Lyapunov Exponents without Rescaling and Reorthogonalization

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We present a new method for the computation of Lyapunov exponents utilizing representations of orthogonal matrices applied to decompositions of M or $M\tilde{M}$ where M is the tangent map. This method uses a minimal set of variables, does not require renormalization or reorthogonalization, can be used to efficiently compute partial Lyapunov spectra, and does not break down when the Lyapunov spectrum is degenerate. [S0031-9007(98)05948-1]

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Chaotic dynamics has been investigated in a very large class of systems, including astrophysical, biological, and chemical systems, mechanical devices, models of the weather, lasers, plasmas, and fluids, to mention a few. Lyapunov exponents provide the single most important quantitative characterization of the exponential divergence of initially nearby trajectories, which is the hallmark of chaos. Recent applications of these exponents include the connection between chaotic dynamics and transport theory in statistical mechanics [1,2] and galactic dynamics [3].

Several methods exist for computing Lyapunov exponents [4–8]. However, no single method appears to be optimal. For example, *QR* and SVD (singular value decomposition) methods [5,6] require frequent renormalization (to combat exponential growth of the separation vector between the fiducial and nearby trajectories) and reorthogonalization (to overcome the exponential collapse of initially orthogonal separation vectors onto the direction of maximal growth). The existing continuous versions of the *QR* and SVD methods also suffer from the additional disadvantage of being unable to compute the partial Lyapunov spectrum using a fewer number of equations/operations than required for the computation of the full spectrum [6]. Further, the continuous SVD method breaks down when computing degenerate Lyapunov spectra [6]. The symplectic method [7] is applicable only to Hamiltonian systems (and a few generalizations thereof) and has proven difficult to extend to systems of moderate size, although this is possible in principle [9]. It also does not permit easy evaluation of partial Lyapunov spectra.

The widespread perception that some form of explicit rescaling and reorthogonalization is necessary lies at the heart of most methods for computing Lyapunov exponents. In this Letter, we propose a general method which analytically obviates the need for rescaling and reorthogonalization. Our new method also does away with the other shortcomings listed above: A partial Lyapunov spectrum can be computed using a fewer number of equations as compared to the computation of the full spectrum, there is no difficulty in evaluating degenerate Lyapunov spectra, the equations are straightforward to generalize to higher dimensions, and the method uses the minimal set of dynamical variables. Since our method is based on exact differential equations for the Lyapunov exponents, global invariances of the Lyapunov spectrum can be preserved.

The key feature of our approach is the use of explicit group theoretical representations of orthogonal matrices. This results in a set of coupled ordinary differential equations for the Lyapunov exponents along with the various angles parametrizing the orthogonal matrices. The system of differential equations is treated as an initial value problem and solved numerically to obtain the Lyapunov exponents. In the preferred variant of our method, the equations are only partially coupled leading to easy evaluation of the incomplete Lyapunov spectrum. An interesting consequence of our methodology is the natural separation between "slow" (the exponents) and "fast" (the angles) pieces in the evolution equations. (This fact can be used to provide speed-up in numerical implementations.) Since the structure of the coupled differential equations is of a special form, they may also turn out to be useful for analytic studies of evolution in tangent space.

To begin, we consider an n dimensional continuous-time dynamical system,

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

where $\mathbf{z} = (z_1, z_2, \ldots, z_n)$ and $\mathbf{F}$ is an n-dimensional vector field. Let $\mathbf{Z}(t) = \mathbf{z}(t) - \mathbf{z}_0(t)$ denote deviations from the fiducial trajectory $\mathbf{z}_0(t)$. Linearizing Eq. (1) around this trajectory, we obtain

$$\frac{d\mathbf{Z}}{dt} = \mathbf{DF}(\mathbf{z}_0(t), t) \cdot \mathbf{Z}\,, \tag{2}$$

where $\mathbf{DF}$ denotes the $n \times n$ Jacobian matrix.

Integrating the linearized equations along the fiducial trajectory yields the tangent map $M(\mathbf{z}_0(t), t)$ which takes the initial variables $\mathbf{Z}^{\text{in}}$ into the time-evolved variables $\mathbf{Z}(t) = M(t)\mathbf{Z}^{\text{in}}$ [the dependence of M on the fiducial trajectory $\mathbf{z}_0(t)$ is understood]. Let Λ be an $n \times n$ matrix

given by $\Lambda = \lim_{t\to\infty}(M\tilde{M})^{1/2t}$, where $\tilde{M}$ denotes the matrix transpose of M. The Lyapunov exponents then equal the logarithm of the eigenvalues of Λ [4].

