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Dynamical averaging in terms of periodic orbits

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Abstract

Periodic orbit theory methods for evaluation of average values of observables for chaotic dynamical systems are reviewed and illustrated by several examples, such as evaluation of the Lyapunov exponents and the diffusion constants.

In chaotic dynamics detailed prediction is impossible, as any finitely specified initial condition, no matter how precise, will fill out the entire accessible phase space (similarly finitely grained) in finite time. Hence for chaotic dynamics one does not attempt to follow individual trajectories to asymptotic times; what is possible (and sensible) is description of the geometry of the set of possible outcomes, and evaluation of the asymptotic time averages. Examples of such averages are transport coefficients for chaotic dynamical flows, such as the escape rate, mean drift and the diffusion rate; power spectra; and a host of mathematical constructs such as the generalized dimensions, Lyapunov exponents and the Kolmogorov entropy. Here we shall outline how such averages are evaluated within the framework of the periodic orbit theory. The key idea is to replace the expectation values of observables by the expectation values of generating functionals. This associates a Ruelle operator with a given observable, and leads to cycle averaging formulas for its dynamical averages. In contradistinction to averages evaluated on finite approximations to Cantor sets, these formulas are exact, and highly convergent for nice hyperbolic dynamical systems. We illustrate the utility of such cycle expansions by several examples, such as evaluation of the Lyapunov exponents and the diffusion constants.

1. Dynamical averaging

Consider a d -dimensional dynamical system described by d first order ordinary differential equations

$$\frac{dx_i}{dt} = F_i(x), \quad i = 1, 2, \dots, d. \quad (1)$$

The trajectory passing through point x is parameterized by the integral of the above equations:

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$$x_i(t) = \int_0^t d\tau F_i(x) \equiv f_i^t(x), \quad x_i = x_i(0).$$

The flow might describe a trajectory of a particle moving in a potential, evolution of concentrations of a set of chemicals, a discrete time mapping $x_n = f^n(x)$, or even a renormalization operator flow describing a transition to chaos.

1.1. Time averaging

Let $\phi(\tau, x(\tau))$ be any “observable” evaluated on a trajectory $x(\tau) = f^\tau(x)$. Function ϕ can be a scalar, a vector, a tensor; for example, the coordinate $\phi_i(\tau, x) = x_i(\tau)$. The integral of an observable along the trajectory is

$$\Phi^t(x) = \int_0^t d\tau \phi(\tau, x(\tau)), \quad x = x(0). \quad (2)$$

A familiar example of such function for Hamiltonian flows is the action associated with a trajectory,

$$\Phi^t(x) = S(q(t), q(0)) = \int_0^t d\mathbf{q}(\tau) \cdot \mathbf{p}(\tau), \quad x_i = (\mathbf{q}, \mathbf{p}).$$

The *time average* of the observable along the trajectory is given by

$$\langle \phi(x) \rangle = \lim_{t \rightarrow \infty} \frac{1}{t} \Phi^t(x). \quad (3)$$

If ϕ does not behave too wildly as a function of time – for example, $\phi_i = x_i$ is bounded for bounded dynamical systems – $\Phi^t(x)$ is expected to grow not faster than t , and the limit (3) might exist. In other contexts, such as in the case of anomalous diffusion, $\Phi^t(x)$ is not proportional to t but some function of t such as t^α ; in such cases (3) has to be suitably redefined.

However, $\langle \phi(x) \rangle$ is a very wild function of x ; for a nice hyperbolic system it takes the same value $\langle \phi \rangle$ for almost all initial x , but a different value on any periodic orbit, i.e. on a dense set of initial points. For example, for an open system such as the Sinai gas (an infinite 2D periodic array of scattering disks) the phase space is dense with initial x which correspond to periodic runaway trajectories. The mean distance squared traversed by such trajectory grows as $x(t)^2 \sim t^2$, and its contribution to the diffusion rate $D \approx x(t)^2/t$, (3) evaluated with $\phi(x) = x(t)^2$, diverges. Hence for chaotic dynamical systems robust averaging requires also averaging over the initial x and worrying about the measure of the “pathological” trajectories.

