How Long Do Numerical Chaotic Solutions Remain Valid?

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Dynamical conditions for the loss of validity of numerical chaotic solutions of physical systems are already understood. However, the fundamental questions of "how good" and "for how long" the solutions are valid remained unanswered. This work answers these questions by establishing scaling laws for the shadowing distance and for the shadowing time in terms of physically meaningful quantities that are easily computable in practice. The scaling theory is verified against a physical model. [S0031-9007(97)03523-0]

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In studying their systems, physical scientists write differential equations derived from fundamental laws. These equations are then used to understand, analyze, predict, and control the system's behavior, provided one is able to determine the solutions. As the role of nonlinearity grows in importance for the study of physics, solutions often cannot be obtained in closed form, and numerical solutions must be relied on. Computers are now an integral part of the physicist's *modus operandi*.

A basic question always present when obtaining numerical solutions is to what extent they are valid. This question is especially meaningful when dealing with chaotic dynamics, since local sensitivity to small errors is the hallmark of a chaotic system. Floating-point calculations commonly used to approximate solutions of differential equations or compute discrete maps produce *pseudotrajectories*, which differ from true trajectories by new, small errors at each computational step. Despite the sensitive dependence on initial conditions, the methods of shadowing have shown that for chaotic systems that are hyperbolic [1] or nearly hyperbolic [2], locally sensitive trajectories are often *globally insensitive*, in that there exist true trajectories with adjusted initial conditions, called shadowing trajectories, very close to long computer-generated pseudotrajectories. A dynamical system is hyperbolic if phase space can be spanned locally by a fixed number of independent stable and unstable directions which are consistent under the operation of the dynamics.

In the absence of hyperbolic structure, much less is known about the validity of long computer simulations. Recently it was shown that trajectories of a chaotic system with a fluctuating number of positive finite-time Lyapunov exponents fail to have long shadowing trajectories [3]. In other words, they are globally sensitive to small errors. The hyperchaotic system of [3] has two positive Lyapunov exponents, although finite-time approximations of the smaller of the two fluctuate about zero, due to visits of the trajectory to regions of the attractor with a varying number of stable and unstable directions. The destruction of hyperbolicity caused by this phenomenon leads to global sensitivity—only relatively short pseudotrajectories will be approximately matched by true system trajectories.

Our discussion of the global sensitivity of trajectories for these nonhyperbolic systems is limited in this Letter to the comparison between physical models and computer simulations, but the same questions arise whenever comparing the time behavior of two systems evolving under similar, but slightly different dynamical rules. For example, a natural system and its theoretical *model* differ by modeling errors. In the presence of fluctuating Lyapunov exponents, global sensitivity may lead to trajectory mismatch, in particular when long times are considered. The result is that no trajectory of the theoretical model matches, even approximately, the true system outcome over long time spans.

Although the dynamical reasons and conditions for the loss of validity of chaotic solutions have been identified [1–5], the central and most practical question of all for physical scientists remained to be answered: If the numerical solutions are valid, "how good" are they and "for how long" are they valid? In this work, we answer these questions by establishing fundamental scaling laws in terms of physically meaningful quantities that are easily obtained in practice when doing computer simulations of physical systems. We answer the "how good" question by obtaining a quantitative rule governing the *shadowing distance*, the pointwise distance from the shadowing trajectory to the pseudotrajectory, and we answer the "for how long" question by obtaining a quantitative rule governing the *shadowing time*, the length of true shadowing trajectories. We find that the expected shadowing distance and time have power law dependencies on the size of the one-step error made in the computer simulation. The exponents of the power laws depend on the mean and variance of the Lyapunov exponent nearest to zero, quantities that are easily computable in practice. The greater the finite-time fluctuation about zero, the smaller the power law exponent, resulting in large shadowing distances and valid trajectories of limited length.

We begin with a statistical description of the pointwise shadowing distance. For our purposes, a pseudotrajectory is a discrete list of numbers generated according to a computer-implemented evolution rule, such as a Runge-Kutta approximation to the solution of a differential equation. Typically, at each of a number of discrete steps, there is a small discrepancy between the rule and the governing equation, due to the truncation error of the rule or the rounding properties of the computer. Shadowing theory shows that, under certain conditions, there is another true trajectory, with a slightly adjusted initial condition, that follows very closely to (shadows) the pseudotrajectory. The *pointwise shadowing distances* are the stepwise distances between it and the true shadowing trajectory. The maximum such distance may be considered the "global error" of the original calculation.

