Progress of Theoretical Physics, Vol. 83, No. 5, May 1990

Comparison of Different Methods for Computing Lyapunov Exponents

Karlheinz GEIST, Ulrich PARLITZ and Werner LAUTERBORN

Institut für Angewandte Physik, Technische Hochschule Darmstadt Schlossgartenstrasse 7, D-6100 Darmstadt

(Received January 25, 1990)

Different discrete and continuous methods for computing the Lyapunov exponents of dynamical systems are compared for their efficiency and accuracy. All methods are either based on the QR or the singular value decomposition. The relationship between the discrete methods is discussed in terms of the iteration algorithms and the decomposition procedures used. We give simple derivations of the differential equations for continuous methods proposed recently and show that they cannot be recommended because of their long computation time and numerical instabilities. The methods are tested with the damped and driven Toda chain and the driven van der Pol oscillator.

§ 1. Introduction

The main aim of this paper is to compare different approaches for computing the spectrum of Lyapunov exponents that have been proposed during the last years.[1)~7)] We consider discrete ($t \in \boldsymbol{Z}$) or continuous ($t \in \boldsymbol{R}$) dynamical systems (M, ϕ) that are defined by a diffeomorphic flow map acting on an m-dimensional state space M:

$$\begin{aligned} &\phi^t : M \to M\,, \\ &\quad \boldsymbol{x} \mapsto \phi^t(\boldsymbol{x})\,. \end{aligned} \tag{1}$$

A continuous dynamical system is usually given by an ordinary differential equation

$$\dot{\boldsymbol{y}} = v(\boldsymbol{y})\,, \qquad \boldsymbol{y} = \boldsymbol{y}(\boldsymbol{x}; t) = \phi^t(\boldsymbol{x}) \in M\,, \quad t \in \boldsymbol{R}\,. \tag{2}$$

The computation of the Lyapunov exponents is based on the linearized flow map

$$\begin{aligned} &D_x\phi^t : T_xM \to T_{\phi^t(x)}M\,, \\ &\qquad \boldsymbol{u} \mapsto D_x\phi^t(\boldsymbol{u})\,. \end{aligned} \tag{3}$$

With respect to the orthonormal standard basis $\{\boldsymbol{e}_1, \cdots, \boldsymbol{e}_m\}$ in the tangent spaces T_xM and $T_{\phi^t(x)}M$ the linearized flow map $D_x\phi^t$ is given as the invertible $m \times m$ flow matrix $Y = Y(\boldsymbol{x}; t)$. For discrete dynamical systems Y is obtained as the product of the Jacobi matrices of the map $\phi^t (t=1)$ at the successive orbit points $\boldsymbol{x}_j := \phi^j(\boldsymbol{x})$ $(1 \le j \le n)$. When dealing with continuous systems the associated matrix variational equations

$$\dot{Y} = JY\,, \quad Y(\boldsymbol{x}; 0) = I \tag{4}$$

have to be integrated simultaneously with the differential equations (2) in order to obtain $D_x\phi^t$ as the $m \times m$ matrix Y. Here $J = J(\boldsymbol{y}(\boldsymbol{x}; t)) = ((\partial v_i / \partial y_j)|_{\boldsymbol{y}(x;t)})$ denotes the Jacobi matrix of partial derivatives of the vector field v at the point $\boldsymbol{y}(\boldsymbol{x}; t)$. The initial condition of the differential equation (4) in this case is the identity matrix I. The *Lyapunov exponents* λ_i are given by the logarithms of the eigenvalues μ_i $(1 \leq i \leq m)$ of the positive and symmetric matrix

$$\Lambda_x := \lim_{t\to\infty} [Y(\boldsymbol{x}; t)^{\mathrm{tr}} Y(\boldsymbol{x}; t)]^{1/2t}, \tag{5}$$

where $Y(\boldsymbol{x}; t)^{\mathrm{tr}}$ denotes the transpose of $Y(\boldsymbol{x}; t)$. The existence of Λ_x for ρ-almost all $x \in M$ (ρ denotes an ergodic ϕ-invariant probability measure on the state space M) is based on the multiplicative ergodic theorem proved by Oseledec in 1968.[8] The Lyapunov exponents are ρ-almost everywhere constant and describe the way nearby trajectories converge or diverge in the state space of a dynamical system by measuring the mean logarithmic growth rates

$$\lambda_i = \lim_{t\to\infty} \frac{1}{t} \ln \| Y(\boldsymbol{x}; t)\boldsymbol{u} \|, \quad (1 \leq i \leq m) \tag{6}$$

of perturbations $\boldsymbol{u} \in \mathrm{Eig}(\Lambda_x; \mu_i)$ of the local flow in direction of the eigenspaces $\mathrm{Eig}(\Lambda_x; \mu_i) := \{\boldsymbol{u} \in T_x M | \Lambda_x \boldsymbol{u} = \mu_i \boldsymbol{u}\}$ of the limit matrix Λ_x. More details on the meaning of Lyapunov exponents and related quantities may be found in the articles of Benettin et al.[4] Eckmann and Ruelle,[6] Johnson, Palmer and Sell,[9] Paladin and Vulpiani[10] and Lauterborn and Parlitz.[11]

In § 2 two matrix decompositions are introduced that constitute the basis of two different ways for computing the Lyapunov spectrum. According to Eq. (8) or (13) in the following chapter it can in principle be computed by a single singular value (SV) or QR decomposition for a sufficiently large chosen time t $(t \to \infty)$. Practically, however, the computation of the flow matrix Y fails for large times t, because the column vectors of Y in general converge very fast to the subspace of $T_{\phi^t(x)}M$ with the largest expansion rate.[5] This can be avoided with the help of suitable reorthonormalization schemes where one may distinguish *discrete* and *continuous* methods. The *discrete* methods iteratively approximate the Lyapunov exponents in a finite number of (discrete) time steps and therefore apply to iterated maps and continuous dynamical systems where the linearized flow map is evaluated at discrete times.

Discrete methods that use the QR decomposition are discussed in § 3.1. This decomposition may be performed by the well-known Gram-Schmidt orthonormalization procedure (GS) or a sequence of Householder transformations (see Appendix A). The GS procedure was first used by Shimada and Nagashima[3] and Benettin, Galgani, Giorgilli and Strelcyn,[4] although they formally do not refer to the QR decomposition. The use of Householder transformations instead of the GS procedure was suggested by Eckmann and Ruelle[6] because of their superior numerical properties. A method is called *continuous* when all relevant quantities are obtained as solutions of certain ordinary differential equations, i.e., continuous methods can only be formulated for continuous dynamical systems, not for maps. This kind of methods for computing the Lyapunov spectrum has been proposed by several authors.[1),2),7),12),13] In the case of the QR decomposition differential equations for the orthogonal matrix Q and the diagonal elements of R are needed to determine the Lyapunov spectrum. In § 3.2 two derivations are given. The first one only holds for the case of the complete spectrum.

The second derivation yields the desired differential equations when only k ($k<m$) Lyapunov exponents are to be computed. In this case rectangular $m\times k$ matrices Q are considered and the matrix identity $QQ^{\mathrm{tr}}=I$ cannot be used anymore. Therefore this second approach leads to more complicated differential equations than the first one. We discuss the problems that occur when these algorithms are used.

In § 4 another method for computing the spectrum of Lyapunov exponents is considered that is based on the singular value decomposition SVD of the flow matrix Y. In contrast to the discrete versions of the QR algorithm discussed in § 3.1 for the SV decomposition no iterative procedure is known to the authors that avoids the typical numerical collapse. Therefore we resume here only the continuous method introduced by Greene and Kim[1] with slight modifications that are necessary to avoid numerical overflow problems. It shows the same numerical inefficiency as the continuous methods based on the QR decomposition. A further disadvantage of this method is the fact that its differential equations become singular when the Lyapunov spectrum to be computed is degenerate, i.e., $\lambda_i\simeq\lambda_{i+1}$ for at least one $1\leq i\leq m-1$, which is the normal case for periodic and quasiperiodic attractors (see, e.g., Geist and Lauterborn.[14),15)]) The continuous methods based on the SV decomposition are therefore not suitable for the computation of Lyapunov diagrams like those shown in Refs. 14), 15).

We conclude with a final discussion of our experiences with the different methods.

