0.0001 |
| $z_{4}=1.3$ | -0.1892 | -0.2095 | -0.1795 | -0.1738 | -0.1793 | -0.1806 |
|  | (0.0000) | (0.0000) | (0.0000) | (0.0000) | (0.0000) | (0.0000) |
|  |  |  |  | [492.09] | [7658.6] | [39012.8] |

${ }^{\text {a }}$ Sum of the exponents and CPU time in sec are given in ( ) and [ ], respectively.
is no significant difference between the three algorithms as far as the convergence of the Lyapunov exponents is concerned. It is noteworthy that the differential method works well for even systems with degenerate spectra like the coupled quartic oscillators.

On the whole, the standard method seems to have an edge over the new method as far as the CPU time for the computation of the Lyapunov spectrum is concerned. The differential version of the standard method generally consumes more CPU time compared to the other two methods. For some systems like the anisotropic Kepler problem


Fig. 1. Plot of the maximal Lyapunov exponent for the coupled quartic oscillator system with $\alpha=8$.
and the Rössler hyperchaos system, there are numerical overflow problems, whatever be the values of $\beta$ and the error tolerance $\epsilon$ one chooses for this algorithm. In fact, it appears that the value of $\beta$ has to be significantly higher than $-\lambda_{n}$ (indicated by the stability analysis) for these systems, for reasonable convergence.

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 both for small and large energies. For large energies ( $\sim 25000$ ), since the energy varied by $\sim 15$ when we used the RKQC routine, we also used a symplectic procedure which eliminates secular variations in the energy [13]. With this routine, the CPU times were nearly the same for both the 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 spectrum 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. The differential version of the standard method led to a numerical overflow problem, corresponding to this initial condition.

In the standard method, after solving for the fiducial trajectory, the equations for the tangent flow are linearized equations. In differential method, corresponding to continuous GSR, these equations are nonlinear. 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 differential version of the standard method and the new method less efficient and can even lead to inaccuracies, in strongly chaotic situations.

## 5. Lyapunov eigenvectors

Earlier we had defined the matrix $d_{i j}$ as

$$
\begin{equation*}
d_{i j}=\left(\mathbf{e}_{i}(t), \hat{\mathbf{e}}_{j}(t)\right) . \tag{58}
\end{equation*}
$$

Consider the quantities

$$
\bar{d}_{i j}=\left\{\begin{array}{cl}
d_{i j} / d_{j j}, & i \geq j,  \tag{59}\\
=0, & i<j .
\end{array}\right.
$$

Define the vectors $\bar{d}_{i}$ as

$$
\begin{equation*}
\bar{d}_{1}=\left(\bar{d}_{11}, \bar{d}_{21}, \bar{d}_{31}, \ldots\right), \quad \bar{d}_{2}=\left(0, \bar{d}_{22}, \bar{d}_{32}, \ldots\right), \text { etc. } \tag{60}
\end{equation*}
$$

Let $\mathbf{D}_{1}, \mathbf{D}_{2}, \ldots, \mathbf{D}_{n}$, be the orthonormal set of vectors obtained from $\bar{d}_{i}^{\prime}$ by the Gram-Schmidt procedure, starting with $\bar{d}_{1}$. It can now be shown that $\mathbf{D}_{1}, \mathbf{D}_{2}, \ldots, \mathbf{D}_{n}$, are the eigenvectors of $\tilde{M} M$ or the Lyapunov eigenvectors corresponding to the eigenvalues $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n}[3]$. In this section, we consider the computation and convergence of these eigenvectors corresponding to the systems considered in Section 4.

In the standard method, we have to compute $\mathbf{e}_{i}(t)$ and $\hat{\mathbf{e}}_{i}(t)$ separately to obtain $\bar{d}_{i j}$. As all the vectors $\mathbf{e}_{j}(t)$ tend to align along $\hat{\mathbf{e}}_{1}$, both $d_{i j}=\left(\mathbf{e}_{i}(t), \hat{\mathbf{e}}_{j}(t)\right)$ and $d_{j j}=\left(\mathbf{e}_{j}(t), \hat{\mathbf{e}}_{j}(t)\right)$ would tend to zero for $j>1$. As $\bar{d}_{i j}$ is the ratio of $d_{i j}$ and $d_{j j}$, it would be difficult to compute them for large $t$, in this method. Even then, the procedure seems to give reasonable results for all the systems, we have considered.