1.2. Space averaging

The *expectation value* $\langle \phi \rangle$, the asymptotic time and space average over the “phase space” M (d -dimensional integral over $x_i \in M$, where x_i are the d coordinates of the dynamical system) is not of a particularly tractable form:

$$\begin{aligned}
 \langle \phi \rangle &= \frac{1}{|M|} \int_M dx \langle \phi(x) \rangle, \quad |M| = \int_M dx = \text{volume}, \\
 &= \lim_{t \rightarrow \infty} \frac{1}{t|M|} \int_M dx \int_0^t d\tau \phi(\tau, f^\tau(x)). \tag{4}
 \end{aligned}$$

Such averages are more conveniently studied by introducing an auxiliary variable β , and investigating instead of $\langle \phi \rangle$ the expectation value of

$$\langle e^{\beta \cdot \Phi^t} \rangle = \frac{1}{|M|} \int_M dx e^{\beta \cdot \Phi^t(x)} = \frac{1}{|M|} \int_M dx dy \delta(y - f^t(x)) e^{\beta \cdot \Phi^t(x)}. \tag{5}$$

For example, if the observable is a d -dimensional vector $\phi_i(\tau, x)$, then β is a conjugate vector $\beta \in \mathbb{R}^d$; if the observable is a $[d \times d]$ tensor, β is also a rank-2 tensor, and so on. The auxiliary variable β usually has no particular physical meaning.

2. Evolution operator formalism

Formally, all we have done above is to insert the identity

$$1 = \int_M dy \delta(y - f^t(x)), \tag{6}$$

i.e. we are averaging over trajectories that remain in M for all times. However, this substitution enables us to shift the focus from studying individual trajectories $f^t(x)$ to the evolution of the totality of initial conditions. The kernel of (5) is the Ruelle (or the evolution) operator [1]

$$\mathcal{L}^t(y, x) = \delta(y - f^t(x)) e^{\beta \cdot \Phi^t(x)}. \tag{7}$$

The integral over the observable Φ is additive along the trajectory

$$\Phi^{t_1+t_2}(x) = \int_0^{t_1} d\tau \phi(\tau, x(\tau)) + \int_{t_1}^{t_1+t_2} d\tau \phi(\tau, x(\tau)) = \Phi^{t_1}(x) + \Phi^{t_2}(x(t_1))$$

either if the observable is periodic, $\phi(\tau + t_1, x(\tau)) = \phi(\tau, x(\tau))$, or if it has no explicit dependence on τ , $\phi(\tau, x) = \phi(x)$ (why we might care about periodic observables will become clear in Section 4.4). If $\Phi^t(x)$ is additive along the trajectory, the Ruelle operator has the semigroup property: $\int dz \mathcal{L}^{t_2}(y, z) \mathcal{L}^{t_1}(z, x) = \mathcal{L}^{t_2+t_1}(y, x)$. This semigroup property is the reason why (5) is preferable to (4) as a starting point for evaluation of dynamical averages; their value in the asymptotic $t \rightarrow \infty$ limit can be recovered by means of evolution operators. If the limit $\langle \phi(x) \rangle$, Eq. (3) exists for “almost all” initial x , the expectation value (5) is an integral over exponentials, which therefore also grows exponentially with time

$$\langle e^{\beta \cdot \Phi^t} \rangle \sim \frac{1}{|M|} \int_M dx e^{t\beta \cdot \langle \phi(x) \rangle} \sim e^{tQ(\beta)},$$

and the function

$$Q(\beta) = \lim_{t \rightarrow \infty} \frac{1}{t} \log \langle e^{\beta \cdot \Phi^t} \rangle \tag{8}$$

also exists. \mathcal{L}^t is a linear operator acting on a distribution of initial conditions $\rho(x)$, $x \in M$, so the $t \rightarrow \infty$ limit will be dominated by $e^{tQ(\beta)}$, the leading eigenvalue of \mathcal{L}^t ,

$$(\mathcal{L}^t \circ \rho_\beta)(y) \equiv \int_M dx \delta(y - f^t(x)) e^{\beta \cdot \Phi^t(x)} \rho_\beta(x) = e^{tQ(\beta)} \rho_\beta(y), \quad (9)$$

where $\rho_\beta(x)$ is the corresponding eigenfunction. For $\beta = 0$ the Ruelle operator (7) is a dynamical flows generalization of the Perron-Frobenius operator of probability theory, with $\rho_0(x)$ the natural measure [1–3]. If the system is bounded and no trajectories escape, the leading eigenvalue of \mathcal{L}^t is exactly 1, i.e. $Q(0) = 0$. The expectation value $\langle e^{\beta \cdot \Phi^t} \rangle$ is a generating function for the moments of ϕ , and averages such as (4) are recovered by evaluating the derivatives of $Q(\beta)$

$$\left. \frac{\partial Q}{\partial \beta_i} \right|_{\beta=0} = \lim_{t \rightarrow \infty} \frac{1}{t} \langle \Phi_i^t \rangle = \langle \phi_i \rangle, \quad (10)$$

$$\left. \frac{\partial^2 Q}{\partial \beta_i \partial \beta_j} \right|_{\beta=0} = \lim_{t \rightarrow \infty} \frac{1}{t} (\langle \Phi_i^t \Phi_j^t \rangle - \langle \Phi_i^t \rangle \langle \Phi_j^t \rangle) = \lim_{t \rightarrow \infty} \frac{1}{t} \langle (\Phi_i^t - t \langle \phi_i \rangle) (\Phi_j^t - t \langle \phi_j \rangle) \rangle \quad (11)$$

and so forth.