§ 2. Matrix decompositions

2.1. *Singular value decomposition*

Let

$$Y=UFV^{\mathrm{tr}} \tag{7}$$

be the *singular value decomposition* (SVD) of $Y=Y(\boldsymbol{x};t)$ into the product of the orthogonal matrices U and V and the diagonal matrix $F=\mathrm{diag}(\sigma_1(t),\cdots,\sigma_m(t))$.[16)] The diagonal elements $\sigma_i(t)$ ($1\leq i\leq m$) of F are called the *singular values* of Y. The SVD is unique up to permutations of corresponding columns, rows and diagonal elements of the matrices U, V and F. In those cases where all singular values are different a unique decomposition can be achieved by the additional request of a strictly monotonically decreasing singular value spectrum, i.e., $\sigma_1(t)>\sigma_2(t)>\cdots>\sigma_m(t)$. Multiplying Eq. (7) with the transpose $Y^{\mathrm{tr}}=VFU^{\mathrm{tr}}$ from the left shows, that the squares of the singular values $\sigma_i(t)$ of Y are the eigenvalues of the matrix $Y^{\mathrm{tr}}Y$ (see, e.g., Lorenz[17)]). Therefore Eq. (5) implies the relation

$$\lambda_i=\ln\mu_i=\lim_{t\to\infty}\ln[\sigma_i^2(t)]^{1/2t}=\lim_{t\to\infty}\frac{1}{t}\ln[\sigma_i(t)] \tag{8}$$

between the Lyapunov exponents λ_i, the eigenvalues μ_i of Λ_x and the singular values $\sigma_i(t)$ ($1\leq i\leq m$).

The singular value decomposition permits an impressive geometric illustration of the meaning of the Lyapunov exponents. Multiplying Eq. (7) with V from the right

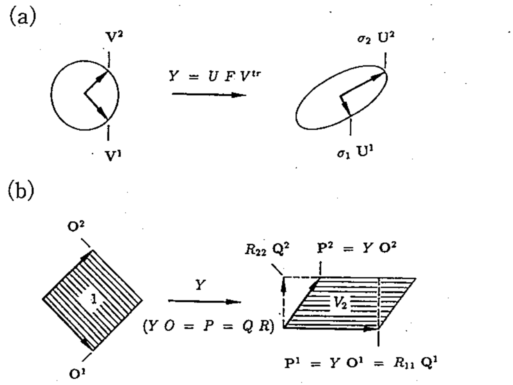

Fig. 1. Geometric illustration of (a) the SV and (b) the QR decomposition.

yields

$$YV^i = \sigma_i(t)U^i, \qquad (1 \le i \le m) \qquad (9)$$

where the V^i and U^i $(1 \le i \le m)$ are the column vectors of the matrices V and U. When following the orbit γ_x a (infinitesimal) small sphere around the initial point x (the unit sphere $S^m(x) := \{u \in T_xM \mid \|u\| = 1\}$ in the tangent space T_xM) is deformed (by the linearized flow map $D_x\phi^t$: $T_xM \to T_{\phi^t(x)}M$) to an ellipsoid $E^m(x; t) := D_x\phi^t(S^m(x))$ with principal axes $\sigma_i(t)U^i$ $(1 \le i \le m)$ (Fig. 1(a)). The mean logarithmic expansion rates of the principal axes give the Lyapunov exponents.

2.2. *QR decomposition*

Another way to look at the Lyapunov spectrum is to ask how the volumes V_k of k-dimensional parallelepipeds $[P^1(t), \cdots, P^k(t)]$ $(1 \le k \le m)$ in the m-dimensional tangent space $T_{\phi^t(x)}M$ grow (or shrink) in time. The axes of the parallelepipeds are given by $P^i(t) := D_x\phi^t(O^i) = YO^i$ where $\{O^1, \cdots, O^m\}$ denotes an orthonormal basis of T_xM chosen at random.[4),6)] The orthonormal basis vectors $O^i (1 \le i \le m)$ define orthogonal $m \times k$ matrices $O := (O^1, \cdots, O^k)(1 \le k \le m)$. It turns out that the sum of the first k Lyapunov exponents λ_i $(1 \le i \le k \le m)$ gives the desired growth rates

$$\lambda^k := \lim_{t \to \infty} \frac{1}{t} \ln[V_k] = \sum_{i=1}^{k} \lambda_i, \qquad (10)$$

when the Lyapunov exponents constitute a monotonically decreasing sequence (see, e.g., Benettin et al.[4)]). The volume V_k $(1 \le k \le m)$ can be computed with the help of the uniquely defined *QR decomposition*

$$P = QR = (Q^1, \cdots, Q^k)\begin{pmatrix} R_{11} & * & \cdots & * \\ 0 & R_{22} & \ddots & \vdots \\ \vdots & \ddots & \ddots & * \\ 0 & \cdots & 0 & R_{kk} \end{pmatrix} \qquad (11)$$

of the $m \times k$ parallelepiped matrix $P := (P^1, \cdots, P^k)$ into the product of an orthogonal $m \times k$ matrix Q $(Q^{i\,tr} Q^j = \delta_{ij}$ for $1 \le i, j \le k)$ and an upper triangular $k \times k$ matrix R with positive diagonal elements $R_{ii} > 0$ $(1 \le i \le k)$ (see Fig. 1(b)):

$$V_k = \prod_{i=1}^{k} R_{ii}. \qquad (12)$$

Substituting the volumes V_k $(1 \le k \le m)$ in Eq. (10) by the products (12) yields:

$$\lambda_i = \lim_{t \to \infty} \frac{1}{t} \ln[R_{ii}]. \quad (1 \le i \le m) \qquad (13)$$

For almost all orthogonal bases $\{\boldsymbol{O}^1, \cdots, \boldsymbol{O}^m\}$ the diagonal elements R_{ii} $(1 \le i \le m)$ of R are, in the limit $t \to \infty$, ordered according to their size. In the following we take $\boldsymbol{O}^i := \boldsymbol{e}_i$ as it is done usually. In particular cases however this special choice of $\{\boldsymbol{O}^1, \cdots, \boldsymbol{O}^m\}$ can destroy the asymptotic monotony of the R_{ii} $(1 \le i \le m)$ (for an example see § 5).

§ 3. QR decomposition based methods

3.1. *Discrete methods*

The discretization $t_j := j \cdot \Delta t$ $(0 \le j \le n)$ of the continuous time variable t $(t = n \cdot \Delta t)$ enables the stepwise computation of the QR decomposition of the $m \times k$ parallelepiped matrix P $(1 \le k \le m)$, where Δt has to be chosen sufficiently small to avoid the numerical problems mentioned above. The different algorithms for computing the QR decomposition of P for discretized continuous systems or iterated maps are summarized in the following diagram:

$$
\begin{tikzcd}
\boldsymbol{R}^k \arrow[rrrrr, "R"] \arrow[d, "Q^0:=O"'] \arrow[drrrrr, "P"] & & & & & \boldsymbol{R}^k \arrow[d, "Q"] \\
\boldsymbol{R}^m \arrow[rrrrr, "Y"] \arrow[d, phantom, "\cong" description] & & & & & \boldsymbol{R}^m \arrow[d, phantom, "\cong" description] \\
T\boldsymbol{x}_0M \arrow[d, phantom, "\cong" description] & T\boldsymbol{x}_1M \arrow[d, phantom, "\cong" description] & T\boldsymbol{x}_2M \arrow[d, phantom, "\cong" description] & & T\boldsymbol{x}_{n-1}M \arrow[d, phantom, "\cong" description] & T\boldsymbol{x}_nM \arrow[d, phantom, "\cong" description] \\
\boldsymbol{R}^m \arrow[r, "Y^0"] & \boldsymbol{R}^m \arrow[r, "Y^1"] & \boldsymbol{R}^m \arrow[r, dashed] & \cdots \arrow[r] & \boldsymbol{R}^m \arrow[r, "Y^{n-1}"] & \boldsymbol{R}^m \\
\boldsymbol{R}^k \arrow[u, "Q^0:=O"] \arrow[r, "R^0"'] \arrow[ur, dashed, "P^0"'] & \boldsymbol{R}^k \arrow[u, "Q^1"] \arrow[r, "R^1"'] \arrow[ur, dashed, "P^1"'] & \boldsymbol{R}^k \arrow[u, "Q^2"] \arrow[r, dashed] \arrow[ur, dashed] & \cdots \arrow[r] \arrow[ur, dashed] & \boldsymbol{R}^k \arrow[u, "Q^{n-1}"] \arrow[r, "R^{n-1}"'] \arrow[ur, dashed, "P^{n-1}"'] & \boldsymbol{R}^k \arrow[u, "Q^n"']
\end{tikzcd}
\tag{14}
$$

