Traces and determinants of strongly stochastic operators

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Periodic orbit theory allows calculations of long-time properties of chaotic systems from traces, dynamical zeta functions, and spectral determinants of deterministic evolution operators, which are in turn evaluated in terms of periodic orbits. For the case of stochastic dynamics a direct numerical evaluation of the trace of an evolution operator is possible as a multidimensional integral. Techniques for evaluating such path integrals are discussed. Using as an example the logistic map $f(x)=\lambda x(1-x)$ with moderate to strong additive Gaussian noise, rapid convergence is demonstrated for all values of λ with strong noise as well as at fixed $\lambda=5$ for all noise levels. [S1063-651X(99)10604-4]

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I. INTRODUCTION

Periodic orbit theory is a remarkable tool in classical [1–3] and quantum [4,5] chaotic systems, permitting the evaluation of long-time properties, such as escape rates, dynamical averages, and energy levels in terms of short unstable recurrent motions, that is, periodic orbits or "cycles." In classical hyperbolic systems with known topology, such as the repeller of the map $5x(1-x)$ discussed below, convergence can be impressive: the escape rate is computed to nine digits from the eight cycles of period 4 or less. The lowest energy levels of helium [6] are computed to an accuracy far better than would be expected from a semiclassical approximation. Even when there is intermittency, hence hyperbolicity is lost, it is possible to get sensible results using special techniques in both the classical [7,8] and quantum [9] cases.

Recently the theory has been extended to classical systems with weak additive noise, using Feynmann diagrams [10] or smooth conjugacy techniques [11]. There are a number of motivations for such extensions: noise at some level is present in all physical systems; it regularizes the theory, replacing Dirac δ functions by smooth kernels (see below) and fractal distributions by smooth functions. There is also some hope that the noise may effectively truncate the theory, rendering irrelevant contributions from periodic orbits longer than the finite memory of the system.

The result of these investigations is a weak noise perturbation theory, representing the trace of the evolution operator and derived quantities as a power series expansion in σ, the noise level. The coefficients are combinations of higher derivatives of the map evaluated at the periodic orbits of the deterministic unperturbed system. Numerically, the coefficients themselves converge at a similar rate to the classical periodic orbit theory, but the power series in σ is useful only for weak noise, say, $\sigma<0.03$, suggesting the following question, the subject of this paper:

To what extent does periodic orbit theory survive strong noise, and how fast does it converge?

Strong noise differs qualitatively from weak noise in a number of respects: The stochastic dynamics is equally close to many slightly different deterministic dynamical systems; so, the concept of a unique perturbation theory becomes less defined, in addition to the lack of convergence of such a theory. Also, Gaussian noise has no preferred status; for weakly stochastic systems, all types of noise distributions with a given variance σ^2 are identical to order σ^2.

The approach taken here is that the relevant quantity, the trace of an evolution operator, is evaluated numerically, using very little detailed information about the dynamics, in particular without reference to periodic orbits. The method is general enough to include any type of dynamics (hyperbolic, intermittent, attracting) and uncorrelated noise, subject to smoothness of both dynamics and the noise distribution, with the latter decaying exponentially at large distances. Here, as in Refs. [10,11] the noise is additive, but this is not a necessary condition.

From the trace, it is straightforward to construct the spectral determinant, and hence highly convergent expansions for escape rates and dynamical averages, in the spirit of cumulant expansions, as in standard periodic orbit theory. This has some similarities to Ref. [12], where various approximations to the quantum trace are compared.

Section II outlines the formalism required for the calculation; in particular, casting the trace as a multidimensional integral. Section III discusses numerical approaches for evaluating this integral. The results are given in Sec. IV and discussed in Sec. V.

II. FORMALISM

The goal is to determine the long-time properties of stochastic dynamical systems, here one-dimensional maps with additive noise:

$$x_{n+1}=f(x_n)+\sigma\xi_n, \tag{1}$$

where $f(x)$ is a known function, for example the logistic map,

$$f(x)=\lambda x(1-x). \tag{2}$$

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σ is a measure of the strength of the noise and ξ_n are independent identically distributed random variables with unit variance,

$$\langle \xi_m \xi_n \rangle = \delta_{mn}, \tag{3}$$

such as a normalized Gaussian distribution. The methods used here are equally applicable to σ and ξ that depend on x, and non-Gaussian noise distributions.

Instead of the Langevin form (1), it is more convenient to consider the discrete Fokker-Planck equation for a probability distribution $\rho(x)$ transported by the dynamics and diffusing due to the noise:

$$\rho_{n+1}(x) \equiv \mathcal{L}[\rho_n](x) = \int \delta_\sigma(x - f(x'))\rho_n(x')dx', \tag{4}$$

where $\delta_\sigma(y)$ is the noise kernel, for example,

$$\delta_\sigma(y) = \frac{e^{-y^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}}, \tag{5}$$

reducing to a Dirac δ in the deterministic $\sigma=0$ limit.