In the differential version of the standard method, it has been shown that $\bar{d}_{i j}$ satisfy the following differential equations [3]:

$$
\begin{equation*}
\frac{\mathrm{d}}{\mathrm{~d} t} \bar{d}_{i j}=\sum_{k=j+1}^{i} \frac{d_{k k}}{d_{j j}} \bar{d}_{i k}\left(G_{j k}+G_{k j}\right), \quad i>j \tag{61}
\end{equation*}
$$

So the eigenvectors are obtained by direct integration of these equations. This procedure does not pose any problem as we do not come across division by small numbers here. Indeed we find that the eigenvectors converge much more rapidly than the Lyapunov exponents in all the cases, as anticipated by Goldhirsch et al. [3].

In the new method, the orthonormal vectors $\hat{\mathbf{e}}_{i}(t)$ are just the columns of the orthogonal matrix $Q$. However, it is not straightforward to compute $\mathbf{e}_{i}(t)$ in this method. So we do not consider this method further here.

We summarize the results for the Lyapunov eigenvectors in Table 2 for the same systems with the same parameters and initial conditions as in Table 1. As remarked earlier, the vectors converge sufficiently fast and the two methods yield essentially identical results. Now for a Hamiltonian system, the tangent map matrix $M$ satisfies the 'sympletic condition'

$$
\begin{equation*}
\tilde{M} S M=S, \tag{62}
\end{equation*}
$$

with

$$
S=\left[\begin{array}{ccc}
0 & \vdots & I  \tag{63}\\
\cdots & \cdots & \cdots \\
-I & \vdots & 0
\end{array}\right],
$$

where 0 and $I$ are $(n / 2) \times(n / 2)$ null matrix and identity matrix, respectively, [14]. It can be shown that if $\mathbf{D}$ is an eigenvector corresponding to eigenvalue $\lambda$, then the eigenvector corresponding to the eigenvalue $-\lambda$ is $S \mathbf{D}$ [1]. This

Table 2
Comparison of the Lyapunov eigenvectors computed using the differential and the standard methods for some systems with $n=2,3$ and $4^{\text {a }}$