The diagram (14) is commutative, since the flow matrix $Y = Y^{n-1} \cdots Y^0$ can be expressed as the product of the matrices Y^j at the successive orbit points $\boldsymbol{x}_j := \phi^{t_j}(\boldsymbol{x}_0) \in M (0 \le j \le n-1)$ by the chain rule and $P = QR$ and $Y^{j-1}Q^{j-1} = Q^j R^{j-1}$ $(1 \le j \le n)$ by definition of the QR decomposition (11). The diagonal "maps" P^j $(0 \le j \le n-1)$ are only important for continuous dynamical systems as will be discussed below. In that case the matrices Y^j and P^j $(0 \le j \le n-1)$ can be obtained by integrating the matrix variational equations (4) with the $m\times m$ unit matrix I ($I_{ij}=\delta_{ij}$ for $1\leq i\leq m, 1\leq j\leq m$) or the orthogonal $m\times k$ matrices Q^j ($Q^{j\mathrm{tr}}Q^j=I$) as initial conditions, respectively. It is easy to show that $Y^jQ^j=P^j$ $(0\leq j\leq n-1)$, because the relation $d/dt(Y^jQ^j)=d/dt(Y^j)Q^j$ implies that Y^jQ^j and P^j are systems of fundamental solutions of the matrix variational equations (4) with the same initial conditions Q^j $(0\leq j\leq n-1)$ at times $t=0$ (see, e.g., Ref. 18)). The commutativity of (14) and the uniqueness of the QR decomposition (11) imply:

$$R_{ii}=\prod_{j=0}^{n-1}R_{ii}^j . \quad (1\leq i\leq k) \tag{15}$$

Substituting the diagonal elements of R in Eq. (13) by the product (15) yields

$$\lambda_i=\frac{1}{\Delta t}\lim_{n\to\infty}\frac{1}{n}\sum_{j=0}^{n-1}\ln[R_{ii}^j] . \tag{16}$$

The iterative computation of the diagonal elements R_{ii}^j $(1\leq i\leq k,\ 0\leq j\leq n-1)$ of R^j can now be realized by two different "iteration paths" in the diagram (14). The first one is the so-called *treppen-iteration algorithm*

$$Y^{j-1}Q^{j-1}=Q^jR^{j-1} , \quad (1\leq j\leq n) \tag{17}$$

by Eckmann and Ruelle,[6] where the Y^{j-1} are $m\times m$ matrices, the Q^{j-1} are $m\times k$ matrices and the R^{j-1} are $k\times k$ matrices. Thus only the first k rows of Y^{j-1} $(1\leq j\leq n)$ are needed for this algorithm. In the case of an iterated map ϕ these rows are easily computed in terms of the relevant partial derivatives of ϕ at the points $\boldsymbol{x}_{j-1}:=\phi^{j-1}(\boldsymbol{x})$. For continuous dynamical systems however the numerical integration of the complete set of m^2 matrix variational equations (4) is required to determine the first k rows of Y^{j-1} $(1\leq j\leq n)$. To characterize the dynamics of high-dimensional systems often the knowledge of a small number k of the Lyapunov exponents $\lambda_1, \cdots, \lambda_k$ $(k\ll m)$ is sufficient (see, e.g., Geist and Lauterborn[14),15)] and Dressler[19),20)]). The time consuming integration of "superfluous" differential equations should therefore be avoided as far as possible. This can be done by bypassing the explicit numerical computation of the complete $m\times m$ matrices Y^{j-1} and the matrix multiplications $Y^{j-1}Q^{j-1}$ in algorithm (17) by utilizing the (dashed) diagonals in diagram (14). In this way one obtains the *diagonal algorithm*

$$P^{j-1}=Q^jR^{j-1} , \quad (1\leq j\leq n) \tag{18}$$

the principle of which has been used by Shimada and Nagashima,[3)] Benettin et al.[4)] and Wolf et al.[5)]

3.2. *Continuous methods*

3.2.1. Differential equations for the complete Lyapunov spectrum

If Y is replaced by the product QR in the matrix variational equations (4) we obtain

$$\dot{Q}R+Q\dot{R}=JQR . \tag{19}$$

Multiplying (19) with $Q^{-1}=Q^{\mathrm{tr}}$ from the left and R^{-1} from the right yields

$$Q^{tr}\dot{Q}-Q^{tr}JQ=-\dot{R}R^{-1}. \tag{20}$$

The right-hand side of Eq. (20) is an upper triangular matrix. The components of the skew symmmetric matrix

$$S:=Q^{tr}\dot{Q} \tag{21}$$

are therefore given by the equation

$$S_{ij}=\begin{cases} (Q^{tr}JQ)_{ij}, & i>j \\ 0, & i=j \\ -(Q^{tr}JQ)_{ji}. & i<j \end{cases} \tag{22}$$

The matrix S may be used to define the desired differential equation for Q:

$$\dot{Q}=QS. \tag{23}$$

By (20) and (22) the equations for the diagonal elements of R are given by

$$\frac{\dot{R}_{ii}}{R_{ii}}=(Q^{tr}JQ)_{ii}. \quad (1\leq i\leq m) \tag{24}$$

To determine the Lyapunov exponents λ_i only the logarithms $\rho_i:=\ln(R_{ii})$ of the diagonal elements of R are of interest. According to (24) they fulfill the equations

$$\dot{\rho}_i=(Q^{tr}JQ)_{ii}. \qquad (1\leq i\leq m) \tag{25}$$

Thus to compute the spectrum of Lyapunov exponents only Eqs. (23) and (25) have to be solved simultaneously with the equations of motion (2). The quantities $\rho_i(t)/t$ converge to the Lyapunov exponents $\lambda_i(1\leq i\leq m)$ in the limit $t\to\infty$.

3.2.2. Differential equations for the largest k Lyapunov exponents

In the derivation of differential equation (23) for the orthogonal matrix Q from the definition (21) of S we have used the matrix identity $QQ^{tr}=I$. This is not possible in the case where only the largest k Lyapunov exponents are to be computed. Then R is a $k\times k$ matrix and Q is a $m\times k$ matrix. Therefore the identity $Q^{tr}Q=I$ holds but not $QQ^{tr}=I$.

In the following a derivation of the differential equations for Q and the diagonal elements R_{ii} $(1\leq i\leq m)$ of R is given where the identity $QQ^{tr}=I$ is not used. Equation (19) directly implies the differential equation

$$\dot{Q}=JQ-QW \tag{26}$$

for Q, where $W:=\dot{R}R^{-1}$ is a $k\times k$ upper triangular matrix. From (26) it follows:

$$W=Q^{tr}JQ-Q^{tr}\dot{Q}=Q^{tr}JQ-S. \tag{27}$$

As W is upper triangular and S skew symmetric it is easy to see that the equations

$$W_{ij}=\begin{cases} (Q^{tr}JQ)_{ij}+(Q^{tr}JQ)_{ji}, & i<j \\ (Q^{tr}JQ)_{ij}, & i=j \\ 0, & i>j \end{cases} \tag{28}$$

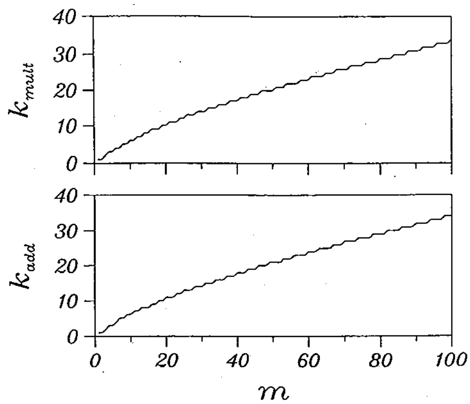

Fig. 2. Operations count for the two continuous QR methods for computing the Lyapunov exponents given in § 3.2. In the Eqs. (26), (28) and (29) for the $m\times k$ case $n_{\rm add}(m, k):=[2m^2k+mk^3+mk^2-k^2-k]/2$ additions and $n_{\rm mult}(m, k):=[mk(2m+3k+k^2)]/2$ multiplications occur. In the $m\times m$ case (Eqs. (22), (23) and (25)) $n_{\rm add}(m):=[5m^3-4m^2-m]/2$ additions and $n_{\rm mult}(m):=[5m^3+m^2]/2$ multiplications are to be computed. Thus for k larger than the critical value $k_{\rm add}(m):=\max\{k\in N|n_{\rm add}(m, k)\le n_{\rm add}(m)\}$ ($k_{\rm mult}(m):=\max\{k\in N|n_{\rm mult}(m, k)\le n_{\rm mult}(m)\}$) the computation of the largest k exponents needs more additions (multiplications) than the determination of the complete spectrum. The dependence of the quantities $k_{\rm add}$ and $k_{\rm mult}$ on the state space dimension m is shown in the figure.

for the components of W hold. Knowing W as a function of J and Q, the differential equation (26) can be solved to obtain $Q(t)$. The differential equations for the logarithms $\rho_i(t)$ of the diagonal elements R_{ii} of R are given in terms of W:

$$\dot{\rho}_i = W_{ii}\,. \quad (1\le i\le m) \tag{29}$$

For k larger than a critical value the computation of the largest k exponents is more expensive than the determination of the complete Lyapunov spectrum (see Fig. 2).