Long-time properties of the dynamics are obtained from the leading eigenvalue(s) of the linear evolution operator $\mathcal{L}$, which are (the inverses of) solutions of the characteristic equation

$$\det(1 - z\mathcal{L}) = 0. \tag{6}$$

For example, the probability of a point initially in an open system remaining there after n iterations is typically proportional to $e^{-\gamma n}$ where the escape rate γ is related to the leading zero z_0 by

$$\gamma = -\ln z_0. \tag{7}$$

Dynamical averages and diffusion coefficients can be obtained from the leading zero of appropriately weighted evolution operators [1–3].

The spectral determinant (6) of an infinite dimensional operator may be defined by its cumulant expansion in powers of z, using the matrix relation $\ln\det = \mathrm{tr}\ln$ and Taylor expanding the logarithm:

$$\begin{aligned}\det(1 - z\mathcal{L}) &= \exp\left(-\sum_{n=1}^{\infty}\frac{z^n}{n}\mathrm{tr}\,\mathcal{L}^n\right)\\ &= 1 - z\ \mathrm{tr}\,\mathcal{L} + \frac{z^2}{2}[(\mathrm{tr}\,\mathcal{L})^2 - \mathrm{tr}\,\mathcal{L}^2] - \dots\\ &\equiv \sum_{n=0}^{\infty} Q_n z^n. \end{aligned}\tag{8}$$

Q_n may be obtained from all the traces $\mathcal{L}^m$ with $m \leqslant n$, and an approximation for z_0 is obtained by numerical root finding on the nth degree polynomial given by the truncation of the determinant. The above expression for Q_n quickly gets complicated; it is easier to expand the derivative

$$-z\frac{d}{dz}\det(1 - z\mathcal{L}) = \det(1 - z\mathcal{L})\sum_{n=1}^{\infty} z^n\,\mathrm{tr}\,\mathcal{L}^n, \tag{9}$$

which leads to the recursive equation

$$Q_n = \frac{1}{n}\left(\mathrm{tr}\,\mathcal{L}^n - \sum_{m=1}^{n-1} Q_m\,\mathrm{tr}\,\mathcal{L}^{n-m}\right). \tag{10}$$

The utility of the cumulant expansion as a method to calculate the leading eigenvalue(s) depends on a rapid decrease of the Q_n with n, corresponding to widely spaced eigenvalues. For example, an isolated fixed point of stability Λ without noise has eigenvalues $z_m = |\Lambda|\Lambda^m$, $m = 0,1,2,\dots$ and cumulants $Q_n \sim \Lambda^{-n(n+1)/2}$. This superexponential convergence is characteristic of hyperbolic systems, and also, judging by the results below, stochastic systems. For other classes of operators more general methods may be required.

The trace in Eq. (10) is straightforward to write down as an n-dimensional integral, a discrete periodic chain reminiscent of a path integral, obtained in Ref. [13],

$$\mathrm{tr}\,\mathcal{L}^n = \int \prod_{j=0}^{n-1} dx_j \prod_{j=0}^{n-1} \delta_\sigma(x_{j+1} - f(x_j)), \tag{11}$$

where the index j is cyclic, so $x_n = x_0$. In the noiseless ($\sigma = 0$) limit, the integrand is a product of Dirac δ functions, and the trace is given by a sum over the fixed points of f^n, that is, the n cycles of f. In Refs. [10,11] the weak noise limit is obtained by a saddlepoint expansion of the integral around these cycles. Here, the integral is performed numerically, up to $n=5$, as described in the following section.

III. NUMERICAL METHODS

The required quantities, $\mathrm{tr}\,\mathcal{L}^n$, are n-dimensional integrals, which in the case of weak noise ($\sigma \ll 1$) have a large number of sharp peaks surrounding the periodic points of the deterministic map. Obtaining an accurate numerical estimate of the integral for any $n>2$ seems prohibitively difficult, since Monte Carlo approaches take too long to converge, and direct integration schemes require a small step size, but cover a large configuration space. See Ref. [14] for more discussion.

In the case of Gaussian (or similar) noise and smooth dynamics $f(x)$ the integrand is smooth and decays exponentially fast at the boundaries. This in turn implies that the simplest possible integration algorithm, summing the integrand at a cubic array of coordinate values, converges faster than any power of the step size, and is typically exponential once the step size is smaller than σ.

This remarkable convergence rate for smooth, exponentially decaying integrands follows from the observation that by multiplying the terms near the boundary by appropriate factors, it is possible to obtain algorithms of higher and higher order in the step size [14]. Exponentially decaying integrands are impervious to any such coefficients, and so converge faster than any power of the step size.