What are such formulas good for? A typical application is to the problem of describing a particle scattering elastically off a 2D triangular array of disks. If the disks are sufficiently large to block any infinite length free flights, the particle will diffuse chaotically, and the transport coefficient of interest is the diffusion constant given by $x(t)^2 \approx 4Dt$. In contrast to D estimated numerically from trajectories $x(t)$ for finite but large t , the above formulas yield an expression for D evaluated in the $t \rightarrow \infty$ limit. For example, for $\phi_i = x_i$ and zero mean drift $\langle x_i \rangle = 0$, the diffusion constant is given by the curvature of the leading eigenvalue exponent $Q(\beta)$ at $\beta = 0$:

$$D \equiv \lim_{t \rightarrow \infty} \frac{1}{2dt} \langle x(t)^2 \rangle = \frac{1}{2d} \sum_i \left. \frac{\partial^2 Q}{\partial \beta_i^2} \right|_{\beta=0}. \quad (12)$$

As we shall see below, evolution operator formalism yields an explicit closed form expression for D .

2.1. Fredholm determinants, Ruelle zeta functions

Extraction of the spectrum of \mathcal{L} commences with the evaluation of the trace

$$\text{tr } \mathcal{L}^t = \int dx e^{\beta \cdot \Phi^t(x)} \delta(x - f^t(x)).$$

As the relation between evolution operators and the associated Fredholm determinants, Ruelle zeta functions and cycle expansions is discussed at length in literature (see for example Ref. [4,5]), here and in the next section we only state the results needed for understanding the central formula of this paper, cycle averaging formula (21). For a continuous time hyperbolic flow one obtains [6]

$$\text{tr } \mathcal{L}^t = \sum_{p \in \mathcal{P}} \tau_p \sum_{r=1}^{\infty} \frac{\delta(t - \tau_p r)}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} e^{r\beta \cdot \Phi_p}, \quad (13)$$

where the sum is over all prime (i.e., nonrepeating) cycles p whose period τ_p divides t , and $\mathbf{J}_p(x) = Df^{\tau_p}(x)_\perp$ is the Jacobian (monodromy matrix) transverse to the flow.

The above trace formula has a simple geometrical interpretation. Prime cycles partition the phase space into closed tubes of length τ_p and thickness $1/|\det(\mathbf{1} - \mathbf{J}_p)|$; the trace picks up a periodic orbit contribution only when the time t equals a prime period or its repeat, hence the time delta function $\delta(t - \tau_p r)$. Finally, $e^{r\beta \cdot \Phi_p}$ is the mean value of $e^{\beta \cdot \Phi^t(x)}$ evaluated on this part of phase space, so the trace formula is nothing but the integral $\int_{\mathcal{M}} dx e^{\beta \cdot \Phi^t(x)}$ partitioned by the intrinsic topology of the flow, and discretized as a sum over neighborhoods of periodic orbits. The beauty of the formula is that it is coordinatization independent: both $\det(\mathbf{1} - \mathbf{J}_p) = \det(\mathbf{1} - \mathbf{J}^{\tau_p}(x))$ and $\Phi_p = \Phi^{\tau_p}(x)$ are independent of the starting periodic point x ; for the Jacobian \mathbf{J}_p this follows from the chain rule for derivatives, and for Φ_p from the fact that the integral is evaluated on a closed loop. The sum over time delta functions is smoothed over by taking a Laplace transform,

$$\text{tr } \mathcal{L}(s) \equiv \int_0^\infty dt e^{-st} \text{tr } \mathcal{L}^t.$$

The identity $\text{tr } \mathcal{L}(s) = \frac{d}{ds} F(\beta, s)$ then yields [6] the periodic orbit formula for the Fredholm determinant of the evolution operator (7)

$$F(\beta, s) = \prod_{p \in \mathcal{P}} \exp \left(- \sum_{r=1}^\infty \frac{1}{r} \frac{e^{\beta \cdot \Phi_p - s\tau_p r}}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} \right). \tag{14}$$

Values of s for which $F(\beta, s)$ vanishes yield the eigenvalues of the operator \mathcal{L} .