§ 4. Singular value decomposition based continuous method

Similar to the continuous QR method we will now formulate differential equations for the quantities that are needed to compute the Lyapunov spectrum in terms of the singular value decomposition SVD.

To avoid computational difficulties with the exponentially increasing or decreasing diagonal elements σ_i $(1\le i\le m)$ of the matrix F we consider the diagonal matrix

$$E:=\ln(F)=\mathrm{diag}(\varepsilon_1, \cdots, \varepsilon_m) \tag{30}$$

with elements $\varepsilon_i:=\ln(\sigma_i)$ $(1\le i\le m)$. Differentiation with respect to time yields

$$\dot{E}=F^{-1}\dot{F}=F^{-1}\dot{U}^{\rm tr}UF+F^{-1}U^{\rm tr}JUF+V^{\rm tr}\dot{V}\,, \tag{31}$$

where the derivative $\dot{F}$ of F is given by substituting the flow matrix Y in the matrix variational equations (4) by its singular value decomposition $Y=UFV^{\rm tr}$ (7). To eliminate V in Eq. (31) the sum $\dot{E}+\dot{E}^{\rm tr}=2\dot{E}$ is computed where the term $V^{\rm tr}\dot{V}+\dot{V}^{\rm tr}V$ vanishes due to the orthogonality of V. With the abbreviations

$$A:=U^{\rm tr}\dot{U}=-\dot{U}^{\rm tr}U\,,$$

$$B:=-F^{-1}AF\,,$$

$$C:=U^{\rm tr}JU\,,$$

$$D := F^{-1} C F\,, \tag{32}$$

this yields the following differential equation for E:

$$2\dot{E} = B + B^{\mathrm{tr}} + D + D^{\mathrm{tr}}\,. \tag{33}$$

The right-hand side of Eq. (33) depends on the matrices J, $F = \exp(E)$, U and $\dot{U}$. To separate the time derivatives $\dot{E}$ and $\dot{U}$ of E and U the components of the matrices B and D have to be considered. They are given by the equations

$$B_{ij} = -A_{ij}\frac{\sigma_j}{\sigma_i}\,,$$

$$D_{ij} = C_{ij}\frac{\sigma_j}{\sigma_i}\,. \tag{34}$$

The orthogonality of U implies that A is skew symmetric and thus $B_{ii} = -A_{ii} = 0$ $(1 \le i \le m)$. The diagonal elements $\dot{\varepsilon}_i = \dot{\sigma}_i / \sigma_i$ of $\dot{E}$ therefore fulfill the equation

$$\dot{\varepsilon}_i = C_{ii}\,, \tag{35}$$

which can be used to compute the quantities $\varepsilon_i(t)/t \xrightarrow{t \to \infty} \lambda_i$ $(1 \le i \le m)$. By means of the off-diagonal elements in Eq. (33) the $m(m-1)/2$ equations

$$\begin{aligned} 0 &= B_{ij} + B_{ji} + D_{ij} + D_{ji} \\ &= -A_{ij}\frac{\sigma_j}{\sigma_i} - A_{ji}\frac{\sigma_i}{\sigma_j} + C_{ij}\frac{\sigma_j}{\sigma_i} + C_{ji}\frac{\sigma_i}{\sigma_j}\,, \qquad i > j \end{aligned} \tag{36}$$

for the components of A can be derived. To remove troublesome exponentially growing quantities equation (36) is multiplied by σ_i/σ_j and the critical terms σ_i^2/σ_j^2 are replaced by

$$h_{ij} := \exp(2(\varepsilon_i - \varepsilon_j))\,, \quad (1 \le i, j \le m, i \ne j) \tag{37}$$

to get

$$A_{ij} = \begin{cases} \dfrac{C_{ji} + C_{ij} h_{ji}}{h_{ji} - 1}\,, & i < j \\ 0\,, & i = j \\ \dfrac{C_{ij} + C_{ji} h_{ij}}{1 - h_{ij}}\,. & i > j \end{cases} \tag{38}$$

By means of matrix A the desired differential equation for U can be formulated as

$$\dot{U} = UA\,. \tag{39}$$

For nondegenerate Lyapunov spectra $\{\lambda_i\}$ the singular values $\sigma_i(t) \sim \exp(\lambda_i t)$ constitute in general a strictly monotonically decreasing sequence $\sigma_1 > \cdots > \sigma_m$ for $t \to \infty$ and the quantities $h_{ij} \sim \exp(2t(\lambda_i - \lambda_j))$ converge to zero very fast for $i > j$. This means that the skew symmetric matrix A in (39) tends to the matrix S of Eq. (21) in the limit $t \to \infty$.

It should be noted that Eq. (39) becomes singular for attractors with degenerate

Lyapunov spectra because $\lambda_i=\lambda_j$ $(1\leq i, j\leq m, i\neq j)$ implies $\lim_{t\to\infty}h_{ij}(t)=1$. For this reason and the fact that the continuous SVD method needs even more operations than the continuous QR method we have not investigated the $m\times k$ case although the SV decomposition is well defined for rectangular matrices, too.[16)]

§ 5. Numerical results

The implemented methods for computing Lyapunov exponents are given in Table I. Four of these methods are discrete QR methods where different iteration algorithms (Eqs. (17) and (18)) and different procedures for the QR decomposition are used. The GS method is based on the usual Gram-Schmidt orthonormalization procedure as well as the RGS method where the orthogonalization is repeated (see Appendix A.1). In the case of the H1 and the H2 method Householder transformations are used for the QR decomposition. H1 is based on the treppen-iteration algorithm (17) whereas H2 is given by the diagonal algorithm (18). The continuous QR methods CQR for the complete Lyapunov spectrum is implemented as described in § 3.2.1. A continuous singular value method CSV has also been tested for a special low dimensional example as will be discussed in the following.

The first dynamical system used to compare these methods is a damped and driven Toda chain of $N=15$ unit masses $m_i=1$ and periodic boundary conditions $q_0=q_N$, $q_{N+1}=q_1$ with the $[(2N-2)+1]$-dimensional state space $M=\boldsymbol{R}^{2N-2}\times S^1$:

$$\begin{pmatrix} \dot{d}_i \\ \dot{v}_i \\ \dot{\vartheta} \end{pmatrix} = V\begin{pmatrix} d_i \\ v_i \\ \vartheta \end{pmatrix} := \begin{pmatrix} v_i - v_{i+1} \\ [(K_{i-1}-K_i)-(D_{i-1}-D_i)+F_i]/m_i \\ \omega_0/2\pi \end{pmatrix}. \tag{40}$$

Here q_i denotes the elongation of the ith mass m_i from its equilibrium position, $v_i:=\dot{q}_i$ its velocity, $d_i:=q_i-q_{i+1}$ the relative elongations of adjacent masses, $K_i:=\exp(d_i)-1$ the exponential restoring force of the spring between the ith and $(i+1)$-th mass, $D_i:=(v_{i+1}-v_i)d$ the internal dissipation force proportional to the relative velocities of the masses with damping coefficient d and $F_i(t):=a\sin(\omega_0 t)\delta_{i,1}$ a single-frequency external force with driving amplitude a and frequency ω_0. This system possesses quasiperiodic solutions with two and three incommensurate fre-

Table I. Classification of the implemented methods for computing Lyapunov exponents.