Note also, that having chosen, say, x_0 and x_1, and the argument of the exponential, $-(x_1 - f(x_0))^2/(2\sigma^2)$ happens to be too small, it is not necessary to consider the other x_j. This provides a very substantial savings in time for $n>2$.

Finally, the integral is symmetric under a cyclic interchange of the x_j: this implies an additional saving of a factor n. The logic required here is not trivial since the contribution differs depending on whether some of the x_j are identical. For example, for $n=4$, choose two values x_{min} and x_{max} beyond which there is no possible contribution. Then sum $x_{min} \leqslant x_0 \leqslant x_{max}$, defining x_0 to be the largest of the x_j, and the one occurring first, if more than one are maximum. Sum $x_{min} \leqslant x_1 \leqslant x_0$, checking that the argument of the exponential is not too small. Sum $x_{min} \leqslant x_2 \leqslant x_0$, again checking the argument of the exponential. Then sum $x_{min} \leqslant x_3 < x_0$, and multiply each contribution by 4. If $x_2 = x_0$, the x_j could form a 2 cycle repeated twice, so when $x_3 = x_1$ count the term twice instead of four times, and stop the sum over x_3 to avoid double counting. Finally, the repeated fixed point $x_0 = x_1 = x_2 = x_3$ has been excluded, so sum this explicitly and count it once. The case $n=5$ is simpler as there is only a repeated fixed point, but there are more possibilities for which of the x_j are maximum.

Even with the above short cuts, large n, small σ, and stringent precision requirements can lead to sums of 10^9 terms. This means it is advisable to group them in size (using the argument of the exponential) as they are summed; then, combine the groups from smallest to largest to minimize roundoff error.

Given the above algorithm the step size h is decreased until two successive estimates agree to within a specified precision (for example, ten digits). Since the amount of time increases as h^{-n}, the optimal sequence is probably $h_j = h_0 e^{-j/n}$. Note that large initial values of h can lead to a zero result as the entire contribution region may be missed.

With the above algorithm, calculation of the trace up to $n=5$ with $\sigma \geqslant 0.01$, and $n=6$ for somewhat higher values of σ, is feasible for the case of Gaussian noise and smooth one-dimensional dynamics.

IV. RESULTS

The logistic map $f(x) = \lambda x(1-x)$ for various values of λ exhibits most of the behaviors observed in one-dimensional maps. For all $\lambda \geqslant 1$ any initial x outside the range $[0,1]$ ends up at $-\infty$, while the behavior of points within this range depend on λ as follows: For $0 \leqslant \lambda \leqslant 1$, the point $x=0$ is a stable fixed point, marginally so at $\lambda=1$, and then unstable for $\lambda > 1$. For $1 \leqslant \lambda \leqslant 3$, the fixed point $x = 1 - 1/\lambda$ is stable, and then bifurcates to a stable cycle of period 2. This cycle in turn becomes unstable, bifurcating to a 4 cycle, then an 8 cycle, and so on, to $\lambda \approx 3.57$ at which point a chaotic attractor forms. The period doubling cascade in the presence of weak noise may be described by the renormalization approach of Ref. [13]. At larger values of λ more stable cycles are created, including a 3 cycle, which is stable at $\lambda = 3.84$, leading to a pattern of alternating stable ‘‘windows’’ surrounded by nonattracting unstable cycles and chaotic attractors containing many unstable cycles. At $\lambda=4$ the attractor fills the interval $[0,1]$, and in this case, the Ulam map, the dynamics is exactly solvable. For $\lambda > 4$ almost all initial conditions leave the interval, but infinitely many unstable cycles remain, the closure of which forms a fractal repeller with a well-defined escape rate.

Imposing additive noise to the logistic map leads to escape for all $\lambda > 0$, although this may be very unlikely if σ is small. At $\lambda = 2$, for example, every point (except the endpoints) is attracted to the stable fixed point at $x = 1/2$, and the noise must move the trajectory out of the interval to escape. In cases like this, the stochastic behavior is analogous to quantum tunneling, and is exponentially suppressed for small σ. At bifurcation points, including $\lambda = 1$, the stability of the relevant cycles is marginal, leading to intermittency. Marginal cycles are difficult to treat using cycle expansions, and it is one of the goals of this paper to understand how this poor convergence is modified by the presence of noise.

TABLE I. Convergence of the spectral determinant, as measured by $-\log_{10}|Q_5|$, where Q_5 is the coefficient of z^5 in the cumulant expansion (8) for various types of dynamics of the logistic map (2). Larger numbers imply faster convergence, giving roughly the number of converged digits in the escape rate calculated to $n=4$.

