New Method for Computing Finite-Time Lyapunov Exponents

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We present a novel method for computing *finite-time* Lyapunov exponents and vectors, via generalizing a correction given by Goldhirsch, Sulem, and Orszag [Physica (Amsterdam) **27D**, 311 (1987)] into higher-order corrections. This method is a generalized *LR* method, which is, in contrast to the existing methods, applicable to multidimensional systems with degenerate spectra. The efficiency and accuracy is demonstrated by applying it to multidimensional dynamical systems. Without these corrections, we could not accurately detect, as an example, the coexistence of qualitatively different Lyapunov instabilities along a trajectory for a multidimensional oscillator system.

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The spectrum of Lyapunov exponents (LEs) provides quantitative characterization of a dynamical system. LEs of a reference trajectory measure the exponential rates of principal divergences of the initially neighboring trajectories [1]. Motion with at least one positive LE has a strong sensitivity to small perturbations of the initial conditions and is said to be chaotic. In contrast, the principal divergences in regular motion, such as quasiperiodic motion, are at most linear in time, and then the leading LE should be zero in this case. The LEs have been studied both theoretically and experimentally in a wide range of systems [2,3] to elucidate the connections to the physical phenomena of importance, such as nonequilibrium relaxation and transports [4,5].

The existence of LEs is proved under a general condition [6]. However, the convergence of LEs is found to be quite slow (algebraically) in time for a generic dynamical system [7], due to its nonhyperbolicity [8]. In a nonhyperbolic system, chaotic and regular motions coexist in the phase space, which introduces large variations in local instability *along a reference chaotic trajectory*. The variations are related to the alternations between qualitatively different motions, such as chaotic and quasiregular, laminar motions in two-dimensional systems [9] and random and cluster motions in high-dimensional systems [10]. These variations are quantified by *finite-time* Lyapunov exponents (FTLEs), the exponential rates of principal divergences during finite-time intervals. Recent understandings of shadowability (i.e., computability of chaotic systems) [11,12], the mixing process in two-dimensional incompressible flow, entropy production in an advection-diffusion equation, and dynamo phenomena [13] have been widely developed with the essential use of FTLEs and finite-time Lyapunov vectors (FTLVs).

For a nonhyperbolic system, there exist time intervals where part of the FTLEs accumulate around zero. Hence the FTLE spectra are (quasi-)degenerate, which impede us to accurately compute the FTLEs with the existing numerical methods, the *QR* and the singular value decomposition (SVD) methods [7,14]. The *QR* methods, based on the matrix factorization of *QR* decomposition (QRD) [15], are effective and widely used algorithms for computing the LEs [1,16–19]. However, for the FTLEs, these methods introduce errors that decrease only algebraically in time [7]. Goldhirsch, Sulem, and Orszag have derived a correction for the standard *QR* method [7,20]. This correction is rather effective for nondegenerate spectra, but insufficient to accurately compute FTLEs with (quasi-)degenerate spectra. On the other hand, the SVD methods, based on the matrix factorization of SVD [15], are accurate algorithms for computing FTLEs [7,14]. However, the SVD methods have a severe limitation of being applicable only to continuous-time systems with nondegenerate spectra [14].

In this Letter, by generalizing the correction given by Goldhirsch *et al.* to higher-order corrections, we develop a new, accurate method for computing FTLEs and FTLVs, which is applicable even when the spectrum is degenerate. We demonstrate the accuracy, efficiency, and usefulness of our method, by applying it to multidimensional dynamical systems.

