Continuous time algorithm for Lyapunov exponents. I

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The Lyapunov exponent algorithm of Benettin *et al.* [C. R. Acad. Sci. Paris **286A**, 431 (1978); Meccanica **15**, 9 (1980)] and of Shimada and Nagashima [Prog. Theor. Phys. **61**, 1605 (1979)] is converted to a continuous time algorithm. The Gram-Schmidt orthonormalization process is incorporated into the differential equations, making orthogonalization continuous. Differential equations for the k-dimensional fiducial volumes are also derived. It is further shown that this algorithm is a factorization of the fundamental matrix Φ in the form $\Phi(t) = E(t)W(t)E^{-1}(t_0)$, where $E(t)$ is orthonormal and $W(t)$ is upper triangular. Numerical stability of the algorithm is considered, and it is shown that the standard Gram-Schmidt process can be used to stabilize the (possibly) unstable equations of motion for the orthonormal basis vectors. A numerical example is presented.

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I. INTRODUCTION

A nonlinear system of differential equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) \tag{1}$$

can (at worst) be integrated numerically to produce a trajectory $\mathbf{x}(\mathbf{x_0}, t)$, a function of time t, and the initial conditions $\mathbf{x}(t_0) = \mathbf{x}_0$ at the starting time. Neighboring trajectories obey the *variational equations*

$$\delta\dot{\mathbf{x}} = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right|_{\mathbf{x}(t)} \delta\mathbf{x} = A(t)\delta\mathbf{x}, \tag{2}$$

where $\delta\mathbf{x}$ is the presumed infinitesimal displacement from the reference orbit. These are a set of time-dependent linear differential equations, and their stability is governed in the general case by their Lyapunov exponents.

The first successful algorithm for calculating the entire spectrum of Lyapunov exponents is due to Benettin and co-workers [1,2] and to Shimada and Nagashima [3]. We will term this method the "standard" algorithm for calculating Lyapunov exponents. Another method for calculating Lyapunov exponents propagates the exterior products of reference solutions directly [4,5]. Although these latter algorithms may be computationally more efficient, we will restrict our attention to the reformulation of the "standard" algorithm.

We will (roughly) follow the notation of [3], although the methods are virtually identical. They begin by integrating N reference solutions $\mathbf{u}_k(t)$ to (2) over a finite time interval τ, starting from initial conditions $\mathbf{u}_k(t_0) = \mathbf{e}_k(t_0)$, an orthonormal basis. At the end of the time interval, the volumes of the k-dimensional parallelepipeds ($k = 1, 2, \ldots, N$) spanned by the vectors $\mathbf{u}_k(t)$ are calculated

$$V_k = \left\| \bigwedge_{j=1}^{k} \mathbf{u}_j(t) \right\|, \tag{3}$$

where $\wedge$ is the outer product, and $\| \; \|$ is a norm.

At this point, the vectors $\mathbf{u}_k(t)$ are orthonormalized by the Gram-Schmidt procedure. That is, new orthonormal vectors $\mathbf{e}_k(t_0 + \tau)$ are calculated according to

$$\mathbf{e}_1 = \mathbf{u}_1 / \| \mathbf{u}_1 \|, \tag{4}$$

$$\mathbf{e}_2 = \{\mathbf{u}_2 - (\mathbf{u}_2 \cdot \mathbf{e}_1)\,\mathbf{e}_1\} / \| \mathbf{u}_2 - (\mathbf{u}_2 \cdot \mathbf{e}_1)\,\mathbf{e}_1 \|, \tag{5}$$

and, in general,

$$\mathbf{e}_k = \left\{ \mathbf{u}_k - \sum_{j=1}^{k-1} (\mathbf{u}_k \cdot \mathbf{e}_j)\,\mathbf{e}_j \right\} \Bigg/ \left\| \mathbf{u}_k - \sum_{j=1}^{k-1} (\mathbf{u}_k \cdot \mathbf{e}_j)\,\mathbf{e}_j \right\|. \tag{6}$$

The Gram-Schmidt procedure leaves invariant the k-dimensional subspaces spanned by the vectors $\mathbf{u}_1$, $\mathbf{u}_2, \ldots, \mathbf{u}_k$ in constructing the new k-dimensional subspace spanned by $\mathbf{e}_1$, $\mathbf{e}_2$, $\ldots$, $\mathbf{e}_k$.