If one is interested only in the leading eigenvalue of \mathcal{L}^t , the size of the p cycle neighborhood $1/|\det(\mathbf{1} - \mathbf{J}_p^r)|$ can be approximated by $1/|A_p|^r$, the dominant term in the $t \rightarrow \infty$ limit, where $A_p = \prod_e A_{p,e}$ is the product of the expanding eigenvalues of the Jacobian \mathbf{J}_p . Performing the r sum, the Fredholm determinant is thus approximated by the Ruelle zeta function [1]

$$1/\zeta(\beta, s) = \prod_{p \in \mathcal{P}} (1 - t_p), \quad t_p = \frac{1}{|A_p|} e^{\beta \cdot \Phi_p - s\tau_p}. \tag{15}$$

The Ruelle zeta function is useful because it also vanishes at e^{ts} equal to $e^{tQ(\beta)}$, the *leading* eigenvalue of \mathcal{L}^t , defined implicitly as the largest solution of either of the equations

$$F(\beta, Q(\beta)) = 0, \quad 1/\zeta(\beta, Q(\beta)) = 0. \tag{16}$$

In practice Fredholm determinants and Ruelle zeta functions are preferable to the trace (13) because they are much easier to compute; the main difference is that while a trace diverges at an eigenvalue, they vanish at s corresponding to an eigenvalue, and are analytic in s in its neighborhood.

3. Cycle expansions

The above infinite products can be rearranged as expansions with improved convergence properties [4,5]. To present the result we expand the zeta function (15) as a formal power series,

$$\begin{aligned} 1/\zeta &= \prod_p (1 - t_p) = 1 - \sum_{p_1+\dots+p_k} t_{p_1+\dots+p_k}, \\ t_{p_1+\dots+p_k} &= (-1)^{k+1} t_{p_1} t_{p_2} \dots t_{p_k}, \end{aligned} \tag{17}$$

where the prime on the sum indicates that the sum is over all distinct non-repeating combinations of prime cycles. For $k > 1$, $t_{p_1+\dots+p_k}$ are weights of “pseudocycles”; they are sequences of shorter cycles that shadow a cycle with symbol sequence $p_1 p_2 \dots p_k$ along segments p_1, p_2, \dots, p_k .

The simplest example is the cycle expansion for a system described by a complete binary symbolic dynamics. In this case the Euler product (15) is given by

$$\begin{aligned} 1/\zeta = & (1 - t_0)(1 - t_1)(1 - t_{01})(1 - t_{001})(1 - t_{011})(1 - t_{0001})(1 - t_{0011})(1 - t_{0111}) \\ & \times (1 - t_{00001})(1 - t_{00011})(1 - t_{00101})(1 - t_{00111})(1 - t_{01011})(1 - t_{01111}) \dots \end{aligned}$$

and the first few terms of the expansion (17) ordered by increasing total pseudocycle length are:

$$\begin{aligned} 1/\zeta = & 1 - t_0 - t_1 - t_{01} - t_{001} - t_{011} - t_{0001} - t_{0011} - t_{0111} - \dots \\ & - t_{0+1} - t_{0+01} - t_{01+1} - t_{0-001} - t_{0+011} - t_{001+1} - t_{011+1} - t_{0+01+1} - \dots \end{aligned}$$

We refer to such series as *cycle expansions*.

The next step is the key step: regroup the terms into the dominant *fundamental* contributions t_f and the decreasing *curvature* corrections c_n . For the binary case this regrouping is given by

$$\begin{aligned} 1/\zeta = & 1 - t_0 - t_1 - [(t_{01} - t_1 t_0)] - [(t_{001} - t_{01} t_0) - (t_{011} - t_{01} t_1)] \\ & - [(t_{0001} - t_0 t_{001}) + (t_{0111} - t_{011} t_1) + (t_{0011} - t_{001} t_1 - t_0 t_{011} + t_0 t_{01} t_1)] - \dots \\ = & 1 - \sum_f t_f - \sum_n c_n . \end{aligned} \tag{18}$$

We refer to such regrouped series as *curvature expansions*. The separation into “fundamental” and “curvature” parts of cycle expansions is possible only for dynamical systems whose symbolic dynamics has finite grammar. The fundamental cycles t_0, t_1 have no shorter approximants; they are the “building blocks” of the dynamics in the sense that all longer orbits can be approximately pieced together from them. The fundamental part of a cycle expansion is given by the sum of the products of all nonintersecting loops of the associated Markov graph [7]. The terms grouped in brackets are the curvature corrections; the terms grouped in parenthesis are combinations of longer orbits and their shorter “shadowing” approximants. If all orbits are weighted equally ($t_p = z^{n_p}$), such combinations cancel exactly. If the flow is continuous and smooth, orbits of similar symbolic dynamics will traverse the same neighborhoods and will have similar weights, and the weights in such combinations will almost cancel. The utility of cycle expansions, in contrast to direct averages over periodic orbits such as the trace formulas (see (37) below), lies precisely in this organization into nearly cancelling combinations: cycle expansions are dominated by short cycles, with long cycles giving exponentially decaying corrections.