Let us consider continuous- or discrete-time dynamical systems in n-dimensional phase space $x = (x^1, x^2, \ldots, x^n)$, whose equations of motion are, respectively, given by

$$\frac{dx^j(t)}{dt} = f^j(x(t)) \quad \text{or} \quad x^j(t) = F^j(x(t-1)) \qquad (1)$$

for $j = 1, 2, \ldots, n$. We write the solution of Eq. (1) starting from x_0 at $t = 0$ as $x(t, x_0)$. The stability matrix from a time t_i to a later time t_f along a reference trajectory $x(t, x_0)$ is the $n \times n$ Jacobian matrix $M(t_f, t_i)$ whose j-k element is $\partial x^j(t_f, x_0)/\partial x^k(t_i, x_0)$. Hence an infinitesimal perturbation $v = (v^1, v^2, \ldots, v^n)$ at $t = t_i$ is transformed to $M(t_f, t_i)\, v$ at $t = t_f$. Note that $M(t_f, t_i)$ has the relation $M(t_f, t_i) = M(t_f, 0)M(t_i, 0)^{-1}$, where $M(t, 0)$ obeys the linear variational equations of Eq. (1) with the initial conditions $M(0, 0) = I$ ($\equiv$ the $n \times n$ identity matrix).

Now we introduce the FTLEs and the FTLVs from the SVD [15] of the stability matrix

$$M(t_f, t_i) = U(t_f, t_i)D(t_f, t_i)V(t_f, t_i)^T = \sum_{j=1}^{n} u_j(t_f, t_i)\mu_j(t_f, t_i)v_j(t_f, t_i)^T, \quad (2)$$

where U, V are orthogonal matrices $U = [u_1, u_2, \ldots, u_n]$, $V = [v_1, v_2, \ldots, v_n]$ [21], and D is a diagonal matrix $D = \mathrm{diag}(\mu_1, \mu_2, \ldots, \mu_n)$ [22]. The singular values μ_j are the square roots of non-negative eigenvalues of the symmetric matrix $M^T M$. They are, without loss of generality, assumed to be ordered as $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. From Eq. (2), the jth FTLEs, FTLVs, and left FTLVs in the time interval from t_i to t_f are given by $\lambda_j(t_f, t_i) = \log\mu_j(t_f, t_i)/(t_f - t_i)$, $v_j(t_f, t_i)$, and $u_j(t_f, t_i)$, respectively. The ordinary, i.e., infinite-time, LEs and Lyapunov vectors are given by the $t_f \to \infty$ limits of FTLEs and FTLVs.

Now we develop a numerical method for computing FTLEs and FTLVs. The first step of our method is the procedure of the standard QR method [1,16], which is based on the QRD of the stability matrix: $M(t, 0) = Q(t, 0)R(t, 0)$, where upper triangular $R(t, 0)$ with non-negative diagonal elements and orthogonal $Q(t, 0)$ are evaluated as follows [1,16,23]. By dividing time into intervals τ ($t_k = k\tau$ for $k = 1, 2, \ldots$), $M(t, 0)$ is represented as $M(t, 0) = T_n T_{n-1} \cdots T_1$ for $t = n\tau$, with $T_k = M(t_k, t_{k-1})$. Then, with utilizing QRD repeatedly, Q_k and R_k ($k = 1, 2, \ldots$) are introduced as follows:

$$T_1 = Q_1 R_1; \qquad T_k Q_{k-1} = Q_k R_k \qquad (k \geq 2). \quad (3)$$

These matrices satisfy $M(t, 0) = Q_n R_n R_{n-1} \cdots R_1$, and thus $R(t, 0) = R_n R_{n-1} \cdots R_1$. The standard QR method evaluates the jth LE as $\lim_{t\to\infty} \sum_{k=1}^{n} (1/t) \log(R_k)_{j,j}$.