The integration is then reinitialized with new $\mathbf{u}_k(t_0 + \tau) = \mathbf{e}_k(t_0 + \tau)$, and carried forward to $t = t_0 + 2\tau$. The whole cycle is repeated over a long time interval. Standard existence theorems guarantee that the k-dimensional Lyapunov exponents are given by the limits

$$\lambda^{(k)} = \lim_{n\to\infty} \frac{1}{n\tau} \sum_{j=1}^{n} \frac{\ln V_k(t_0 + j\tau)}{\ln V_k(t_0 + (j-1)\tau)} \tag{7}$$

and that these limits exist.

One potential problem with this algorithm is that all vectors $\mathbf{u}_k$ tend towards the direction in space associated with the largest positive Lyapunov exponent. If the renormalization time τ is too long, the Gram-Schmidt procedure can fail, or become quite inaccurate. Thus, in choosing τ it helps to already know the largest positive exponent. Some authors have gone so far as to recommend renormalization after *every* time step. If this is to be done, then renormalization is virtually a continuous process. We explore this possibility in the next section.

II. A DIFFERENTIAL GRAM-SCHMIDT ALGORITHM

Begin the integration of $\dot{\mathbf{u}}_i = A(t)\mathbf{u}_i$ with a set of orthonormal unit vectors

$$\mathbf{u}_i(t_0) = \mathbf{e}_i(t_0)\,. \tag{8}$$

Now, integrating over an infinitesimal time interval, from t_0 to $t_0 + \delta t$, we have

$$\mathbf{u}_i(t_0 + \delta t) \approx \mathbf{e}_i(t_0) + A(t_0)\mathbf{e}_i(t_0)\delta t\,. \tag{9}$$

The $\mathbf{u}_i$ are no longer orthonormal at $t = t_0 + \delta t$. To reorthogonalize them, we invoke the standard Gram-Schmidt algorithm.

For the first vector we have

$$\mathbf{e}_1(t_0 + \delta t) = \mathbf{u}_1(t_0 + \delta t)/\parallel \mathbf{u}_1(t_0 + \delta t) \parallel\,, \tag{10}$$

where $\parallel\ \parallel$ can be any Riemannian norm. Using the usual Euclidean norm on rectangular coordinates, and using (9) to expand the norm to the first order in δt, gives

$$\begin{aligned}\parallel \mathbf{u}_1(t_0 + \delta t) \parallel^{-1} &\approx \parallel \mathbf{e}_1(t_0) \parallel^{-1} \\ &\quad -\tfrac{1}{2} \parallel \mathbf{e}_1(t_0) \parallel^{-3} 2\mathbf{e}_1 \cdot A(t_0)\mathbf{e}_1(t_0)\delta t + O(\delta t^2) \\ &= 1 - \mathbf{e}_1(t_0) \cdot A(t_0)\mathbf{e}_1\delta t + O(\delta t^2)\end{aligned} \tag{11}$$

since $\parallel \mathbf{e}_1(t_0) \parallel = 1$. Inserting this into (10) and again retaining only first-order terms yields

$$\begin{aligned}\mathbf{e}_1(t_0 + \delta t) \approx\ & \mathbf{e}_1(t_0) + A(t_0)\mathbf{e}_1(t_0)\delta t \\ & -[\mathbf{e}_1(t_0) \cdot A(t_0)\mathbf{e}_1(t_0)]\mathbf{e}_1(t_0)\delta t + O(\delta t^2)\,.\end{aligned} \tag{12}$$

Taking the term $\mathbf{e}_1(t_0)$ to the right side, dividing by δt, and proceeding to the limit easily gives

$$\frac{d}{dt}\mathbf{e}_1 = A\mathbf{e}_1 - (\mathbf{e}_1 \cdot A\mathbf{e}_1)\,\mathbf{e}_1 \tag{13}$$

as the differential equation satisfied by $\mathbf{e}_1(t)$.