| System with initial condition | Lyapunov eigenvectors |  |
| :--- | :--- | :--- |
|  | Standard method | Differential method |
| Driven van der Pol oscillator $(n=2)$ |  |  |
| $z_{1}=-1.0$ | $D_{1}(0.894,0.447)$ | $D_{1}(0.894,0.447)$ |
| $z_{2}=1.0$ | $D_{2}(-0.447,0.894)$ | $D_{2}(-0.447,0.894)$ |
| Lorenz system $(n=3)$ | $D_{1}(0.004,0.040,-0.999)$ |  |
| $z_{1}=0.0$ | $D_{2}(-0.789,-0.614,-0.028)$ | $D_{1}(0.004,0.040,-0.999)$ |
| $z_{2}=1.0$ | $D_{3}(-0.614,0.788,0.029)$ | $D_{2}(-0.789,-0.614,-0.028)$ |
| $z_{3}=0.0$ |  | $D_{3}(-0.614,0.788,0.029)$ |
| Anisotropic Kepler Problem $(n=4)$ | $D_{1}(0.230,0.139,-0.868,-0.417)$ |  |
| $z_{1}=1.0$ | $D_{2}(-0.291,0.262,-0.427,0.815)$ | $D_{1}(0.233,0.136,-0.863,-0.428)$ |
| $z_{2}=2.0$ | $D_{3}(-0.373,0.854,0.187,-0.309)$ | $D_{2}(-0.288,0.263,-0.438,0.810)$ |
| $z_{3}=1.0$ | $D_{4}(0.850,0.427,0.171,0.255)$ | $D_{3}(-0.371,0.855,0.188,-0.309)$ |
| $z_{4}=0.5$ |  | $D_{4}(0.851,0.425,0.170,0.256)$ |
| Rössler hyperchaos $(n=4)$ | $D_{1}(0.660,0.081,-0.051,0.745)$ | $D_{1}(0.660,0.081,-0.052,0.745)$ |
| $z_{1}=-20.0$ | $D_{2}(-0.749,0.115,0.022,0.653)$ | $D_{2}(-0.749,0.111,0.022,0.653)$ |
| $z_{2}=0.0$ | $D_{3}(-0.014,-0.928,0.347,0.137)$ | $D_{3}(0.030,0.991,0.005,-0.134)$ |
| $z_{3}=0.0$ | $D_{4}(-0.058,-0.345,-0.936,0.025)$ | $D_{4}(0.050,-0.003,0.998,0.025)$ |
| $z_{4}=15.0$ |  |  |
| Coupled quartic oscillator $(n=4, \alpha=6)$ | $D_{1}(0.687,0.685,0.162,0.182)$ | $D_{1}(0.684,0.684,0.178,0.185)$ |
| $z_{1}=0.8$ | $D_{2}(-0.223,0.241,0.672,-0.663)$ | $D_{2}(-0.234,0.241,0.666,-0.666)$ |
| $z_{2}=0.5$ | $D_{3}(0.670,-0.666,0.231,-0.232)$ | $D_{3}(0.666,-0.666,0.241,-0.234)$ |
| $z_{3}=1.0$ | $D_{4}(-0.170,-0.173,0.684,0.688)$ | $D_{4}(-0.185,-0.178,0.684,0.684)$ |
| $z_{4}=1.3$ |  | $D_{1}(0.503,-0.352,0.583,-0.533)$ |
| Coupled quartic oscillator $(n=4, \alpha=8)$ | $D_{1}(0.503,-0.351,0.581,-0.535)$ | $D_{2}(0.635,0.740,0.085,0.204)$ |
| $z_{1}=0.8$ | $D_{2}(0.634,0.744,0.080,0.196)$ | $D_{4}(0.580,-0.088,-0.201,0.633,0.743)$ |
| $z_{2}=0.5$ | $D_{3}(-0.084,-0.192,0.638,0.741)$ |  |
| $z_{3}=1.0$ | $D_{4}(0.581,-0.536,-0.498,0.356)$ |  |
| $z_{4}=1.3$ |  |  |

${ }^{\text {a }}$ The eigenvectors are at $t=1000$ for the differential method and at $t=1000,35,150,170,200,20$, respectively, from top to bottom for the standard method.
symmetry is very evident in our numerical values of the eigenvectors in the case of coupled quartic oscillators, but is satisfied only approximately in the case of the highly nonlinear anisotropic Kepler problem. It is to be noted that the eigenvectors are dependent upon the initial conditions and are only 'local' properties.

## 6. Conclusions

In a recently proposed new method [5], the Lyapunov exponents $\delta$, are computed directly, so to say, by utilizing representations of orthogonal matrices, applied to the tangent map. In this paper, we have established the connection between this method and a 'differential formulation' of the standard procedure to compute the Lyapunov spectra. We have also used the standard decomposition $S O(4) \sim S O(3) \times S O(3)$ to simplify the calculations for $n=4$, which are otherwise very involved. It has been claimed that the new method has several advantages over the existing methods as it does not require renormalization or reorthogonalization and requires lesser number of equations. This led us to make a detailed comparison of the new method with the standard method as well as its differential version, as regards accuracy and efficiency, by computing the full Lyapunov spectra of some typical nonlinear systems with 2, 3 and 4 variables. There is reasonable agreement among the three procedures as far as the values of the Lyapunov exponents are concerned. However, the standard method seems to score over the other two, as far as
efficiency (as indicated by the CPU time for a process) is concerned, especially in certain strongly chaotic situations, and is the most 'robust' procedure. The differential version of the standard method relies on a stability parameter and seems to demand a prior estimate of the Lyapunov spectrum. The equations for tangent flow are nonlinear in this version and highly so in the new method. This is what makes them less efficient, though the number of coupled differential equations to be solved is smaller in the new method. However they are still useful as alternative algorithms for the computation of Lyapunov spectra. We have also made a comparative study of the computation of the Lyapunov eigenvectors using the standard method and its differential version. The eigenvectors converge fairly rapidly (compared to the exponents) and the two procedures yield essentially identical results.

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