We now introduce a normalized form of the stability matrix, which gives approximate values of the FTLEs and the FTLVs: $M = Ue^d rV^T$, where U, V are orthogonal, d is diagonal, and r is upper triangular with diagonal elements of unity. These matrices are determined as follows: Since $M(t_f, t_i) = M(t_f, 0)M(t_i, 0)^{-1}$ and $M(t_n, 0) = Q_n R_n R_{n-1} \cdots R_1$, the stability matrix $M(t_f, t_i)$ is represented as $M(t_f, t_i) = Q_f R_f R_{f-1} \cdots R_{i+1} Q_i^T$ ($t_i = i\tau$, $t_f = f\tau$). Then, U and V are chosen as $U = Q_f$, $V = Q_i$. The remaining matrices d and r are given by $d_{j,j} = \log(R_{i+1})_{j,j} + \log(R_{i+2})_{j,j} + \cdots + \log(R_f)_{j,j}$ and $r = e^{-d} R_f R_{f-1} \cdots R_{i+2} R_{i+1}$, respectively. In order to obviate the numeric overflow or underflow, r is computed as $r = r_{f-i} \cdots r_2 r_1$, where $r_1 = e^{-d_1} R_{i+1}$, $r_k = e^{-d_{k+1}} R_{i+k} e^{d_k}$ ($k \geq 2$), and $(d_k)_{j,j} = \log(R_{i+1})_{j,j} + \log(R_{i+2})_{j,j} + \cdots + \log(R_{i+k})_{j,j}$. Estimating U, d, and V are straightforward.

If all off-diagonal elements of r are negligibly small compared to the diagonal elements ($= 1$), then the jth FTLE and (left) FTLV are given by $d_{j,j}/(t_f - t_i)$ and $(u_j)v_j$, respectively. Therefore, we define $\lambda_j^{QR}(t_f, t_i)$ as $d_{j,j}/(t_f - t_i)$. In general, however, r is far from diagonal, and thus λ_j^{QR}, u_j, v_j are not accurate approximations of FTLEs and FTLVs. Figure 1(a) shows errors in the smallest exponents, $|\lambda_2^{QR}(t, 0) - \lambda_2(t, 0)|$, against t for the standard map [24]: $y(t) = y(t-1) - K \sin[x(t-1)]$, $x(t) = x(t-1) + y(t)$. The exact exponents λ_j are directly computed by diagonalizing the symmetric matrix $M^T M$ with high-precision computation to evade its round-off error. The error decreases quite slowly as $\sim 1/t$, which clearly shows that λ_j^{QR} is not a sufficiently accurate approximation.

Now we present our novel method for FTLE(V)s, by correcting the finite-time error in λ^{QR}. To this end, we construct a sequence of refinements $U_{(k)}, d_{(k)}, r_{(k)}, V_{(k)}$ ($k = 0, 1, 2, \ldots$) satisfying $r_{(k)} \to$ diagonal as $k \to \infty$, with the normalization condition that $M = U_{(k)} e^{d_{(k)}} r_{(k)} V_{(k)}^T$ for even k and $M = U_{(k)} r_{(k)}^T e^{d_{(k)}} V_{(k)}^T$ for odd k. Here $U_{(k)}, V_{(k)}$ are orthogonal, $d_{(k)}$ is diagonal, and $r_{(k)}$ is an upper-triangular matrix with diagonal elements of unity. Starting from $U_{(0)} = U$, $d_{(0)} = d$, $r_{(0)} = r$,