The second vector is normalized according to

$$\begin{aligned}\mathbf{e}_2(t_0 + \delta t) = &\{\mathbf{u}_2(t_0 + \delta t) - [\mathbf{u}_2(t_0 + \delta t) \cdot \mathbf{e}_1(t_0 + \delta t)]\,\mathbf{e}_1(t_0 + \delta t)\} \\ &\times \parallel \mathbf{u}_2(t_0 + \delta t) - [\mathbf{u}_2(t_0 + \delta t) \cdot \mathbf{e}_1(t_0 + \delta t)]\,\mathbf{e}_1(t_0 + \delta t) \parallel^{-1}\,.\end{aligned} \tag{14}$$

Expanding to the first order again, the numerator of this expression becomes

$$\mathbf{e}_2 + A\mathbf{e}_2\delta t - (\mathbf{e}_2 \cdot A\mathbf{e}_1)\,\mathbf{e}_1\delta t - (\mathbf{e}_1 \cdot A\mathbf{e}_2)\,\mathbf{e}_1\delta t + O(\delta t^2)\,. \tag{15}$$

Time notation has been suppressed above, since all quantities are evaluated at $t = t_0$. Similarly, the denominator expands to first order as

$$\parallel \cdots \parallel^{-1} \approx 1 - \mathbf{e}_2 \cdot A\mathbf{e}_2\delta t + O(\delta t^2)\,. \tag{16}$$

Inserting these results into (14) and proceeding to the limit as before gives

$$\dot{\mathbf{e}}_2 = A\mathbf{e}_2 - (\mathbf{e}_2 \cdot A\mathbf{e}_2)\,\mathbf{e}_2 - (\mathbf{e}_2 \cdot A\mathbf{e}_1 + \mathbf{e}_1 \cdot A\mathbf{e}_2)\,\mathbf{e}_1 \tag{17}$$

as the differential equation for $\mathbf{e}_2(t)$. Proceeding recursively in this manner, the general $\mathbf{e}_k(t)$ vector obeys the equation of motion

$$\begin{aligned}\frac{d}{dt}\mathbf{e}_k = \quad & A\mathbf{e}_k - (\mathbf{e}_k \cdot A\mathbf{e}_k)\,\mathbf{e}_k \\ & -\sum_{j=1}^{k-1}(\mathbf{e}_k \cdot A\mathbf{e}_j + \mathbf{e}_j \cdot A\mathbf{e}_k)\,\mathbf{e}_j\,.\end{aligned} \tag{18}$$

The Gram-Schmidt orthonormalization process can thus be reduced to a set of differential equations itself, and the $\mathbf{e}_k$ vectors can be propagated instead of the $\mathbf{u}_k$ vectors.

One immediate benefit of this is that the volume of the k-dimensional parallelepiped spanned by the vectors $\mathbf{e}_1$, $\mathbf{e}_2$, ..., $\mathbf{e}_k$ at t_0 is very easy to calculate. Since $V_k(t_0)$ is just the k-dimensional unit cube, we have $V_k(t_0) = 1$. The limit for the k-dimensional Lyapunov exponent is

$$\lambda^{(k)} = \lim_{n\to\infty} \frac{1}{n\tau}\sum_{i=0}^{n-1} \ln\left\{\frac{V_k(t_i + \tau)}{V_k(t_i)}\right\}\,, \tag{19}$$

where the renormalization time interval is τ, and the renormalization times $t_i = t_{i-1} + \tau$ are evenly spaced. We have let the renormalization process become a continuous process with time. Identifying $\tau = \delta t$, this becomes

$$\lambda^{(k)} = \lim_{n\to\infty} \frac{1}{n}\sum_{i=0}^{n-1}\left\{\frac{\ln V_k(t_i + \delta t) - \ln V_k(t_i)}{\delta t}\right\} \tag{20}$$

using the basic property of the logarithm. But in the limit, this is just

$$\begin{aligned}\lambda^{(k)} &= \lim_{t\to\infty} \frac{1}{t - t_0}\int_{t_0}^{t} \frac{d}{d\tau}\ln V_k(\tau)\,d\tau \\ &= \lim_{t\to\infty} \frac{1}{t - t_0}\{\ln V_k(t) - \ln V_k(t_0)\}\,,\end{aligned} \tag{21}$$

where τ is a variable of integration. This states that the Lyapunov exponent is (quite literally) the average logarithmic rate of increase of the volume V_k.