A cycle expansion is in essence not much more than a Taylor expansion in a topological cycle length in the following sense; if the number of cycles and their weights grow not faster than exponentially with the cycle length, and we multiply each cycle p by a factor z^{n_p} , $n_p =$ symbol string length of p , the cycle expansion converges for sufficiently small z . The pleasant surprise is that after the prime cycles and the pseudocycles have been grouped into subsets of equal topological length, the dummy variable can be set equal to $z = 1$, as the coefficients in this Taylor expansion can be proven to fall off exponentially or even faster [4,5], guaranteeing the analyticity of $F(\beta, s)$ for s values well beyond those for which the trace formula diverges.

Cycle expansions of Fredholm determinants are obtained in the same way, by grouping together contributions of cycles and pseudocycles of the same symbolic dynamics length.

3.1. Cycle formulas for dynamical averages

The cycle averaging formulas for the slope and the curvature of $Q(\beta)$ are obtained by taking the derivatives of the Eq. (16):

$$0 = \frac{d}{d\beta} F(\beta, Q(\beta)) = \frac{\partial F}{\partial \beta} + \frac{\partial Q}{\partial \beta} \frac{\partial F}{\partial s} \Big|_{s=Q(\beta)} \implies \frac{\partial Q}{\partial \beta} = -\frac{\partial F}{\partial \beta} / \frac{\partial F}{\partial s}. \quad (19)$$

The second derivative of $F(\beta, Q(\beta)) = 0$ yields

$$\frac{\partial^2 Q}{\partial \beta^2} = - \left[\frac{\partial^2 F}{\partial \beta^2} + 2 \frac{\partial Q}{\partial \beta} \frac{\partial^2 F}{\partial \beta \partial s} + \left(\frac{\partial Q}{\partial \beta} \right)^2 \frac{\partial^2 F}{\partial s^2} \right] / \frac{\partial F}{\partial s}. \quad (20)$$

With $F \rightarrow 1/\zeta$ the same formulas apply. Substituting (17) we obtain the cycle averaging formulas [4] for the expectation value of the observable (10) and its variance (11)

$$\langle \phi \rangle = \frac{\langle \Phi \rangle_p}{\langle \tau \rangle_p}, \quad \langle (\phi - \langle \phi \rangle)^2 \rangle = \frac{1}{\langle \tau \rangle_p} \langle (\Phi - \tau \langle \phi \rangle)^2 \rangle_p \quad (21)$$

where $\langle \Phi \rangle_p$ and $\langle \tau \rangle_p$ are respectively the mean cycle Φ and the mean cycle period

$$\langle \Phi \rangle_p \equiv -\frac{\partial}{\partial \beta} \frac{1}{\zeta} = \sum' \Phi_{p_1+\dots+p_k} f_{p_1+\dots+p_k}, \quad \langle \tau \rangle_p \equiv \frac{\partial}{\partial s} \frac{1}{\zeta} = \sum' \tau_{p_1+\dots+p_k} f_{p_1+\dots+p_k},$$

the integrals over the pseudocycles are given by

$$\Phi_{p_1+\dots+p_k} = \Phi_{p_1} + \Phi_{p_2} \cdots + \Phi_{p_k}, \quad \tau_{p_1+\dots+p_k} = \tau_{p_1} + \tau_{p_2} \cdots + \tau_{p_k},$$

and $\langle \cdots \rangle_p$ stands for the average over prime cycles. For bounded flows both $\beta = 0$ and $Q(0) = 0$, so

$$\langle \Phi \rangle_p = \sum' (-1)^{k+1} \frac{\Phi_{p_1+\dots+p_k}}{|A_{p_1} \cdots A_{p_k}|}, \quad \langle \tau \rangle_p = \sum' (-1)^{k+1} \frac{\tau_{p_1+\dots+p_k}}{|A_{p_1} \cdots A_{p_k}|}. \quad (22)$$

The mean cycle period $\langle \tau \rangle_p$ fixes the normalization of the unit of time. For example, if we have evaluated a billiard expectation value $\langle \phi \rangle$ in terms of continuous time, and would like to also have the corresponding average $[\phi]$ measured in discrete time given by the number of reflections off billiard walls, the two averages are related by $[\phi] = \langle \phi \rangle \langle \tau \rangle_p / \langle n \rangle_p$, where n_p is the number of bounces along the cycle p .