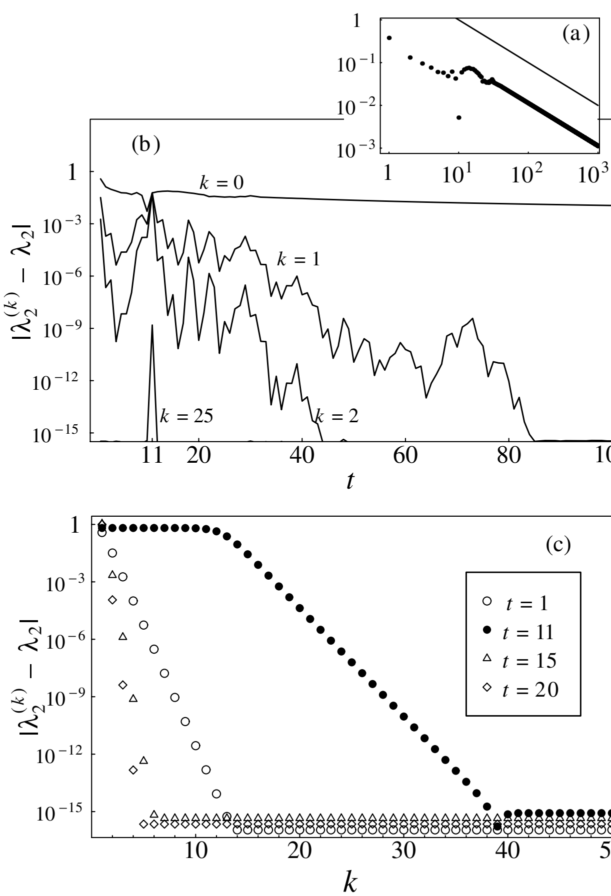

FIG. 1. The finite-time errors for $K = 1.5$, $(x(0), y(0)) = (1.1\pi, 0)$: (a) The errors in the QR method, $|\lambda_2^{QR}(t, 0) - \lambda_2(t, 0)|$, are plotted against t. (The solid line is $10/t$ for eye guidance.) The kth corrected errors in the smallest exponents are plotted: (b) $|\lambda_2^{(k)}(t, 0) - \lambda_2(t, 0)|$ vs t for $k = 0, 1, 2, 25$; (c) $|\lambda_2^{(k)}(t, 0) - \lambda_2(t, 0)|$ vs k for $t = 1, 11, 15, 20$.

$V_{(0)} = V$, we generate the successors $d_{(k)}$, $r_{(k)}$ $(k \geq 1)$ by

$$r^T_{(k-1)} = \mathcal{Q}_{(k)}\mathcal{R}_{(k)} \quad \text{(QRD)},$$
$$r_{(k)} = e^{-d_{(k-1)}}\mathcal{D}^{-1}_{(k)}\mathcal{R}_{(k)}e^{d_{(k-1)}},$$
$$d_{(k)} = \log(\mathcal{D}_{(k)}) + d_{(k-1)}, \tag{4}$$

where $\mathcal{D}_{(k)}$ is the diagonal matrix equal to the diagonal part of $\mathcal{R}_{(k)}$. The matrices $U_{(k)}, V_{(k)}$ are given by $U_{(k)} = U_{(0)}\mathcal{Q}_{(2)}\mathcal{Q}_{(4)}\cdots\mathcal{Q}_{(2\lfloor k/2\rfloor)}$, $V_{(k)} = V_{(0)}\mathcal{Q}_{(1)}\mathcal{Q}_{(3)}\cdots\mathcal{Q}_{(2\lfloor(k-1)/2\rfloor+1)}$, where $\lfloor x\rfloor$ denotes the largest integer not greater than x. This procedure (4) is intrinsically regarded as the diagonalization of the symmetric matrix M^TM via the LR method [15], except for including the normalization to overcome the large condition number of the stability matrix. Here the matrices $e^{d_{(k)}}r_{(k)}$ and $r^T_{(k)}e^{d_{(k)}}$ correspond, respectively, to the upper- and lower-triangular matrices, R and L, of the LR method. As a result of the general property of the LR method [15], this iterative procedure always converges to the exact SVD exponentially, which enables us to accurately obtain FTLEs and FTLVs.

Using $U_{(k)}$, $V_{(k)}$, $d_{(k)}$, we define the kth corrected FTLE and (left) FTLVs as $\lambda^{(k)}_j(t_f, t_i) = d_{(k)j,j}/(t_f - t_i)$ and the jth column vector of $(U_{(k)})V_{(k)}$, respectively. Note that the first corrected exponent $\lambda^{(1)}_j(t, 0) = (d_{j,j} + \log\mathcal{D}_{(1)j,j})/t$ is the same as the correction proposed by Goldhirsch *et al.* for nondegenerate spectra systems in [7,20]. Namely, our correcting procedure is a generalization of the correction proposed by them.