Some confusion might arise at this point, since it would seem that $V_k(t) = 1$ for all time, since we have arranged the $\mathbf{e}_k$ vectors to always be orthonormal. However, the rate of change of V_k must be computed *with respect to the* $\mathbf{u}_k$ *vectors*, since only they are solutions to the original variational equations $\dot{\mathbf{u}}_k = A\mathbf{u}_k$. We have trivially

$$\frac{d}{dt}\ln V_k = \frac{1}{V_k}\frac{d}{dt}V_k\,, \tag{22}$$

where we must calculate dV_k/dt using the $\mathbf{u}_k$ vector solutions. Now, since

$$V_1 = (\mathbf{u}_1 \cdot \mathbf{u}_1)^{1/2} \tag{23}$$

we have easily

$$\frac{d}{dt}V_1 = \frac{1}{2V_1} 2\mathbf{u}_1 \cdot \frac{d\mathbf{u}_1}{dt} = \mathbf{e}_1 \cdot A\mathbf{e}_1 \tag{24}$$

since at the beginning of a time step we have $\mathbf{u}_1 = \mathbf{e}_1$, making $V_1 = 1$, and of course using $\dot{\mathbf{u}}_1 = A\mathbf{u}_1$.

At the beginning of a time step, V_2 is just the unit square, with sides aligned with the orthogonal $\mathbf{u}_1$,$\mathbf{u}_2$ axes. Along its side parallel to the $\mathbf{u}_2$ axis, it is gaining area at the rate $\mathbf{u}_1 \cdot \dot{\mathbf{u}}_1$, while along its other face its rate of change of area is just $\mathbf{u}_2 \cdot \dot{\mathbf{u}}_2$. Both faces, of course, have unit length, and are perpendicular. So we find

$$\frac{d}{dt}V_2 = \mathbf{e}_1 \cdot A\mathbf{e}_1 + \mathbf{e}_2 \cdot A\mathbf{e}_2 \,. \tag{25}$$

Similarly, V_3 is initially a unit cube, gaining or losing volume at its three perpendicular unit area faces at the rates $\mathbf{u}_k \cdot \dot{\mathbf{u}}_k = \mathbf{e}_k \cdot A\mathbf{e}_k$, where $k = 1, 2, 3$. In general, then,

$$\frac{d}{dt}V_k = \sum_{j=1}^{k} \mathbf{e}_j \cdot A\mathbf{e}_j \,. \tag{26}$$

Furthermore, since with respect to the $\mathbf{e}_k$ basis we will always have each fiducial volume equal to a unit k-dimensional hypercube at the beginning of the time step, we have

$$\frac{d}{dt}\ln V_k = \frac{\dot{d}}{dt}V_k = \sum_{j=1}^{k} \mathbf{e}_j \cdot A\mathbf{e}_j \,. \tag{27}$$

This remarkable equation accentuates the fact that linear systems are *scale invariant*. That is, the rate of change of $\ln V_k$ should *not* depend on the absolute size of V_k, nor on the scale of the $\mathbf{u}_k$ solutions. Note that the derivatives of the $\ln V_k$ are calculated *directly* from the variational equations, not from allowing $\mathbf{u}_k$ solutions to grow by a (hopefully) manageable amount before renormalization. We note in passing that in an N-dimensional space, this states that

$$\frac{d}{dt}\ln V_N = \boldsymbol{\nabla} \cdot \mathbf{f} \,, \tag{28}$$

where $\boldsymbol{\nabla}\cdot$ is the divergence operator, and $\mathbf{f}$ are the original equations of motion.