As we shall explain in Section 5.1, the above averages are not what one would intuitively write down. Note also that the cycle averaging formulas, in contrast to some of the earlier analytic work [8], require no knowledge of explicit eigenvalues of the Perron-Frobenius operator (i.e., the natural measure ρ_0). This is one of the main virtues of the cycle expansions: their evaluation *does not* require construction of the (coordinate dependent) eigenfunctions.

4. Applications of cycle expansions

The cycle averaging formulas (21) are the main result of the periodic orbit theory applied to evaluation of dynamical averages. We now give a few examples of their applicability. An application to the evaluation of correlation functions, formulated very much in the same spirit as this paper, was given recently by Eckhardt and Grossmann [10]. A few more examples of “thermodynamic” averages are given in Refs. [4,12].

4.1. Probability conservation

If the system is bounded, all trajectories remain confined for all times and the leading eigenvalue (9) must equal 1, $Q(0) = 0$. Probability conservation thus provides the first and a very useful check of the quality of finite cycle truncations of cycle expansions: the dynamical zeta function (15) should have its first zero at $\beta, s = 0$

$$1/\zeta(0,0) = 1 + \sum'_{p_1+\dots+p_k} \frac{(-1)^k}{|A_{p_1} \cdots A_{p_k}|} = 0. \quad (23)$$

4.2. Lyapunov exponents

The largest Lyapunov exponent μ of a given dynamical trajectory is given by the $t \rightarrow \infty$ limit of $\frac{1}{t} \log |Df^t(x)|$, where $|Df^t(x)|$ is the absolute value of the largest eigenvalue of the linearized flow. The corresponding “observable” (2)

$$\Phi^t(x) = t\mu(x) = \log |Df^t(x)|$$

is additive for 1D maps by the chain rule formula for the derivative of the iterated map f^t . For higher-dimensional flows only stability matrices are multiplicative, not individual eigenvalues, and the construction of the correct Ruelle operator for evaluation of the Lyapunov spectra for higher-dimensional flows is not trivial; it requires an extension of evolution equations to the flow in the tangent space, and was given only recently [13]. However, the modification affects only the nonleading eigenvalues of the evolution operator, and the Ruelle zeta function and the associated cycle averaging formula (21) for the largest Lyapunov exponent are of the expected form

$$\mu = \frac{1}{\langle \tau \rangle_p} \sum'_{p_1+\dots+p_k} (-1)^{k+1} \frac{\tau_{p_1} \mu_{p_1} + \cdots + \tau_{p_k} \mu_{p_k}}{|A_{p_1} \cdots A_{p_k}|}, \quad (24)$$

with $\mu_p = \ln |A_p^{\max}|/\tau_p$ the Lyapunov exponent of the p cycle, and A_p^{\max} its largest eigenvalue. The above cycle averaging formula has been applied to many 1D maps, 2D maps and 3D flows, and works well in practice.

4.3. Diffusion

Consider a d -dimensional flow on a periodic potential and let $\hat{x}(t)$ be the trajectory of the initial point $x(0)$. The cycle expansion for the diffusion constant (12) with zero mean drift $\langle \hat{x}_i \rangle = 0$ is given by [14–16]

$$D = \frac{1}{2d} \frac{\langle \hat{x}^2 \rangle_p}{\langle \tau \rangle_p} = \frac{1}{2d} \frac{1}{\langle \tau \rangle_p} \sum'_{p_1+\dots+p_k} (-1)^{k+1} \frac{(\hat{x}_{p_1} + \cdots + \hat{x}_{p_k})^2}{|A_{p_1} \cdots A_{p_k}|}. \quad (25)$$

The alert reader should immediately protest that $x_p = x(\tau_p) - x(0)$ is manifestly equal to zero for a periodic orbit. That is correct; \hat{x}_p in the above formula refers to a displacement on a periodic lattice, while p refers to closed orbit of the dynamics reduced to the fundamental cell, with x_p belonging to the closed prime orbit p . Even so, this is not an obvious formula. Globally periodic orbits have $\hat{x}_p^2 = 0$, and contribute only to the time normalization $\langle \tau \rangle_p$. The mean square displacement $\langle \hat{x}^2 \rangle_p$ gets contributions only from the periodic runaway trajectories; they are closed in the fundamental cell, but on the periodic lattice each one grows like $\hat{x}(t)^2 = (t/\tau_p)^2 \hat{x}_p^2 \sim t^2$. Nevertheless, thanks to the exponential suppression of long cycles by the $1/|A_p|$ weights, the mean $\hat{x}(t)^2$ grows linearly with t . If the system is not hyperbolic, the suppression of long cycles

can be weaker, $1/|A_p| \approx 1/\tau_p^\alpha$ rather than $1/|A_p| \approx e^{-\tau_p \mu}$ (here μ is the Lyapunov exponent), and the diffusion can be anomalous [20].