It is clear that M is of central importance in the evaluation of Lyapunov exponents. Its evolution equation can easily be derived,

$$\frac{dM}{dt} = \mathbf{D}\mathbf{F}M\,. \tag{3}$$

Instead of a brute force attack, our purpose is now to write M (or some variant thereof) in such a way that the resulting evolution equations are intrinsically well behaved. One way to do this is to follow the approach of Ref. [7] and introduce the matrix $A \equiv M\tilde{M}$. The evolution equation for A follows from (3)

$$\frac{dA}{dt} = \mathbf{D}\mathbf{F}A + A\tilde{\mathbf{D}\mathbf{F}}\,. \tag{4}$$

The matrix A is symmetric and positive definite [4]. Hence, it can be written as an exponential of a symmetric matrix B [10]: $A = e^B$. Furthermore, any symmetric matrix can be diagonalized using orthogonal matrices [10]. Thus, $A = e^{ODO^{-1}}$, where O is an $n \times n$ orthogonal matrix, D is an $n \times n$ diagonal matrix, and $O^{-1} = \tilde{O}$. From standard properties of matrix exponentials, it follows that $A = Oe^D O^{-1}$. There is no need for rescaling since the diagonal matrix D is already in the exponent (the diagonal elements are just the Lyapunov exponents multiplied by time).

To proceed further, we use an easy to obtain explicit representation of the orthogonal matrix O from group representation theory [11]. One advantage is that a minimum number of variables is used to characterize the system: $n(n-1)/2$ in O and further n variables in D, for a total of $n(n+1)/2$. Another advantage is that numerical errors can never lead to loss of orthogonality. Finally, the dynamical equations (4) are solved numerically.

Instead of using the above approach we now describe a variant of this idea which has certain further advantages. As is well known [10], the matrix M can be written as the product $M = QR$ of an orthogonal $n \times n$ matrix Q and an upper-triangular $n \times n$ matrix R with positive diagonal entries. Substituting this into Eq. (3), we obtain

$$\dot{Q}R + Q\dot{R} = \mathbf{D}\mathbf{F}QR\,, \tag{5}$$

where the overdot denotes a time derivative. Multiplying the above equation by $\tilde{Q}$ from the left and R^{-1} from the right, we get

$$\tilde{Q}\dot{Q} + \dot{R}R^{-1} = \tilde{Q}\mathbf{D}\mathbf{F}Q\,. \tag{6}$$

Note that $\tilde{Q}\dot{Q}$ is a skew(anti)-symmetric matrix for any orthogonal matrix Q and $\dot{R}R^{-1}$ is still an upper-triangular matrix.

As before, we now employ an explicit representation of the orthogonal matrix Q representing it as a product of $n(n-1)/2$ orthogonal matrices, each of which corresponds to a simple rotation in the (i,j)th plane $(i<j)$. Denoting the matrix corresponding to this rotation by $O^{(ij)}$, its matrix elements are given by

$$\begin{aligned} O^{(ij)}_{kl} &= 1 \quad \text{if } k = l \neq i,j\,; \\ &= \cos\phi \quad \text{if } k = l = i \text{ or } j\,; \\ &= \sin\phi \quad \text{if } k = i,\ l = j\,; \\ &= -\sin\phi \quad \text{if } k = j,\ l = i\,; \\ &= 0 \quad \text{otherwise.} \end{aligned} \tag{7}$$

Here ϕ denotes an angle variable. Thus, the $n \times n$ matrix Q is represented by

$$Q = O^{(12)}O^{(13)}\cdots O^{(1n)}O^{(23)}\cdots O^{(n-1,n)}. \tag{8}$$

Hence Q is parametrized by $n(n-1)/2$ angles which we denote by θ_i $[i = 1,\ldots,n(n-1)/2]$. These angles will be collectively denoted by θ.