We can now summarize the continuous time version of the algorithm of Benettin and co-workers and Shimada and Nagashima. The orthonormal basis vectors $\mathbf{e}_k$ obey the differential equations

$$\begin{aligned}\frac{d}{dt}\mathbf{e}_k = \; & A\mathbf{e}_k - (\mathbf{e}_k \cdot A\mathbf{e}_k)\,\mathbf{e}_k \\ & - \sum_{j=1}^{k-1} (\mathbf{e}_k \cdot A\mathbf{e}_j + \mathbf{e}_j \cdot A\mathbf{e}_k)\,\mathbf{e}_j\end{aligned} \tag{29}$$

while the fiducial volume elements obey

$$\frac{d}{dt}\ln V_k = \sum_{j=1}^{k} \mathbf{e}_j \cdot A\mathbf{e}_j \,. \tag{30}$$

Initial conditions for the $\mathbf{e}_k$ are not important so long as they are orthonormal. The coordinate basis vectors make an obvious choice. Initial conditions for the $\ln V_k$ are trivially zero, since initially $V_k = 1$. Then the k-dimensional Lyapunov exponent is

$$\lambda^{(k)} = \lim_{t\to\infty} \frac{1}{t - t_0} \ln V_k(t) \,. \tag{31}$$

The one-dimensional Lyapunov exponents λ_k are related to the k-dimensional exponents by

$$\lambda^{(k)} = \sum_{j=1}^{k} \lambda_j \,. \tag{32}$$

So if the one-dimensional exponents are desired, Eq. (30) is replaced by

$$\frac{d}{dt}\ln S_k = \mathbf{e}_k \cdot A\mathbf{e}_k \tag{33}$$

with initial condition $\ln S_k(t_0) = 0$. Then the one-dimensional Lyapunov exponents are given by

$$\lambda_k = \lim_{t\to\infty} \frac{1}{t - t_0} \ln S_k(t) \,. \tag{34}$$

Since orthogonalization is continuous, this method should not suffer from numerical problems of the previous algorithms if the Gram-Schmidt step is delayed too long. The $\mathbf{e}_k$ should stay bounded, relieving worries about the $\mathbf{u}_k$ vectors spanning many orders of magnitude. Only the $\ln V_k$ are unbounded, and the existence of the limits (31) says that their rates of growth should be linear with time, not exponential. Compared to the original method, then, we are propagating $N^2 + N$ differential equations, instead of the N^2 differential equations of the standard algorithm.

III. A MATRIX FACTORIZATION

The general solution to the variational equations (2) is usually written as a matrix Φ, termed the fundamental matrix. It obeys

$$\dot{\Phi} = A(t)\Phi, \quad \Phi(t_0) = I \,. \tag{35}$$

Still further insight can be gained into this algorithm if we consider the factorization of the fundamental matrix Φ as

$$\Phi(t) = E(t)W(t) \,, \tag{36}$$

where the matrix $E(t)$ is orthonormal, and the matrix $W(t)$ is upper triangular. [To be a proper factorization of Φ, we must either take $E(t_0) = I$, or modify (36) to read $E(t)W(t)E^T(t_0)$. We will proceed assuming the former.] This factorization always exists if Φ is nonsingular, and a moment's thought will show that the algorithm for producing it is nothing but the Gram-Schmidt process. Let the columns of Φ [which are individually solutions

to (2)] be $\phi_i(t)$. If the columns of E are $\mathbf{e}_i$, and if the elements of W are

$$W_{ii} = \left\| \phi_i - \sum_{k=1}^{i-1} (\phi_i \cdot \mathbf{e}_k)\, \mathbf{e}_k \right\| \tag{37}$$

and

$$W_{ij} = \phi_j \cdot \mathbf{e}_i, \quad j > i, \tag{38}$$

then Eq. (36) is simply the Gram-Schmidt orthonormalization. It is sometimes called the *polar factorization* of a matrix, from its similarity to the polar decomposition of a complex number.

Taking a time derivative of (36) and substituting into the variational equations (35) gives

$$\dot{E}W + E\dot{W} = AEW. \tag{39}$$

Or, a simple rearrangement yields

$$\dot{W} = \left(E^T A E - E^T \dot{E}\right) W \equiv U(t) W, \tag{40}$$

where the matrix $U(t)$ is, as yet, unspecified. The fact that $E(t)$ is orthonormal means that its inverse is its transpose. But we can now write the above as the pair of matrix equations

$$\dot{W} = UW \tag{41}$$

and

$$E^T \dot{E} = E^T A E - U. \tag{42}$$

The above form is particularly interesting, since as an orthonormal matrix we know that $E^T\dot{E}$ must be a skew symmetric matrix. To see this, take a derivative of $E^TE = I$, and rearrange to find

$$E^T \dot{E} = -\dot{E}^T E = -\left(E^T \dot{E}\right)^T. \tag{43}$$

This shows skew symmetry, as claimed.