A very simple example of applicability of the above formula for the diffusion constant D is offered by an infinite chain of 1D maps, each acting on interval $[n - \frac{1}{2}, n + \frac{1}{2}]$ with a single constant slope branch

$$f_n(\hat{x}) = A(\hat{x} - n) + n, \quad \hat{x} - n \in [-\frac{1}{2}, \frac{1}{2}].$$

If $A > 1$, a fraction of \hat{x} iterate into neighboring intervals, inducing diffusion. The associated map reduced to the fundamental cell $[-\frac{1}{2}, \frac{1}{2}]$ is given by the 3-branch fractional part of f_n

$$f(x) = \begin{cases} Ax + 1 & \text{if } x \in I_a = [-\frac{1}{2}, -\frac{1}{A}], \quad \sigma = -1 \\ Ax & \text{if } x \in I_b = [-\frac{1}{A}, 0], \quad \sigma = 0 \\ Ax & \text{if } x \in I_c = [0, \frac{1}{A}], \quad \sigma = 0 \\ Ax - 1 & \text{if } x \in I_d = [\frac{1}{A}, \frac{1}{2}], \quad \sigma = 1 \end{cases}, \tag{26}$$

where, for $1 < A \leq 3$, the drift per iteration is given by $\sigma(x) = f_0(x) - f(x) \in \{-1, 0, 1\}$, and the total global drift per one fundamental cell p cycle traversal is $\hat{x}_p = \sum_{i \in p} \sigma(x_i)$. The cycle expansions are simple if the Markov partition is finite: the simplest example is given by fixing the stretching factor to $A = 3$. For this slope the four intervals I_a, I_b, I_c, I_d give a complete Markov partition. $f(I_b) = I_a + I_b$, $f(I_c) = I_c + I_d$, so the symbolic dynamics is given by four pruning rules: subsequences $_bc_$, $_bd_$, $_ca_$, $_cb_$ are forbidden. The allowed sequences are walks on the associated Markov graph, and if the map is piecewise linear, the cycle expansion (17) is polynomial in $z = e^{-s}$, with coefficients given by products over all non-intersecting walks on the Markov graph [7]:

$$1/\zeta = 1 - t_a - t_b - t_c - t_d - t_{ab} - t_{cd} + (t_a + t_d)(t_b + t_c) + t_b t_c + t_a b t_c + t_{cd} t_b - (t_a + t_d) t_b t_c$$

For the piecewise linear maps with uniform stretching the weight of a symbol sequence is a product of weights for individual steps, $t_{pq} = t_p t_q$, where p, q stand for

$$t_a = e^{-\beta} z / A, \quad t_b = t_c = z / A, \quad t_d = e^{\beta} z / A, \quad z = e^{-s}$$

$$\frac{1}{\zeta(\beta, s)} = 1 - \frac{z}{A} (2 + e^{-\beta} + e^{\beta}) + \frac{z^2}{A^2} (1 + e^{-\beta} + e^{\beta}).$$

t_a, t_d correspond to translations by $\sigma = \pm 1$ along the 1D chain. For $\beta = 0$ the dynamics is symmetric under $x \rightarrow -x$, and zeta function factorizes into $\zeta = \zeta_s \zeta_a$, product of the zeta functions for the symmetric and antisymmetric subspaces [17]

$$\frac{1}{\zeta(0, s)} = \left(1 - 3\frac{z}{A}\right) \left(1 - \frac{z}{A}\right).$$

The probability conservation serves here as a check; (23) is indeed satisfied, as $A = 3$. The leading (probability conserving) eigenvalue $s = 0$ belongs to the symmetric subspace $1/\zeta_s(0, 0) = 0$, so the derivatives also act only on the symmetric subspace:

$$\langle \tau \rangle_p = \frac{\partial}{\partial s} \frac{1}{\zeta(0, s)} \Big|_{s=0} = \frac{1}{\zeta_a(0, 0)} \frac{\partial}{\partial s} \frac{1}{\zeta_s(0, s)} \Big|_{s=0} = \left(1 - \frac{1}{A}\right) \frac{3}{A}. \tag{27}$$

The cycle averaging formula for the “mean square drift”

$$\langle \hat{x}^2 \rangle_p = - \frac{\partial^2}{\partial \beta^2} \frac{1}{\zeta(\beta, 0)} \Big|_{\beta=0} = \frac{2}{\Lambda} \left(1 - \frac{1}{\Lambda} \right)$$

now yields the diffusion constant

$$D = \frac{1}{2} \frac{\langle \hat{x}^2 \rangle_p}{\langle \tau \rangle_p} = \frac{1}{3}.$$

We would have obtained this result immediately, if we treated $I_b + I_c$ as a single Markov partition interval; however, keeping them separate highlights most of the steps that would be needed in analysis of systems with more complicated symbolic dynamics.