Typical distributions of pointwise shadowing distances are shown in Fig. 1. The two plots show histograms of shadowing distances for simulations of two different dynamical systems. The exponential shape of the histogram of log distances suggests that the distances themselves obey a power law fit. These physical systems are taken from the family of kicked double rotors, which are hyperchaotic systems with two positive Lyapunov exponents for certain parameter settings. The mechanical system is composed of two coupled rods rotating in a horizontal plane (see [3] for more details). One rod receives a periodic delta function kick of constant magnitude ρ. The system is integrable between kicks, so an explicit equation, or discrete map, can be derived which governs the state (consisting of two angles and velocities) at the kick time. The leftmost histogram in Fig. 1(a) corresponds to a pseudotrajectory created by integrating the double rotor map with kick strength $\rho = 8.2$, and artificially adding errors of size $\delta = 10^{-16}$ at each step (at each kick). The true trajectory that shadows was computed in higher precision using the refinement technique [5], and log distances between each point of the two form the exponential distribution shown. In Fig. 1(b), the kick strength ρ has been increased to 8.7, and the exponent of the exponential distribution is much larger.

In Fig. 1, the distribution of shadowing distances over several orders of magnitude occurs because the trajectory experiences nonhyperbolicity due to the varying number of stable and unstable dimensions. Since this nonhyperbolic behavior is reflected by a Lyapunov exponent fluctuating about zero, we use a diffusion approximation to explain the quantitative aspects of the distributions in Fig. 1 in terms of the finite-time Lyapunov exponents of the system. Our answer to the "how good" question is that the shadowing distances y follow a power law distribution cy^{-2m/σ^2}, where $m > 0$ and σ are the mean and standard deviation of the finite-time Lyapunov exponent closest to zero. We hypothesize the exponential distribution of log shadowing distances of Fig. 1 to follow from a biased random walk with drift toward a reflecting barrier. When the pseudotrajectory lies in hyperbolic regions of the attractor, shadowing theory guarantees the existence of a nearby true trajectory. The true trajectory is found by adjusting the points in a consistent manner along the stable and unstable directions. When a nonhyperbolic region is entered, this consistency of adjustments is interrupted by a normally expanding direction becoming momentarily contracting (or vice versa), causing an excursion away from the reflecting barrier at $\log \delta$, as shown in Fig. 1. The one-step error δ serves as a reflecting barrier since new errors are created on each step, so that the correct trajectory can never be expected to lie closer than δ to the pseudotrajectory.

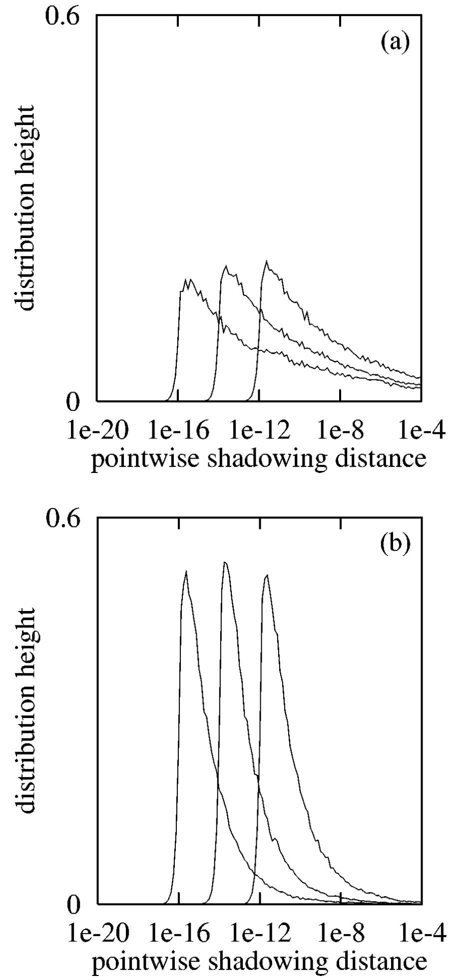

FIG. 1. (a) Distribution of pointwise shadowing distance for a trajectory of the kicked double rotor with $\rho = 8.2$. The three histograms, from left to right, correspond to one-step errors of 10^{-16}, 10^{-14}, and 10^{-12}, respectively. (b) Same as (a), but for $\rho = 8.7$.

The time-t Lyapunov exponents of an m-dimensional system trajectory are the m averages λ_i of the logarithm of local expansion rates along the trajectory of length t, so that an infinitesimal sphere of radius dr at the beginning of the trajectory would evolve to an ellipsoid with axes $\lambda_i^t dr$ after t time units. Distributions of the four time-100 Lyapunov exponents for the kicked double rotor, gathered over a long trajectory, are graphed in Fig. 2. Our diffusion model uses the finite-time Lyapunov exponent closest to zero as the per-step innovation. For the kicked double rotor, we consider only the second largest Lyapunov exponent, since this one reflects the varying number of unstable dimensions along the trajectory.