Since the upper-triangular matrix R has positive diagonal entries, it can be represented as follows:

$$R = \begin{pmatrix} e^{\lambda_1} & r_{12} & \cdots & \cdots & r_{1n} \\ 0 & e^{\lambda_2} & r_{23} & \cdots & r_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & e^{\lambda_n} \end{pmatrix}. \tag{9}$$

The quantities λ_i will be shown to be intimately related to the Lyapunov exponents. Our final equations will be in terms of the λ_i which already appear in the exponent, thus removing the need for rescaling. The quantities r_{ij} represent the supradiagonal terms in R.

Using the above representations of Q and R, we obtain

$$\tilde{Q}\dot{Q} = \begin{pmatrix} 0 & -f_1(\dot{\theta}) & \cdots & -f_{n-1}(\dot{\theta}) \\ f_1(\dot{\theta}) & 0 & \cdots & -f_{2n-3}(\dot{\theta}) \\ \vdots & \vdots & \vdots & \vdots \\ f_{n-1}(\dot{\theta}) & \cdots & f_{n(n-1)/2}(\dot{\theta}) & 0 \end{pmatrix} \tag{10}$$

and

$$\dot{R}R^{-1} = \begin{pmatrix} \dot{\lambda}_1 & r'_{12} & \cdots & \cdots & r'_{1n} \\ 0 & \dot{\lambda}_2 & r'_{23} & \cdots & r'_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dot{\lambda}_n \end{pmatrix}. \tag{11}$$

Here, each of the $n(n-1)/2$ functions f_i depend (in principle) on the time derivatives $\dot{\theta}_i$ of all the angles used to represent Q. In fact, they actually depend only on a subset of the angles. The quantities r'_{ij} are of no concern since they are not present in the final equations.

Substituting the above two expressions in Eq. (6) we obtain

$$\begin{pmatrix} \dot{\lambda}_1 & r''_{12} & \cdots & \cdots & r''_{1n} \\ f_1(\dot{\theta}) & \dot{\lambda}_2 & r''_{23} & \cdots & r''_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ f_{n-1}(\dot{\theta}) & \cdots & \cdots & f_{n(n-1)/2}(\dot{\theta}) & \dot{\lambda}_n \end{pmatrix} = \tilde{Q}\mathbf{DF}Q\,. \tag{12}$$

Denoting the matrix $\tilde{Q}\mathbf{DF}Q$ by S and comparing diagonal elements on both sides of (12) one gets

$$\dot{\lambda}_i = S_{ii}, \qquad i = 1, 2, \ldots, n\,. \tag{13}$$

It can be shown [6] that the Lyapunov exponents are equal to λ_i/t in the limit $t \to \infty$. Thus, the Lyapunov exponents can be obtained by solving the above differential equations for long times. However, since the right-hand side depends on the angles θ_i, we also require differential equations governing the evolution of these angles.

Differential equations for the angles can be obtained by comparing the subdiagonal elements in Eq. (12). This gives

$$f_1(\dot{\theta}) = S_{21}; \quad f_2(\dot{\theta}) = S_{31}; \ldots; f_{n(n-1)/2}(\dot{\theta}) = S_{n,n-1}\,.$$

This set of differential equations can be transformed into a more convenient form [12]

$$\dot{\theta}_i = g_i(\theta), \qquad i = 1, 2, \ldots, n(n-1)/2\,, \tag{14}$$

where the equations for θ_i are decoupled from the equations for λ_i. This avoids potential problems with degenerate Lyapunov spectra. Because of these reasons, the second method just described is to be preferred over the method first discussed. Equations (13) and (14) form a system of $n(n+1)/2$ ordinary differential equations that can be solved to obtain the Lyapunov exponents.

Our system of differential equations has another attractive feature. The equation for λ_1 depends only on the first $(n-1)$ θ_i's (under a suitable ordering) [12]. Therefore, if one is interested in only the largest Lyapunov exponent, one needs to solve only n equations [as opposed to $n(n+1)/2$ for the full spectrum]. The equation for λ_2 depends only on the first $2n-3$ θ_i's. Therefore, to obtain the first 2 Lyapunov exponents, one needs to solve only $2n-1$ equations. In general, to solve for the first m Lyapunov exponents, one has to solve $m(2n-m+1)/2$ equations which is always less than $n(n+1)/2$ (the total number of equations) for $m < n$. This is in contrast to the situation for the conventional continuous QR or SVD methods where it is computationally costlier to evaluate a partial spectrum once a threshold is crossed [6]. The first method discussed above shares this disadvantage.