Now, returning to (42), we can force $E^T\dot{E}$ to be skew symmetric if we choose $U(t)$ upper triangular, with elements

$$U_{ii} = \left(E^T A E\right)_{ii}, \tag{44}$$

$$U_{ij} = \left(E^T A E\right)_{ij} + \left(E^T A E\right)_{ji}, \quad j > i. \tag{45}$$

Then the matrices W and E obey the differential equations (41) and

$$\dot{E} = AE - EU. \tag{46}$$

Since U is upper triangular, (41) will then keep $W(t)$ upper triangular. Similarly, (46) mandates that $E(t)$ remain orthonormal, since we have arranged for $E^T\dot{E}$ to be skew. (Both of these are "mathematical" statements; see the next section for a discussion of numerical behavior.)

Now, the reason for considering this factorization of Φ is that *it is just the algorithm we have been considering.* Writing E in terms of its column vectors $\mathbf{e}_i$, the matrix AE has columns $A\mathbf{e}_i$, and the matrix E^TAE has elements $\left(E^TAE\right)_{ij} = \mathbf{e}_i \cdot A\mathbf{e}_j$. Direct substitution into the differential equation for $\dot{E}$, (46), reproduces (29), column by column. The diagonal elements of W obey $\dot{W}_{ii} = \mathbf{e}_i \cdot A\mathbf{e}_i$. Of course, this is just (33) in another guise. The solution for W_{ii} is

$$W_{ii}(t) = W_{ii}(t_0) \exp\left\{ \int_{t_0}^{t} \mathbf{e}_i \cdot A\mathbf{e}_i dt \right\}. \tag{47}$$

This is the integrated form of (33), so the one-dimensional Lyapunov exponents are given by

$$\lambda_i = \lim_{t\to\infty} \frac{1}{t} \int_{t_0}^{t} \mathbf{e}_i \cdot A\mathbf{e}_i dt. \tag{48}$$

Finally, the upper elements of W can be expressed in terms of convolution integrals. They are not needed if only the Lyapunov exponents are being calculated; it is then only necessary to propagate E and integrate the diagonal elements of W.

IV. NUMERICAL STABILITY

The $\mathbf{e}_k$ equations of motion (29) themselves constitute a nonlinear system of differential equations, and it is quite proper to inquire into *their* stability. The Gram-Schmidt procedure has been incorporated into (29), but it is now in a differential form. It is easy to verify from (29) that $(d/dt)(\mathbf{e}_i \cdot \mathbf{e}_j) = 0$ if and only if the $\mathbf{e}_k$ are an orthonormal basis. But numerical errors can cause the $\mathbf{e}_k$ to wander away from a perfectly orthonormal state. If the equations (29) themselves possess positive Lyapunov exponents, the numerical errors will excite the instability. It would be both impractical and uninteresting to calculate Lyapunov exponents for our method. It is also not necessary.

To check the orthonormality of the $\mathbf{e}_k$ basis, the dot products

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}, \quad i \geq j, \tag{49}$$

where δ_{ij} is Kronecker's delta, can be monitored on a regular basis as the integration proceeds. If the deviation of $\mathbf{e}_i \cdot \mathbf{e}_j$ from δ_{ij} ever exceeds a set tolerance ϵ, the normal Gram-Schmidt procedure can be invoked, and the integration is then restarted. The Gram-Schmidt procedure, of course, leaves invariant the k-dimensional subspaces spanned by the old and new $\mathbf{e}_k$ vectors. In this renormalization the additional contributions to the V_k can be calculated in the normal manner, or if the tolerance ϵ is small enough, they may be ignored.