To obtain the exponential distribution of log shadowing distances shown in Fig. 1 in terms of the finite-time Lyapunov exponent closest to zero, we consider the transition probability P for a continuous diffusion process to be given by Kolmogorov's equation $\frac{\partial P}{\partial t} = \frac{\sigma^2}{2}\frac{\partial^2 P}{\partial x^2} + m\frac{\partial P}{\partial x}$, where the innovations have mean $-m$ and variance σ^2 [6]. The time-invariant equilibrium distribution is found by setting $\partial P/\partial t = 0$; together with the assumptions $0 = P(\infty) = dP/dx(\infty)$ due to the drift $-m < 0$, it follows that the equilibrium is given by an exponential distribution

$$P(x) = \frac{2m}{\sigma^2}\, e^{-2mx/\sigma^2}. \qquad (1)$$

This is consistent with the empirical distributions of Fig. 1, where the distribution of log distances $x = \log_{10}(y)$ have a roughly exponential shape.

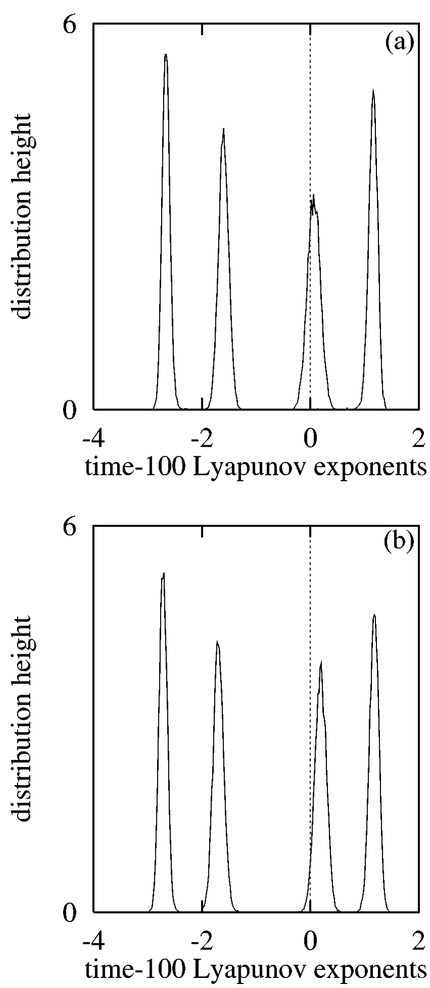

FIG. 2. Distribution of time-100 Lyapunov exponents for the double rotor. (a) $\rho = 8.2$, and (b) $\rho = 8.7$.

A quantitative test of the fitness of the diffusion approximation for shadowing distances is shown in Fig. 3. The close agreement between the exponent measured from the shadowing distance distributions and $2m/\sigma^2$ calculated from finite-time Lyapunov exponents [7] supports the diffusion model explanation of shadowing distance.

The fact that shadowing distances obey a power law distribution with exponent $-2m/\sigma^2$ as a function of one-step error magnitude allows us to infer shadowing time. Shadowing trajectories exist as long as the shadowing distance is small, compared to the size of the attractor. Breakdowns in shadowing (called "glitches" in [3,5]) occur when the reverse happens, namely an excursion far from zero under the diffusion approximation. Therefore, times between glitches are analogous to first passage times of the shadowing distance to approach the order of the attractor length in phase space. The first passage time can be computed from the parameters of the diffusion process. A standard Laplace transform calculation yields the expected time

$$\langle\tau\rangle = \frac{\sigma^2}{2m^2}\left(\delta^{\frac{-2m}{\sigma^2}} - 1\right) - \frac{\ln\delta}{m} \qquad (2)$$

for the shadowing distance to reach 1. Our answer to the "for how long" question is that for small δ, the expected shadowing time τ is governed by the power law

$$\langle\tau\rangle \sim \delta^{\frac{-2m}{\sigma^2}}.$$

To compare actual shadowing times of the kicked double rotor with the power law (3), we have made lengthy calculations summarized in Fig. 4. Shadowing trajectories were calculated for between 500 and 10 000 pseudotrajectories, whose mean shadowing time is plotted as a function of one-step error magnitude. For each fixed kick-strength parameter ρ, log shadowing time shows straight-line behavior as a function of $\log\delta$, supporting the power-law conjecture (3).

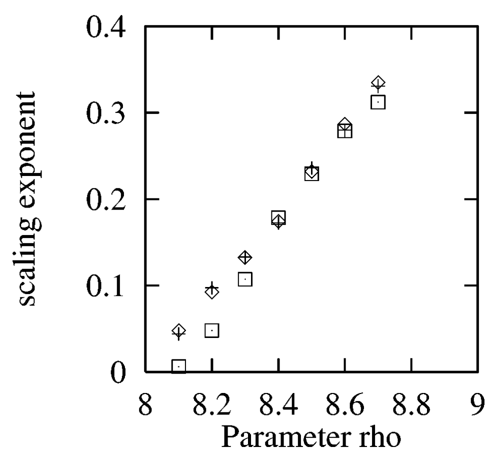

FIG. 3. Comparison of three exponents. Crosses represent the exponent from the power law fit of pointwise shadowing distances from Fig. 1. Diamonds represent $2m/\sigma^2$, calculated from finite-time Lyapunov exponents shown in Fig. 2. Boxes represent the exponent from the power law fit of shadowing times, which are the slopes of the line segments in Fig. 4.