Method	Type	Algorithm	Decomposition of Y	
			Type	Method
GS	discrete	(18)	QR	(A·1)
RGS	discrete	(18)	QR	(A·2)
H1	discrete	(18)	QR	(A·3)~(A·6)
H2	discrete	(17)	QR	(A·3)~(A·6)
CQR	continuous	(22), (23), (25)	QR	—
CSV	continuous	(32), (35), (37)~(39)	SV	—

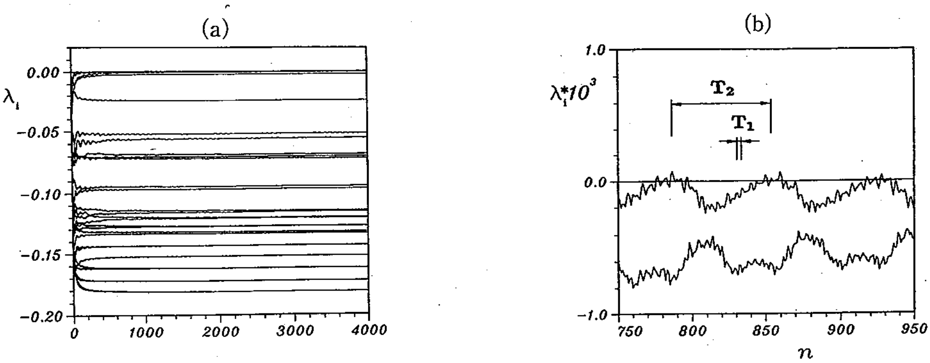

Fig. 3. (a) Numerical estimates of the Lyapunov exponents for a T^3-solution of a damped and driven Toda chain of $N=15$ masses at the driving amplitude $a=3.5$, the driving frequency $\omega_0=1.1237$ and the damping coefficient $d=0.1$ as it develops with the number n of periods $T_0:=2\pi/\omega_0$ of the driving. (b) The second and the third Lyapunov exponent show oscillations with periods $T_1 \simeq 1/(\omega_1^0/2) \simeq 3.4$ and $T_2 \simeq 1/\omega_2^0 \simeq 69.4$, where 1, $\omega_1^0/2 \simeq 0.29786$ and $\omega_2^0 \simeq 0.01440$ are the normalized basic frequencies of the corresponding 3-dimensional double torus $2T^3$ in the state space M. For a more detailed investigation of this attractor see Ref. 15).

quencies as well as high-dimensional strange attractors.[14),15),21)] Their Lyapunov spectra are computed to demonstrate the properties of the different algorithms. Figure 3(a) shows the temporal convergence of the numerical estimates of the complete spectrum of Lyapunov exponents computed with the GS method for a three-frequency quasiperiodic solution of the ($N=15$)-chain (see Fig. 11 in Ref. 15)). Due to the oscillations connected with the structure of the attractor it needs a long time until they arrive at a sufficiently well-defined limit (Fig. 3(b)). The same Lyapunov spectrum has also been computed with the RGS, H1, H2 and CQR method. The corresponding results for the largest and smallest Lyapunov exponent after 500 and 2000 periods of the driving are given in Table II. The differences between the discrete methods are much smaller than the fluctuations of the numerical estimates $\lambda_i(n)$ which converge in the limit $n \to \infty$ to the Lyapunov exponents λ_i. Figure 4 shows the temporal convergence of the numerical estimates of the first, third and fifth Lyapunov exponent of a high dimensional strange attractor of the Toda chain computed with the discrete methods of Table I. The Lyapunov exponents computed with the GS and the RGS method agree within the resolution of the plot. The differences between the other methods are in the order of the fluctuations of the $\lambda_i(n)$.

Table II. Numerical estimates of the Lyapunov exponents λ_1 and λ_{28} after $n=500$ and $n=2000$ periods $T_0=2\pi/\omega_0$ of the driving for the same attractor as in Fig. 3.

Method	λ_1 ($n=500$)	λ_1 ($n=2000$)	λ_{28} ($n=500$)	λ_{28} ($n=2000$)
GS	$-.3878 * 10^{-4}$	$-.7811 * 10^{-4}$	$-.1803$	$-.1812$
RGS	$-.3878 * 10^{-4}$	$-.7811 * 10^{-4}$	$-.1803$	$-.1812$
H1	$-.3880 * 10^{-4}$	$-.7810 * 10^{-4}$	$-.1803$	$-.1812$
H2	$-.3875 * 10^{-4}$	$-.7803 * 10^{-4}$	$-.1803$	$-.1812$
CQR	$-.2218 * 10^{-4}$	—	$-.1804$	—

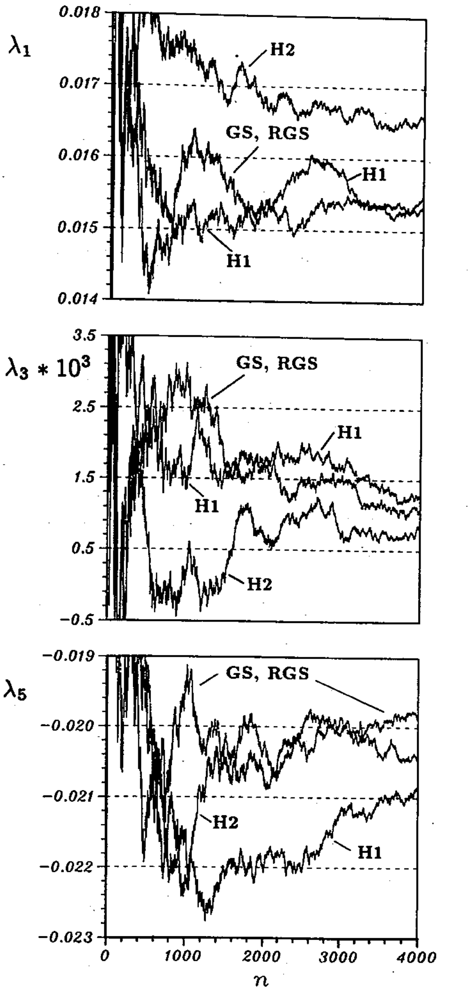

Fig. 4. Numerical estimates of the Lyapunov exponents $\lambda_1 > \lambda_3 > 0 > \lambda_5$ for a high-dimensional strange attractor of a damped and driven Toda chain of $N=15$ masses ($\omega_0=0.9$, $a=6.0$ and $d=0.1$; see Fig. 13 in Ref. 21)).

Table III. Mean relative computation times of the discrete (GS, RGS, H1 and H2) and continuous (CQR) QR decomposition based methods.

Method	CPU-Time
GS	1.00
RGS	1.02
H1	1.07
H2	1.17
CQR	40.00

Table III shows the mean relative computation times. In consequence of the large number of operations the continuous QR method needs up to a factor 40 (!) more CPU-time than the discrete standard methods (see Table III). Therefore the computations have been stopped after 500 periods of the driving because this took already about three hours on a CRAY X-MP/24 with 64-bit arithmetic. Furthermore the differential equations for Q do not assure that Q remains orthogonal during its time evolution and thus nonorthogonal perturbations due to round off errors grow in time (see Fig. 5). To overcome this difficulty Greene and Kim[1] proposed to add an additional correction term $\nu[Q^{tr}Q-I]$ to the right-hand side of the differential equation (23) or (26). For the very special class of dynamical systems with time independent and symmetric Jacobi matrices J they showed that this method preserves the orthogonality of the matrix Q. It should be noted that the necessity for excluding the growth of nonorthogonal perturbations leads to a further increase of the computation time.

In some periodically driven low-dimensional systems of the form

$$\ddot{x}+g(x,\dot{x})=h(t)=h(t+T_0)\,, \tag{41}$$

e.g., the driven van der Pol oscillator,[23]

$$g(x,\dot{x})=d(x^2-1)\dot{x}+x\,,$$

$$h(t)=a\cos(\omega_0 t)\,,$$

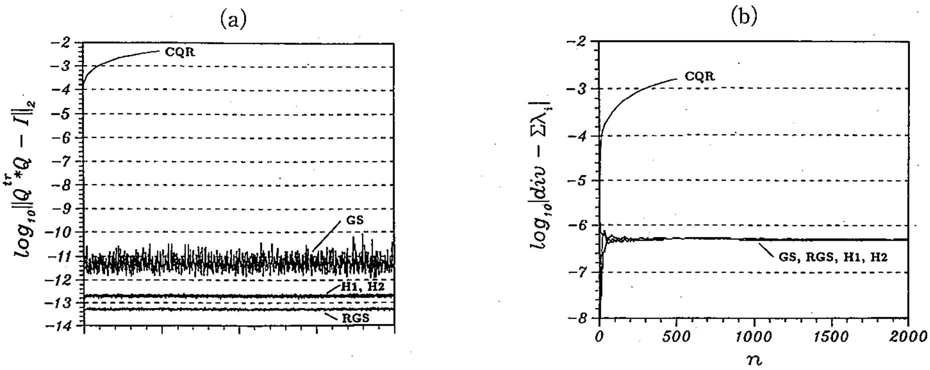

Fig. 5. Check of the orthogonality of $Q(\boldsymbol{x};t)$ for the strange attractor of Fig. 4. (a) Euclidean norm of the matrix $Q^{tr}Q-I$ and (b) divergence of the vector field v minus the sum of the Lyapunov exponents as they develop with the number n of periods of the driving. These two quantities have to vanish for all times because Q is orthogonal and $\sum_{i=1}^{[(2N-2)+1]}\lambda_i=\operatorname{div} V(\boldsymbol{x})=\operatorname{Tr}(J(\boldsymbol{x};t))=-2N\cdot d=-3.0$ has to be constant for all $\boldsymbol{x}\in M$, $t\in\boldsymbol{R}$ by Liouville's theorem (see, e.g., Arnol'd[22]).