Next, we numerically test our correcting procedure using the standard map. The kth corrected errors $|\lambda^{(k)}_2(t, 0) - \lambda_2(t, 0)|$ are plotted in Fig. 1(b) as a function of t [24]. We can see that, for all t computed, the errors rapidly decrease as k increases, with t-dependent convergence rates. For example, the slowest convergence is observed at $t = 11$. To see the detail of the convergences, we plot the errors as a function of k in Fig. 1(c). There are intervals of k in which the errors decrease exponentially, up to precisions close to the floating number precision (16 digits). At $t = 11$, the initial step k_0 at which the interval starts is larger ($k_0 \sim 15$) than that of $t \neq 11$ ($k_0 \sim 1$), because the standard QR method fails to describe the sudden changes in directions of Lyapunov vectors. This is the major reason for the slowest convergence observed at $t = 11$ in Fig. 1(b). These observations show that the higher-order corrections ($k \geq 2$) are generally indispensable. In practice, the correcting procedure is required to be executed until the difference, $|\lambda^{(k)}_j(t, 0) - \lambda^{(k-1)}_j(t, 0)|$, of one step correction (or the magnitude of off-diagonal elements of $r_{(k)}$, $\max\{r_{(k)i,j}; i \neq j\}$) converges to zero with the floating number precision, for the best accuracy of FTLE computation.

The next example is the $(2\Lambda + 1)$-degrees-of-freedom oscillators system (Λ is a non-negative integer), whose Hamiltonian is a ϕ^4-interaction model truncated in reciprocal space:

$$H = \sum_{j=-\Lambda}^{\Lambda}\left(\frac{1}{2}p_jp_{-j} + \frac{\omega_j}{2}q_jq_{-j}\right) + \frac{\lambda}{4}\sum{}' q_{j_1}q_{j_2}q_{j_3}q_{j_4}, \tag{5}$$

where all modes $j = -\Lambda, -\Lambda + 1, \ldots, \Lambda$ satisfy the reality conditions $q_j = q^*_{-j}$; $p_j = p^*_{-j}$, $\omega_j = \sqrt{1 + j^2}$, λ is a nonlinearity parameter, and $\sum' = \sum_{j_1,j_2,j_3,j_4=-\Lambda}^{\Lambda}\delta_{j_1+j_2+j_3+j_4,0}$. This model is a nonhyperbolic dynamical system, which has chaotic trajectories, along which motions change intermittently from irregular to ordered, and vice versa [25]. Examples of typical plots of singular values $\mu_1(t, t_i)$ for ordered and irregular motions [$\Lambda = 2$, $\lambda = (32\pi)^{-1}$] are, respectively, the thick lines in Figs. 2(a) and 2(b). These figures show that the local instability has a qualitative difference that corresponds to the orders of motions: μ_1 increases linearly in time, $t - t_i$, for (a) ordered motions and exponentially for (b) irregular motions.

These singular values are computed by using our method with the relation $\mu_j = \exp[\lambda_j(t - t_i)]$. The accuracy is confirmed by comparing them to the result of the high-precision diagonalization of M^TM, as is done in the standard map. The approximate μ_1 computed via the standard QR method are plotted for comparison, with the thin lines in Figs. 2(a) and 2(b). These figures show