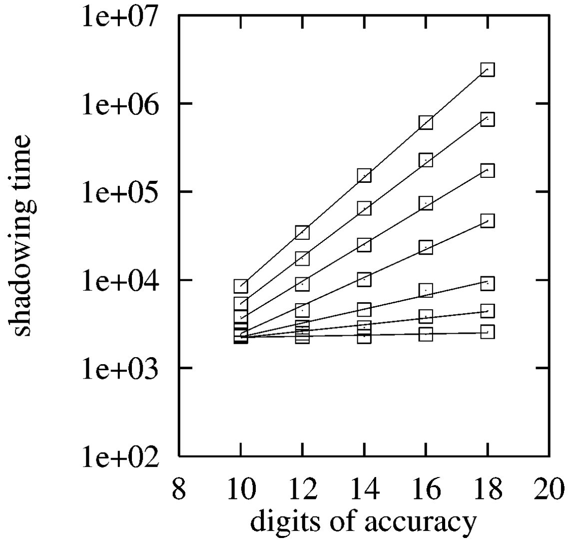

FIG. 4. Squares represent mean number of steps for which a pseudotrajectory of the kicked double rotor with specified one-step accuracy can be shadowed by true trajectory. Straight line on this log-log plot supports a power-law model for shadowing time. The lines drawn are least squares fits, whose slopes are plotted as squares in Fig. 3. The top line corresponds to $\rho = 8.7$. Other lines connect data points corresponding to smaller ρ with a decrement of 0.1; lowest line corresponds to $\rho = 8.1$.

The slopes of the least squares fits from shadowing times in Fig. 4 are plotted as small boxes in Fig. 3 for each of the parameters ρ. According to our heuristic argument above, the slopes should be the power law exponents of (3), and in particular should match $2m/\sigma^2$ measured from the finite-time Lyapunov exponent distributions. Indeed it does for the middle of the parameter range. For $\rho = 8.7$ the fit is not as good; a possible explanation is that using the Lyapunov statistics from only one Lyapunov exponent loses validity when the mean m moves away from zero, as it does for larger ρ. For $8.1 \leq \rho \leq 8.3$ the exponent from $2m/\sigma^2$ is an overestimate because the terms neglected in moving from (2) to (3) have more effect when m approaches 0. Our derivations for shadowing distance and shadowing time are first-order approximations that depend on the existence of one finite-time Lyapunov exponent that is significantly closer to zero than the others.

The fundamental conclusion to be drawn from Fig. 4 is that to obtain a long trajectory which is even approximately correct is for some systems virtually impossible. Dynamical systems like the kicked double rotor that have a finite-time Lyapunov exponent lying close to zero, relative to the variance of its distribution, possess obstructions to the existence (not to mention explicit computation) of true shadowing trajectories close to long pseudotrajectories. Figure 4 shows that the limit for double-precision (10^{-15}) shadowable pseudotrajectories is a few thousand; nor does the situation improve very much for higher precision. The slope of the lowest line, corresponding to $\rho = 8.1$, is almost flat (slope ≈ 0.006), which is to be expected from the power law (3) when $m/\sigma^2 \approx 0$. When the scaling exponent m/σ^2 is close to zero, and increasing the one-step accuracy of the computation results in virtually no improvement in the lengths of shadowable trajectories, it is far from obvious how a long computer simulation should be interpreted.

The fact that for some systems, long computer-generated pseudotrajectories are not matched by true trajectories was first pointed out in [3]. In the present Letter we have shown explicitly how this phenomenon is caused by a Lyapunov exponent fluctuating about zero, and described quantitatively how shadowing breaks down, depending on the proximity of the exponent to zero. Although we have demonstrated fluctuating Lyapunov exponents only for a mechanical system (kicked double rotor), we expect it, and the accompanying global sensitivity of trajectories, to be a common feature of higher-dimensional chaotic dynamical systems.

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[7] The mean m is computed as the mean of the second-largest time-100 Lyapunov exponent, which is an approximation to the (infinite-time) Lyapunov exponent. The standard deviation σ was computed as ten times the standard deviation of the distribution of the second-largest time-100 Lyapunov exponent. Since the diffusion approximation assumes independent and identically distributed innovations, it is important to calculate σ as the time-T Lyapunov exponent multiplied by $\sqrt{T}$ for T beyond the system decorrelation time.