$$\omega_0=2\pi/T_0\,, \tag{42}$$

these problems may be overcome, because the QR decomposition of the flow matrix Y can be done explicitely yielding:

$$\begin{pmatrix} Y_{11} & Y_{12} & Y_{13} \\ Y_{21} & Y_{22} & Y_{23} \\ 0 & 0 & 1 \end{pmatrix}=\begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} R_{11} & R_{12} & R_{13} \\ 0 & R_{22} & R_{23} \\ 0 & 0 & 1 \end{pmatrix}. \tag{43}$$

In this case the orthogonal matrix Q may be parameterized by a single angle α and the differential equation (23) or (26) for Q can be replaced by the differential equation

$$\dot{\alpha}=-\sin^2\alpha-\left(\frac{\partial g}{\partial x}\cos\alpha+\frac{\partial g}{\partial \dot{x}}\sin\alpha\right)\cos\alpha \tag{44}$$

for α. Therefore no problems with the orthogonality of Q can occur but the computation time is still about a factor of two higher than for the discrete standard methods. Note that the simple form of Eq. (43) follows from the special choice $O=I$ for the orthogonal matrix O (see § 2.2). It implies $R_{3,3}(t)=1$, i.e., $\lambda_3=0$. Thus only the nontrivial Lyapunov exponents $\lambda_i=\lim_{t\to\infty}\ln[R_{ii}(t)]/t$ $(i=1,2)$ are (automatically) ordered according to their size. This exceptional role of the trivial exponent occurs in connection with all periodically driven dynamical systems. In contrast to the QR decomposition (43) the singular value decomposition (7) of the flow matrix Y does not yield simple orthogonal matrices U and V that are parameterized (only) by a single angle. To compute the Lyapunov exponents for the complete three-dimensional system one has therefore to solve the general differential equation (39) for the components of the matrix U. This leads to high computational costs and a loss of the orthogonality of U during the computation.

These problems can be avoided by first reducing the dimension of the problem from three to two and then performing the singular value decomposition, because 2×2 orthogonal matrices can always be parameterized by a single angle. The reduction of the dimension results from the fact that the reduced two-dimensional set of variational equations

$$\dot{\tilde{Y}}=\begin{pmatrix} 0 & 1 \\ -\dfrac{\partial g}{\partial x} & -\dfrac{\partial g}{\partial \dot{x}} \end{pmatrix}\tilde{Y}\,, \quad \tilde{Y}(0)=I \tag{45}$$

suffices to compute the two nontrivial Lyapunov exponents λ_1 and λ_2 (see Appendix B). The SV decompostion $\tilde{Y}=\tilde{U}\tilde{F}\tilde{V}^{tr}$ of the reduced flow matrix $\tilde{Y}$ is given by

$$\begin{pmatrix} \tilde{Y}_{11} & \tilde{Y}_{12} \\ \tilde{Y}_{21} & \tilde{Y}_{22} \end{pmatrix}=\begin{pmatrix} \cos\beta & -\sin\beta \\ \sin\beta & \cos\beta \end{pmatrix}\begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix}\begin{pmatrix} \cos\gamma & \sin\gamma \\ -\sin\gamma & \cos\gamma \end{pmatrix}. \tag{46}$$

Substituting $\tilde{U}$ in Eq. (39) yields

$$\dot{\beta}\begin{pmatrix} -\sin\beta & -\cos\beta \\ \cos\beta & -\sin\beta \end{pmatrix}=\begin{pmatrix} \cos\beta & -\sin\beta \\ \sin\beta & \cos\beta \end{pmatrix}A \tag{47}$$

i.e.,

$$\dot{\beta}=A_{21}=-A_{12}\,. \tag{48}$$

The desired differential equations for the angle β and the diagonal elements of $E=\ln(F)$ are therefore given as

$$\dot{\beta}=\frac{C_{21}+C_{12}h_{21}}{1-h_{21}}\,, \tag{49}$$

$$\dot{\varepsilon}_1=C_{11}\,,$$

$$\dot{\varepsilon}_2=C_{22}\,, \tag{50}$$

with

$$h_{21}=\exp(2(\varepsilon_2-\varepsilon_1))\,, \quad (\xrightarrow{t\to\infty}0 \quad \text{if} \quad \lambda_1\neq\lambda_2) \tag{51}$$

and

$$C_{11}=\sin\beta\cos\beta-\left(\frac{\partial g}{\partial x}\cos\beta+\frac{\partial g}{\partial \dot{x}}\sin\beta\right)\sin\beta\,,$$

$$C_{12}=\cos^2\beta+\left(\frac{\partial g}{\partial x}\sin\beta-\frac{\partial g}{\partial \dot{x}}\cos\beta\right)\sin\beta\,,$$

$$C_{21}=-\sin^2\beta-\left(\frac{\partial g}{\partial x}\cos\beta+\frac{\partial g}{\partial \dot{x}}\sin\beta\right)\cos\beta\,,$$

$$C_{22}=-\sin\beta\cos\beta+\left(\frac{\partial g}{\partial x}\sin\beta-\frac{\partial g}{\partial \dot{x}}\cos\beta\right)\cos\beta\,. \tag{52}$$

In contrast to the QR case (Eq. (44)) the right-hand side of Eq. (49) depends via the term h_{21} on the diagonal elements of E (or F) (see Eq. (51)). For nondegenerate Lyapunov exponents $\lambda_1>\lambda_2$ the term h_{21} vanishes for $t\to\infty$ and Eq. (49) becomes

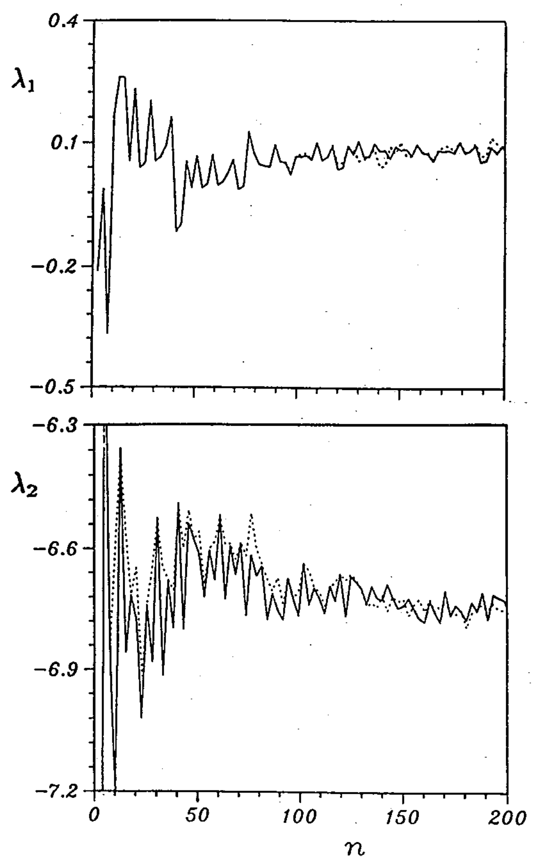

Fig. 6. Numerical estimates of the nontrivial Lyapunov exponents λ_1 and λ_2 of a strange attractor of the driven van der Pol oscillator (41, 42) for $d=5$, $a=5$ and $\omega_0=2.466$. The solid and dashed curves show the results obtained with the CQR and CSV algorithm, respectively. Within the resolution of the plot both curves lie upon each other up to the first peak of λ_2. The dotted curves were computed with the discrete GS method. The large magnitude of the negative exponent is reminiscent of the destroyed strongly attracting torus in the 3-dimensionalstatespace $M := \boldsymbol{R}^2 \times S^1$ and leads to a fast convergence of arbitrarily chosen tangent vectors to the direction of maximal expansion. This example is therefore well suited to study the numerical properties of the different methods for computing Lyapunov exponents. A Poincaré plot of this attractor showing its very thin extension normal to the expanding direction (which is consistent with the Lyapunov dimension of $D_L=2.014$) is given in Ref. 23).

identical to Eq. (44). Already after a short time both continuous methods then yield nearly identical results for the quantities ρ_i and ε_i that are used to compute the Lyapunov exponents (see Eq. (29) or (35), respectively). This fast convergence is demonstrated for a strange attractor of the driven van der Pol oscillator in Fig. 6. The numerical estimates computed with the SV method do not converge faster to the Lyapunov exponents than those computed with the QR methods.