This is possible since at the start of any time step the volume element V_k is supposedly the unit k-dimensional hypercube. If the unit vectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_k$ spanning this cube are out of orthogonality on the order of ϵ, then V_k is in error by the same order of magnitude. If the tolerance ϵ is set one or two orders of magnitude larger than the expected integration error, then the corrections to the value of V_k are of the same order of magnitude as errors introduced by the integration itself. The $\ln V_k$ grow roughly linearly with time, and in a long integration are no longer of order unity. Errors of order ϵ become less

and less important as the integration proceeds. Finally, the accuracy of the final Lyapunov exponents is typically *many* orders of magnitude worse than the integration accuracy, so some inaccuracy in the calculation of the $\ln V_k$ is tolerable.

So, this method has not eliminated the (possible) necessity for Gram-Schmidt reorthogonalizations. However, they are used only as necessary to suppress numerical instabilities in the $\mathbf{e}_k$ equations of motion. They are not used to calculate the Lyapunov exponents.

V. AN EXAMPLE

As an example, we consider the Lorenz problem [6] with nonlinear differential equations

$$\begin{aligned} \dot{x} &= \sigma(y-x)\,, \\ \dot{y} &= (\gamma - z)x - y\,, \\ \dot{z} &= xy - bz\,. \end{aligned} \tag{50}$$

Following Shimada and Nagashima, we take $\sigma = 16$, $\gamma = 40$, and $b = 4$. This problem has several benefits for testing a new algorithm. The divergence of the above system is

$$\nabla \cdot \mathbf{f} = -(\sigma + b + 1) \tag{51}$$

which is constant throughout the space. So with our parameters we already know $\lambda^{(3)} = -21$ from (28). Second, as an autonomous system, a displacement $\mathbf{u}^T = (\dot{x}(t), \dot{y}(t), \dot{z}(t))\delta\tau$ along the state velocity vector (for fixed $\delta\tau$) is an exact solution to (2). To see this, calculate

$$\frac{d\mathbf{f}}{dt} = \frac{\partial \mathbf{f}}{\partial \mathbf{x}}\dot{\mathbf{x}} = A\mathbf{f} \tag{52}$$

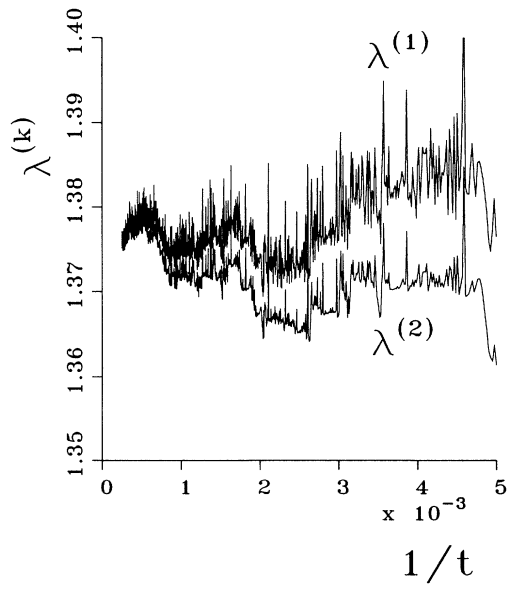

FIG. 1. Convergence of the one- and two-dimensional Lyapunov exponents to a limit, vs inverse time. Oscillations are driven by the chaotic nature of the underlying attractor.

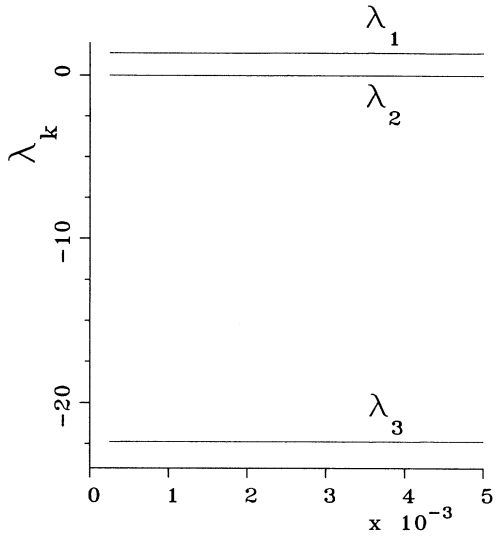

FIG. 2. Convergence of the one-dimensional Lyapunov exponents for the Lorenz problem. The much larger vertical scale hides the oscillations.

for any autonomous system. So in any region in which $\dot{x}$, $\dot{y}$, and $\dot{z}$ are bounded, we will have one of the *one-dimensional* Lyapunov exponents λ_1, λ_2, or λ_3 equal to zero. The strange attractor we will be sampling exists within a bounded region of space, and that bounds the state derivatives.