We end the general analysis of our system of equations by pointing out an interesting fact. From Eq. (13),

$$\dot{\lambda}_1 + \dot{\lambda}_2 + \cdots + \dot{\lambda}_n = \mathrm{Tr}(S)\,. \tag{15}$$

Parametrizing the Jacobian matrix $\mathbf{DF}$ as $[\mathbf{DF}]_{ij} = df_{ij}$ we can evaluate the trace of the matrix S to obtain [12]

$$\dot{\lambda}_1 + \dot{\lambda}_2 + \cdots + \dot{\lambda}_n = df_{11} + df_{22} + \cdots + df_{nn}\,. \tag{16}$$

We now illustrate the second method for a system with 2 degrees of freedom. In this case, Q is parametrized as follows:

$$Q = \begin{pmatrix} \cos\theta_1 & \sin\theta_1 \\ -\sin\theta_1 & \cos\theta_1 \end{pmatrix}, \tag{17}$$

and the upper-triangular matrix R may be written as

$$R = \begin{pmatrix} e^{\lambda_1} & r_{12} \\ 0 & e^{\lambda_2} \end{pmatrix}. \tag{18}$$

Next, we parametrize the Jacobian matrix $\mathbf{DF}$ as follows:

$$\mathbf{DF} = \begin{pmatrix} df_{11} & df_{12} \\ df_{21} & df_{22} \end{pmatrix}. \tag{19}$$

Substituting the above into Eq. (12), we obtain the desired equations for λ_1, λ_2, and θ_1,

$$\begin{aligned} \frac{d\lambda_1}{dt} &= df_{11}\cos^2\theta_1 + df_{22}\sin^2\theta_1 \\ &\quad - \frac{1}{2}(df_{12} + df_{21})\sin 2\theta_1\,, \\ \frac{d\lambda_2}{dt} &= df_{11}\sin^2\theta_1 + df_{22}\cos^2\theta_1 \\ &\quad + \frac{1}{2}(df_{12} + df_{21})\sin 2\theta_1\,, \\ \frac{d\theta_1}{dt} &= -\frac{1}{2}(df_{11} - df_{22})\sin 2\theta_1 \\ &\quad + df_{12}\sin^2\theta_1 - df_{21}\cos^2\theta_1\,. \end{aligned} \tag{20}$$

The above differential equations are numerically integrated forward in time until the desired convergence for the exponents, λ_1/t and λ_2/t, is achieved.

As our first example, we consider the driven van der Pol oscillator,

$$\begin{aligned} \dot{z}_1 &= z_2\,, \\ \dot{z}_2 &= -d(1 - z_1^2)z_2 - z_1 + b\cos\omega t\,. \end{aligned} \tag{21}$$

For the parameter values $d = -5$, $b = 5$, and $\omega = 2.466$, our results are in agreement with values obtained earlier using the symplectic approach [7].

To illustrate the application of the method to a system with more degrees of freedom, we turn to the standard test case of the Lorenz equations [13],

$$\begin{aligned} \dot{z}_1 &= \sigma(z_2 - z_1)\,, \\ \dot{z}_2 &= z_1(\rho - z_3) - z_2\,, \\ \dot{z}_3 &= z_1 z_2 - \beta z_3\,. \end{aligned} \tag{22}$$

For this 3 degrees of freedom system, we need to generalize the equations given in Eq. (20). This can easily be done to obtain six partially coupled differential equations governing the evolution of the three Lyapunov exponents and three angles. We used parameter values of $\sigma = 10$, $\rho = 28$, and $\beta = 8/3$. An extensive comparison of our method against the standard *QR* method with Gramm-Schmidt reorthogonalization (*QR*/GS) [5] was carried out. Both methods were applied to the same fiducial trajectory generated using a fourth order Runge-Kutta (RK4) integrator applied to Eqs. (22) with time step $\epsilon = 0.001$. Error and convergence analysis was carried out by applying the two methods to the fiducial trajectory sampled over time intervals $t_s \geq \epsilon$. Both methods were implemented using RK4 integrators, and with $t_s = \epsilon = 0.001$, both generated essentially identical results. As a function of t_s, both methods were quartically convergent as expected, *QR*/GS possessing a smaller convergence coefficient for the positive Lyapunov exponent and a larger one for the negative exponent. Even for this small system, execution times for both methods were similar. (We did not attempt to fully optimize either of the codes.) For larger systems our method is expected to be more efficient.