§ 6. Conclusions

Different continuous and discrete methods for computing Lyapunov exponents are compared with respect to their efficiency and accuracy. All algorithms are based either on the QR decomposition or the singular value decomposition.

The continuous methods (that are only applicable to differential equations) show several disadvantages. First, they need much more computer time than the discrete methods. Secondly, the orthogonality of the matrices Q or U is destroyed during the computation if no counter-measures are taken (that increase the number of operations furthermore). Thirdly, the computation of only the largest k exponents is not necessarily cheaper than the determination of the whole spectrum. Fourthly, the continuous singular value method diverges for attractors with (almost) degenerate Lyapunov spectra which very often occur in dynamical systems (e.g., periodic windows, quasiperiodic oscillations (see for example, Fig. 3), near bifurcation points, etc.[14),15)]. For these four reasons the continuous methods cannot be recommended.

The quantities $(Q^{tr}JQ)_{ii}$, W_{ii} and C_{ii} $(1 \leq i \leq m)$ occurring in the differential equations (25), (29) and (35) for the Lyapunov exponents can be viewed as "local" divergence rates on the attractor. They depend not only on the point $\boldsymbol{x} \in M$ of the state space M but also on the "history" of the orthogonal matrix Q or U.[32)] These divergence rates occur in a natural way when considering continuous methods and may be viewed as the continuous and high-dimensional analogues of the nonuniformity factor NUF defined for one-dimensional maps by Nicolis, Mayer-Kress and Haubs.[33)] In practice, however, they can be computed with discrete methods, too.

All discrete methods investigated so far are based on the QR decomposition because no discrete algorithm using the singular value decomposition (SVD) is known to the authors. The discrete QR methods are different with respect to the iteration algorithm used (Eq. (17) or (18)) and the procedure for computing the QR decomposition (Gram-Schmidt orthonormalization, repeated GS orthonormalization or Householder transformations). For iterated maps and the investigation of time series[6),24)~27)] it is natural to use algorithm (17) whereas in the case of differential equations only the methods depending on (18) avoid the solution of "superfluous" variational equations. Our investigation of the Toda chain as an example of a high-dimensional continuous dynamical system shows that the differences between the results obtained with the QR decomposition procedures listed above are at most of the order of the fluctuations of the numerical estimates $\lambda_i(n)$ $(\lambda_i(n) \to \lambda_i$ for $n \to \infty)$ of the Lyapunov exponents λ_i $(1 \leq i \leq m)$. Therefore, especially for differential equations where one can reduce the time steps Δt between successive orthonormalizations, the choice of the QR decomposition procedures is not critical. This might be different for some maps with extreme contraction ratios. In that case repeated GS orthonormalizations or Householder transformations with their superior numerical properties are recommended.

Acknowledgements

All computations have been carried out on the CRAY X-MP/24 of the ZIB (Konrad-Zuse-Zentrum für Informationstechnik Berlin) and the SPERRY 1100/82 and VAX8650 of the GWDG (Gesellschaft für wissenschaftliche Datenverarbeitung mbH, Göttingen).

We thank the members of the Nonlinear Dynamics Group at the Institut für Angewandte Physik, Technische Hochschule Darmstadt, for many valuable discussions, especially U. Dressler and J. Holzfuss for the critical reading of the manuscript and the coworkers of the GWDG for their persistent help.

This work was supported by the "Stiftung Volkswagenwerk, Forschungsprojekt-Strukturbildung in gekoppelten nichtlinearen Schwingungssystemen" and the "Sonderforschungsbereich SFB-Nr. 185, Nichtlineare Dynamik, Instabilitäten und Strukturbildung in physikalischen Systemen" of the DFG (Deutsche Forschungsgemeinschaft).

Appendix A
—— *Computation of the QR Decomposition* ——

In the following sections two procedures for computing the QR decomposition of the parallelepiped matrix P (see § 2.2) are recalled.

A.1. Gram-Schmidt orthonormalization

The column vectors $\boldsymbol{Q}^j$ of Q can be determined recursively by the orthogonal projection of the column vectors $\boldsymbol{P}^j$ of P on the column vectors $\boldsymbol{Q}^{j-1}$ $(2\leq j\leq k)$:

$$\begin{aligned}
&R_{11} := \|\boldsymbol{P}^1\|\,,\\
&\boldsymbol{Q}^1 := \boldsymbol{P}^1/R_{11}\,,\\
&R_{ij} := \langle \boldsymbol{Q}^i|\boldsymbol{P}^j\rangle\,,\\
&\bar{\boldsymbol{Q}}^j := \boldsymbol{P}^j - \sum_{i=1}^{j-1} R_{ij}\boldsymbol{Q}^i\,,\\
&R_{jj} := \|\bar{\boldsymbol{Q}}^j\|\,,\\
&\boldsymbol{Q}^j := \bar{\boldsymbol{Q}}^j/R_{jj}\,. \quad (1\leq i\leq j-1,\ 2\leq j\leq k)
\end{aligned} \tag{A·1}$$

Here $\|\boldsymbol{x}\| := \langle \boldsymbol{x}|\boldsymbol{x}\rangle^{1/2}$ denotes the Euclidean norm and $\langle \boldsymbol{x}|\boldsymbol{y}\rangle := \sum_{i=1}^m x_i y_i$ the inner product of the vectors $\boldsymbol{x} := (x_1, \cdots, x_m)^{\mathrm{tr}}$ and $\boldsymbol{y} := (y_1, \cdots, y_m)^{\mathrm{tr}} \in \boldsymbol{R}^m$. For nearly parallel column vectors $\boldsymbol{P}^j$ of P the lengths $\|\bar{\boldsymbol{Q}}^j\|$ of the difference vectors $\bar{\boldsymbol{Q}}^j$ $(2\leq j\leq k)$ are very small. The computation of Q with algorithm (A·1) can therefore lead to errors, which can be avoided by an additional reorthogonalization:

$$\begin{aligned}
&R_{11} := \|\boldsymbol{P}^1\|\,,\\
&\boldsymbol{Q}^1 := \boldsymbol{P}^1/R_{11}\,,\\
&\bar{R}_{ij} := \langle \boldsymbol{Q}^i|\boldsymbol{P}^j\rangle\,,\\
&\bar{\boldsymbol{Q}}^j := \boldsymbol{P}^j - \sum_{i=1}^{j-1} \bar{R}_{ij}\boldsymbol{Q}^i\,,\\
&\tilde{R}_{ij} := \langle \boldsymbol{Q}^i|\bar{\boldsymbol{Q}}^j\rangle\,,\\
&\tilde{\boldsymbol{Q}}^j := \bar{\boldsymbol{Q}}^j - \sum_{i=1}^{j-1} \tilde{R}_{ij}\boldsymbol{Q}^i\,,\\
&R_{ij} := \bar{R}_{ij} + \tilde{R}_{ij}\,,\\
&R_{jj} := \|\tilde{\boldsymbol{Q}}^j\|\,,\\
&\boldsymbol{Q}^j := \tilde{\boldsymbol{Q}}^j/R_{jj}\,, \quad (1\leq i\leq j-1,\ 2\leq j\leq k)
\end{aligned} \tag{A·2}$$

(see Daniel, Gragg, Kaufman and Stewart[28] and Stoer[29]).