				σ		
λ	Type	0.01	0.03	0.1	0.3	1
0	Pure noise	12.7	12.7	12.4	12.7	12.6
1	Intermittent	−2.3	−0.8	1.2	3.8	8.5
2	Stable 1 cycle	2.5	2.2	2.1	5.9	11.8
3	Bifurcation	−0.3	0.7	2.8	7.4	13.2
3.5	Stable 4 cycle	0.3	1.4	3.4	7.8	13.2
3.57	∞ cycle	0.4	1.1	3.6	7.8	13.3
3.72	Chaos	1.5	1.4	4.1	8.0	13.4
3.84	Stable 3 cycle	1.6	2.4	4.6	8.1	13.4
4	Ulam map	2.2	2.9	4.9	8.2	13.8
5	Repeller	9.2	9.1	8.4	9.1	13.3

The results of numerical evaluation of $\mathrm{tr}\,\mathcal{L}^n$ up to $n=5$ are shown in Table I. The spectral determinant is evaluated using Eq. (10), and Q_5, the coefficient of z^5 is noted. Since for the parameters shown, the first zero of the determinant is close to 1, $-\log_{10}|Q_5|$ gives roughly the number of significant digits of z, and hence the escape rate is evaluated to $n=4$. It also gives the approximate range of z over which the $n=4$ approximation is valid.

It is seen that, for the trivial case $\lambda=0$, corresponding to pure noise, and for strong noise $\sigma=1$, the calculation is limited by the double precision arithmetic: evaluation of the trace beyond $n=4$ is superfluous at this level of precision. Almost as precise is the case $\lambda=5$, which has a repeller with complete binary symbolic dynamics in the absence of noise, and hence is an ideal candidate for cycle expansion methods. Nine significant digits are obtained at $n=4$, corresponding to just 8 cycles. The presence of noise makes methods based on enumerating these cycles more difficult [10,11], but convergence is rapid at any noise level.

The other cases, where escape is induced by the presence of noise, do rather poorly for small noise. The significance of $\lambda = 1$, 2, 3, 3.57, 3.84, and 4 are discussed above; the other values in Table I are $\lambda = 3.5$, which contains a stable 4 cycle, and $\lambda = 3.72$ that is not near any large stable window, and numerically exhibits a chaotic attractor, although mathematical proof is difficult. The nature of the underlying attractor seems to have little effect on the rate of convergence, except that the intermittent case ($\lambda=3$ and particularly $\lambda=1$) is divergent at $\sigma=0.01$ to this level of approximation; the escape rate probably converges at impossibly large n, either for the current numerical approach, or for standard cycle expansion techniques. In the other cases, particularly towards larger λ, the expansion appears to be converging, albeit slowly.

V. DISCUSSION

To summarize: It is feasible to evaluate a stochastic trace directly in terms of multidimensional integrals, because the numerical evaluation of such integrals converges exponentially with the number of steps. Cumulant expansions can be applied to classical dynamics with strong external noise, although there is as yet no periodic orbit theory in this regime with which to evaluate the trace. The convergence of the cumulant expansions is improved by the noise, whether the underlying dynamics is hyperbolic, intermittent, or stable. In the case of strong noise ($\sigma > 0.3$ in the present context) or hyperbolic underlying dynamics, the cumulant expansion to fourth order is sufficient to compute the leading eigenvalue to respectable accuracy (roughly eight digits here).

What are the optimal methods for determining the long-time properties of stochastic systems? The strong noise case is best treated by numerical evaluation of the trace, described here, requiring little knowledge of the underlying dynamics. The elements of periodic orbit theory, traces, and determinants indeed survive strong noise and converge rapidly, without reference to periodic orbits. This means that a (hypothetical) periodic orbit approach to strong noise based on cumulant expansions could be expected to converge, but it would be nonunique and nonperturbative, following the discussion in the Introduction. Such nonuniqueness is probably an advantage, permitting a choice of deterministic dynamics with simplified topology.

The weak noise case depends on this underlying dynamics: for the hyperbolic case ($\lambda > 4$), the cycle perturbation theory of [10,11] or numerical evaluation; for noise-induced escape from a strongly chaotic attractor ($\lambda \approx 4$), the analytic methods of [15]; and for tunneling from a stable fixed point, analytic approaches analogous to quantum mechanics.

The intermittent case with weak noise remains an open problem; the results here show that weak noise does not substantially regularize cycle expansions of intermittent systems, at least with respect to the rate of convergence.

Finally, note that the cumulant expansions discussed here are effective only for the first few eigenvalues; more of the spectrum can be found by representing the operator as a matrix in a suitable (truncated) basis and applying standard diagonalization procedures. The convergence of this method for the leading eigenvalue considered here depends on how well the basis represents the leading eigenfunction. Direct diagonalization runs into difficulties in the weakly stochastic intermittent case for reasons related to those of the cumulant expansion: There are many closely spaced eigenvalues converging to a branch cut in the deterministic limit [16].

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