In the Lorenz system of equations, the sum of the three Lyapunov exponents must equal $-(\sigma + \beta + 1)$. With our method, the sum of the three Lyapunov exponents $-(\sigma + \beta + 1) = -13.6666\ldots$ was maintained to nine decimal places, *independent* of the sampling interval over the investigated range, $0.001 \leq t_s \leq 0.02$, a property not shared by *QR*/GS. (The sum of all Lyapunov exponents is an important quantity in stationary, thermostatted nonequilibrium systems since it is directly proportional to the transport coefficients. Recent analytic and numerical results are reported in Refs. [2].)

To summarize, we have described a technique for computing Lyapunov exponents that has several advantages over existing methods. The minimal number of variables is used, rescaling and reorthogonalization are eliminated, partial Lyapunov spectra can be calculated using a fewer number of equations, there are no difficulties with degenerate Lyapunov spectra, and global invariances of the Lyapunov spectrum can be explicitly preserved. The method allows a natural fast/slow split between variables, which may be taken advantage of to improve convergence of the exponents. Moreover, the simple form of the final set of equations may prove to be useful in analytic considerations. Further details will be presented elsewhere [12].

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[1] H. van Beijeren, J. R. Dorfman, E. G. D. Cohen, H. A. Posch, and Ch. Dellago, Phys. Rev. Lett. **77**, 1974 (1996); D. M. Barnett, T. Tajima, K. Nishihara, Y. Ueshima, and H. Furukawa, *ibid.* **76**, 1812 (1996); M. H. Ernst, J. R. Dorfman, R. Nix, and D. Jacobs, *ibid.* **74**, 4416 (1995); E. G. D. Cohen, Physica (Amsterdam) **213A**, 293 (1995); N. I. Chernov, G. L. Eyink, J. L. Lebowitz, and Ya. G. Sinai, Phys. Rev. Lett. **70**, 2209 (1993).

[2] A. Latz, H. van Beijeren, and J. R. Dorfman, Phys. Rev. Lett. **78**, 207 (1997); Ch. Dellago and H. A. Posch, *ibid.* **78**, 211 (1997).

[3] See, e.g., S. Habib, H. E. Kandrup, and M. E. Mahon, Astrophys. J. **480**, 155 (1997); D. Merritt and M. Valluri, *ibid.* **471**, 82 (1996); and references therein.

[4] J.-P. Eckmann and D. Ruelle, Rev. Mod. Phys. **57**, 617 (1985), and references therein.

[5] G. Bennetin, L. Galgani, and J. M. Strelcyn, Phys. Rev. A **14**, 2338 (1976); I. Shimada and T. Nagashima, Prog. Theor. Phys. **61**, 1605 (1979); A. Wolf, J. B. Swift, H. L. Swinney, and J. A. Vastano, Physica (Amsterdam) **16D**, 285 (1985).

[6] K. Geist, U. Parlitz, and W. Lauterborn, Prog. Theor. Phys. **83**, 875 (1990).

[7] S. Habib and R. D. Ryne, Phys. Rev. Lett. **74**, 70 (1995).

[8] F. Christiansen and H. H. Rugh, Nonlinearity **10**, 1063 (1997).

[9] S. Habib and R. D. Ryne, in *Nonlinear Evolution Equations and Dynamical Systems, Proceedings of the 10th Workshop on Nonlinear Evolution Equations and Dynamical Systems, Los Alamos, New Mexico, 1994*, edited by V. G. Makhankov, A. R. Bishop, and D. D. Holm (World Scientific, London, 1995); I. Gjaja, *ibid.*

[10] G. H. Golub and C. F. Van Loan, *Matrix Computations* (Johns Hopkins University Press, Baltimore, 1996), 3rd ed.

[11] I. M. Gelfand, R. A. Minlos, and Z. Ya. Shapiro, *Representations of the Rotation and Lorentz Groups and their Applications* (Pergamon, New York, 1963), pp. 353–354.

[12] T. M. Janaki, G. Rangarajan, S. Habib, and R. D. Ryne (to be published).

[13] E. N. Lorenz, J. Atmos. Sci. **23**, 130 (1963).