A.2. Householder transformations

A QR decompositon procedure characterized by large numerical stability has been found by Householder in 1958.[30] The $m\times k$ matrix $P\equiv P^{(0)}$ is transformed with the help of the symmetric and orthogonal *Householder transformations*

$$H^{(j)} := I - 2\langle \boldsymbol{u}^{(j)} | \boldsymbol{u}^{(j)} \rangle ,$$

$$\boldsymbol{u}^{(j)} := \frac{\boldsymbol{v}^{(j)}}{\|\boldsymbol{v}^{(j)}\|} ,$$

$$\boldsymbol{v}^{(j)} := (0, \cdots, 0, P_{j,j}^{(j-1)}, \cdots, P_{m,j}^{(j-1)})^{\mathrm{tr}} + \mathrm{sign}(P_{j,j}^{(j-1)}) c^{(j)} \boldsymbol{e}_j ,$$

$$c^{(j)} := [\sum_{i=j}^{m} (P_{i,j}^{(j-1)})^2]^{1/2} , \qquad (1 \le j \le k-1) \tag{A·3}$$

into the upper triangular $m \times k$ matrix $R = P^{(k-1)} = H^{(k-1)} \cdots H^{(1)} P$, where $P^{(j)} = H^{(j)} P^{(j-1)}$ $(1 \le j \le k-1)$ (see, e.g., Stoer[29]).

The explicit multiplication of the matrices $H^{(j)}$ $(1 \le j \le k-1)$ can be avoided by applying the $k-1$ Householder steps on the augmented $m \times (k+m)$ matrix

$$(P, I) := \bar{Q}(\bar{R}, \bar{S}) = (\bar{Q}\bar{R}, \bar{Q}\bar{S}) \tag{A·4}$$

(see Mennicken and Wagenführer[31]). In this way one obtains the $m \times (k+m)$ matrix $(\bar{R}, \bar{S})$ and an explicit representation for the orthogonal $m \times k$ matrix $\bar{Q}$:

$$\bar{Q}_{ij} = (\bar{R}, \bar{S})_{j, i+k} . \quad (1 \le i \le m, 1 \le j \le k) \tag{A·5}$$

The numerically computed matrix $\bar{R}$, however, still contains negative diagonal elements. To reach the uniqueness of the QR decomposition of P one therefore has to multiply $\bar{Q}$ and $\bar{R}$ with the diagonal matrix SIGN $(\bar{R})$:=diag (sign$(\bar{R}_{11})$, $\cdots$, sign $(\bar{R}_{kk})$):

$$Q := \bar{Q}\, \mathrm{SIGN}(\bar{R}) ,$$

$$R := \mathrm{SIGN}(\bar{R})\, \bar{R} . \tag{A·6}$$

Appendix B

—— *Lyapunov Exponents of Periodically Driven Oscillators* ——

The Lyapunov exponents $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$ of the reduced system (45) are given in terms of the diagonal elements $\tilde{R}_{11}$ and $\tilde{R}_{22}$ of the corresponding QR decomposition

$$\begin{pmatrix} \tilde{R}_{11} & \tilde{R}_{12} \\ 0 & \tilde{R}_{22} \end{pmatrix} = \tilde{R} = \tilde{Q}^{-1} \tilde{Y} = \begin{pmatrix} \cos\tilde{\alpha} & \sin\tilde{\alpha} \\ -\sin\tilde{\alpha} & \cos\tilde{\alpha} \end{pmatrix} \begin{pmatrix} \tilde{Y}_{11} & \tilde{Y}_{12} \\ \tilde{Y}_{21} & \tilde{Y}_{22} \end{pmatrix} \tag{B·1}$$

of the reduced flow matrix $\tilde{Y}$ (see Eq. (13)). In the 3×3 case the special structure of J and the flow matrix Y (see Eq. (43)) implies the equations

$$0 = -\sin\alpha\, Y_{11} + \cos\alpha\, Y_{22} ,$$

$$R_{11} = \cos\alpha\, Y_{11} + \sin\alpha\, Y_{21} ,$$

$$R_{22} = \sin\alpha\, Y_{12} + \cos\alpha\, Y_{22} , \tag{B·2}$$

for the angle α and the diagonal elements R_{11} and R_{22}. Due to the special structure of J the differential equations for the components Y_{ij} $(i, j = 1, 2)$ are given by

$$\dot{Y}_{11} = Y_{21}\,,$$

$$\dot{Y}_{12} = Y_{22}\,,$$

$$\dot{Y}_{21} = -\frac{\partial g}{\partial x}Y_{11} - \frac{\partial g}{\partial \dot{x}}Y_{21}\,,$$

$$\dot{Y}_{22} = -\frac{\partial g}{\partial x}Y_{12} - \frac{\partial g}{\partial \dot{x}}Y_{22}\,, \qquad (\text{B}\cdot 3)$$

because $Y_{31} = Y_{32} = 0$. Thus the components Y_{ij} and $\tilde{Y}_{ij}$ are solutions of the same differential equation (45) or (B·3). Therefore $\tilde{Y}_{ij} = Y_{ij}$ $(i, j = 1, 2)$, $\tilde{a} = a$ and thus $\tilde{R}_{11} = R_{11}$ and $\tilde{R}_{22} = R_{22}$ by Eqs. (B·1) and (B·2), i.e., the Lyapunov exponents of the reduced system (45) are equal to those of the original system (43).

References

1) J. M. Greene and J.-S. Kim, Physica **D24** (1987), 213.
2) I. Goldhirsch, P.-L. Sulem and S. A. Orszag, Physica **D27** (1987), 311.
3) I. Shimada and T. Nagashima, Prog. Theor. Phys. **61** (1979), 1605.
4) G. Benettin, L. Galgani, A. Giorgilli and J.-M. Strelcyn, Meccanica **15** (1980), 9, 21.
5) A. Wolf, J. B. Swift, H. L. Swinney and J. A. Vastano, Physica **D16** (1985), 285.
6) J.-P. Eckmann and D. Ruelle, Rev. Mod. Phys. **57** (1985), 617.
7) U. Parlitz, Ph. D. Thesis, Georg-August-Universität Göttingen, Göttingen (1987).
8) V. I. Oseledec, Trans. Moscow Math. Soc. **19** (1968), 197.
9) R. A. Johnson, K. J. Palmer and G. R. Sell, Siam J. Math. Anal. **18** (1987), 1.
10) G. Paladin and A. Vulpiani, Phys. Rep. **156** (1987), 147.
11) W. Lauterborn and U. Parlitz, J. Acoust. Soc. Am. **84** (1988), 1975.
12) J. M. Greene and J.-S. Kim, Physica **D36** (1989), 83.
13) M. Rokni and B. S. Berger, Quart. Appl. Math. **45** (1987), 789.
14) K. Geist, Ph. D. Thesis, Georg-August-Universität Göttingen, Göttingen (1989).
15) K. Geist and W. Lauterborn, Physica **D41** (1990), 1.
16) J. J. Dongarra, C. B. Moler, J. R. Bunch and G. W. Stewart, LINPACK User's Guide (SIAM, Philadelphia, Pennsylvania, 1979).
17) E. N. Lorenz, Physica **D13** (1984), 90.
18) H. Grauert and W. Fischer, *Differential und Integralrechnung II*, 3rd ed. (Springer, Berlin, 1978), Satz 2.5, p. 194.
19) U. Dressler, Phys. Rev. **A38** (1988), 2103.
20) U. Dressler, Ph. D. Thesis, Georg-August-Universität Göttingen, Göttingen (1989).
21) K. Geist and W. Lauterborn, Physica **D31** (1988), 103.
22) V. I. Arnol'd, *Gewöhnliche Differentialgleichungen* (Springer, Berlin, 1980).
23) U. Parlitz and W. Lauterborn, Phys. Rev. **A36** (1987), 1428.
24) J.-P. Eckmann, S. O. Kamphorst, D. Ruelle and S. Ciliberto, Phys. Rev. **A34** (1986), 4971.
25) M. Sano and Y. Sawada, Phys. Rev. Lett. **55** (1985), 1082.
26) J. Holzfuss, Ph. D. Thesis, Georg-August-Universität Göttingen, Göttingen (1987).
27) J. Holzfuss and W. Lauterborn, Phys. Rev. **A39** (1989), 2146.
28) J. Daniel, W. B. Gragg, L. Kaufman and G. W. Stewart, Math. Comp. **30** (1976), 772.
29) J. Stoer, *Einführung in die Numerische Mathematik I : unter Berücksichtigung von Vorlesungen von F. L. Bauer, Heidelberger Taschenbücher*, vol. 105, 3rd ed. (Springer, Berlin, 1979).
30) A. S. Householder, J. Assoc. Comput. Math. **5** (1958), 339.
31) R. Mennicken and E. Wagenführer, *Numerische Mathematik 1, rororo vieweg*, vol. 28 (Rowohlt Taschenbuch Verlag GmbH, Reinbeck bei Hamburg, 1977).
32) U. Dressler and G. Mayer-Kress, personal communication.
33) J. S. Nicolis, G. Mayer-Kress and G. Haubs, Z. Naturforsch. **A38** (1983), 1157.