Figure 1 shows the convergence of $\lambda^{(1)}$ and $\lambda^{(2)}$ for the Lorenz system. The integration was performed to $t = 4000$, and renormalization was found to be necessary after time intervals of $\Delta t \approx 1$, with a normalization tolerance $\epsilon = 10^{-7}$. In our method, the $\ln V_k$ are defined as

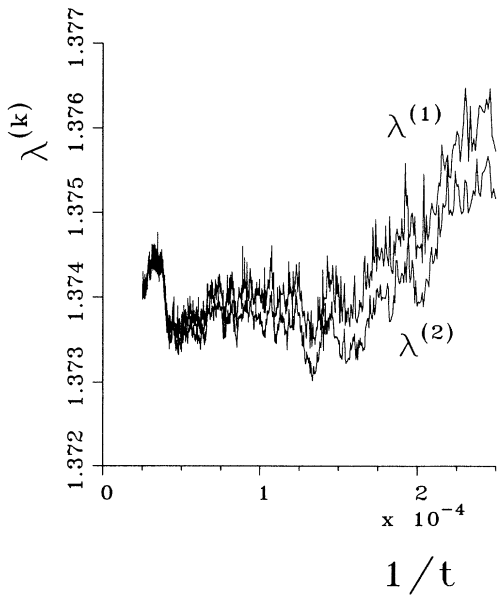

FIG. 3. Convergence of the one- and two-dimensional Lyapunov exponents for a longer integration. This plot shows a great similarity to Fig. 1.

continuous functions of time. As can be seen from Fig. 1, the general trend has superimposed upon it a considerable amount of "noise." [On the other hand, Fig. 1 plots only $\lambda^{(1)}$ and $\lambda^{(2)}$, because the convergence of $\lambda^{(3)}$ with our method, via Eq. (28), is exact after the first time step, and never changes. This will not be true in systems without constant divergence of $\mathbf{f}$.] In reality these are oscillations about the sought-after mean value, and follow the details of the actual trajectory through space (which is usually chaotic). Their amplitude drops off roughly like $1/t$, which necessitates long integrations. Both $\lambda^{(1)}$ and $\lambda^{(2)}$ are clearly converging to a value near 1.37, which is the value cited by Shimada and Nagashima. The fact that $\lambda^{(1)}$ and $\lambda^{(2)}$ are approaching the same limit implies that $\lambda_2 = 0$, as expected.

Figure 2 similarly shows the convergence of the one-dimensional Lyapunov exponents, using the method in the current paper. Again, convergence to previously cited values is apparent. As a final result, we present Fig. 3, which continues the integration from $t = 4000$ to $t = 40\,000$. The portion of the integration shown begins where Fig. 1 ended. One cannot help being struck by the self-similarity of the two plots, especially since the vertical axis scale has been expanded by the same factor of 10 used to expand the integration time scale. This emphasizes the slow numerical convergence of this (and all) Lyapunov exponent methods.

VI. CONCLUSIONS

We have shown that the "standard" algorithm for calculating Lyapunov exponents possesses a true differential form. Potential numerical instabilities in the propagation of the orthonormal basis vectors can be circumvented by employing the Gram-Schmidt method when (and if) needed.

We have also shown that the "standard" algorithm is based on a factorization of the fundamental matrix. In this it is similar to the solutions to the constant coefficient and periodic coefficient cases, which are also based on factorizations of the fundamental matrix. The polar factorization of the standard algorithm is purely real, in opposition to the other two well-known cases. Wiesel [7] has considered factoring Φ into its eigenvectors and eigenvalues, introducing another possible definition for Lyapunov exponents which includes an imaginary part. Exploration of further possible factorizations of Φ is a current research topic.

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