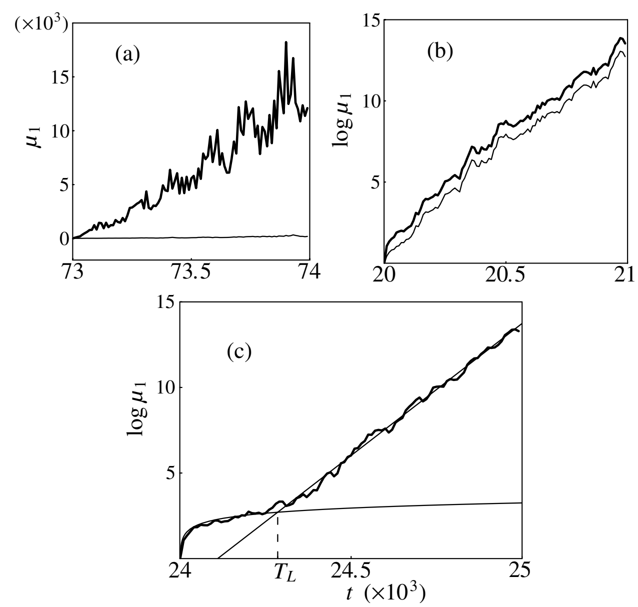

FIG. 2. $\mu_1(t, t_i)$ against t, $t_i < t < t_i + 1000$, for an initial condition [$H(p(0), q(0)) = 300$]: (a) $t_i = 73\,000$ and (b) $t_i = 20\,000$. The thick and the thin lines are our corrected results and the approximate results of the standard QR method, respectively. The thick line in (c) is μ_1 for $t_i = 24\,000$. The thin lines are the fitted lines in the early linear and in the latter exponential stage, respectively. $T_L \sim 24\,300$ is the time at the intersection of these fitted lines.

that the standard QR method does not have enough accuracy both for (a) ordered motions to reproduce the *qualitative* change of μ_1 (the QR approximate μ_1 does not give the original, linear increase and is much smaller than the accurate result) and (b) irregular motions to describe the quantitatively accurate change of $\log\mu_1$ (the approximate $\log\mu_1$ is smaller by an approximately constant gap compared to the accurate result). Therefore, we have again confirmed that our corrections are necessary for accurate computation of local instability in this multidimensional case.

Because of the great accuracy of our method, lifetimes of ordered motions are preciously determined as follows. Figure 2(c) shows a typical plot of μ_1 that changes from linear to exponential increase. The crossover time T_L in Fig. 2(c) corresponds to the change from an ordered to an irregular motion. Thus the lifetime of the ordered motion is accurately given by T_L. Note that our corrections are necessary to obtain lifetimes of ordered motions, because, without these corrections, the qualitative changes, and thus the clear crossover times, generally disappear.

In summary, we have developed a numerical algorithm for computing accurate values of finite-time Lyapunov exponents and vectors, by constructing a correcting procedure to the standard QR method. This procedure is a generalized LR method. As a result, the corrected results exponentially converge to the exact Lyapunov quantities for generic multidimensional dynamical systems including nonhyperbolic systems with (quasi-)degenerate Lyapunov spectra. This method is easy to implement [see Eqs. (3) and (4)] and very efficient, because of the exponential convergence, and because the correcting procedure is called only when the exact quantities are necessary. We have demonstrated the efficiency of our method by applying it both to the standard map and to a multidimensional oscillator system. In the application to the oscillator system, alternations in qualitatively different local instabilities have been found along a trajectory. From crossover times of local instabilities that change from linear to exponential increases, lifetimes of the associated ordered motions are determined accurately.

We expect that this correcting procedure can be applicable for other numerical methods, such as the symplectic method [18,19], and that faster convergence may be accomplished by introducing shifts [15] into the correcting process. We hope that these methods will help us to develop understandings of generic multidimensional nonhyperbolic chaotic systems.

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[21] $[u_1, u_2, \ldots, u_n]$ denotes the matrix whose ith column vector is u_i.

[22] For notational simplicity, the dependencies, on t_i and t_f, of the matrices are omitted.

[23] For a multidimensional chaotic system, the condition number [15] of $M(t, 0)$ becomes exponentially large for large t, which introduces a large amount of errors into the direct evaluation of the QRD (orthonormalizing the column vectors in M).

[24] The behavior of λ_1 is similar to that of λ_2.

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