This formalism works well for simple 1D maps with finite Markov partitions [14], piecewise linear standard map [18], and even infinite partitions [19]. Anomalous diffusion can be treated in a similar way [20]. Regrettably, for physically interesting problems such as the finite horizon Lorentz gas, the convergence of cycle expansions has – so far – been mediocre due to the severe pruning of symbolic dynamics [16,21].

4.4. Power spectra

Pikovsky et al. [22] have applied the cycle averaging formulas to evaluation of the power spectra of chaotic discrete time series. The key idea is to think of the diffusion constant (25) as the value of the power spectrum at zero frequency, and then generalize the diffusion cycle averaging formula to evaluation of the power spectrum at any rational frequency.

Consider $\langle \phi(x) \rangle$, the time averaged observable (3) of the form

$$\hat{x}_t(\omega, x) = \frac{1}{t} \sum_{n=0}^{t-1} x_n e^{in\omega}. \tag{28}$$

where the time is discrete, and $x_n = f^n(x)$. In the $t \rightarrow \infty$ limit this is the *Fourier transform* of the orbit of a dynamical system passing through $x_0 = x$. The power spectrum consists of broad band noise $D(\omega)$ and discrete spectrum $\Delta(\omega)$,

$$\langle |t\hat{x}_t(\omega)|^2 \rangle \sim t^2 \Delta(\omega) + 2tD(\omega),$$

so $D(\omega)$ is the diffusion constant for quantity $\Phi^t(x) = t\hat{x}_t(\omega, x)$, and $\Delta(\omega)$ is its mean drift.

The Fourier transform $\hat{x}_t(\omega)$ is an average of the form $\frac{1}{t} \sum a_n x_n$, where a_n is also an orbit of a dynamical system: in the case of Fourier analysis $a_t = e^{i\theta_t}$, and the extended dynamical system is

$$x_{t+1} = f(x_t)\theta_{t+1} = g_\omega(\theta_t) = \omega + \theta_t \pmod{2\pi} \tag{29}$$

where the θ_t dynamics is the trivial dynamics on the circle. For rational $\omega = 2\pi n/t$ periodic orbits of f^t are also periodic orbits of the extended system, hence the periodic theory can be applied to this problem. We take as the Ruelle operator (where the θ δ -function is taken mod 2π)

$$\mathcal{L}(x, \theta; x', \theta') = \delta(x - f(x')) \delta(\theta - g_\omega(\theta')) \exp\left(\beta x' \frac{1}{2}(e^{i\theta'} + e^{-i\theta'})\right). \tag{30}$$

This operator acts multiplicatively on functions defined on the extended phase space

$$(\mathcal{L}'\psi)(x, \theta) = \int dx' \frac{d\theta'}{2\pi} \delta(x - f'(x')) \delta(\theta - g'_\omega(\theta')) \exp(\beta t |\hat{x}_t| \cos(\theta' + \alpha_t)) \psi(x', \theta'),$$

with α_t the complex phase of \hat{x}_t . However, as the trivial dynamics on the circle is not hyperbolic, care has to be taken [22] in defining \mathcal{L}^t . For the measure uniform in θ , the θ' integration can be shifted to absorb α_t , so the $\mathcal{L}^t \psi$ integrated over x and θ yields

$$\left\langle \int \frac{d\theta}{2\pi} \exp(\beta t |\hat{x}_t| \cos \theta) \right\rangle \rightarrow \left\langle \frac{\exp(\beta t |\hat{x}_t|)}{\sqrt{2\pi\beta t |\hat{x}_t|}} \right\rangle \quad \text{for } t \rightarrow \infty. \tag{31}$$

Apart from a prefactor, the saddle point approximation yields the desired generating function (5). The trace

$$\text{tr } \mathcal{L}^t = \int dx \delta(x - f^t(x)) \int \frac{d\theta}{2\pi} \exp(\beta t |\hat{x}_t(\omega, x)| \cos \theta) \tag{32}$$

can pick up contributions only from the periodic points $x = f^t(x)$. Every periodic point x belongs to some prime cycle p , $x \in \{x_{p,0}, x_{p,1}, \dots, x_{p,\tau_p-1}\}$, where τ_p is the minimal period of x under f , and $x_{p,m} = f^m(x_{p,0})$. The Fourier transform of a single traversal of a prime cycle is given by

$$\hat{x}_p(\omega) = \frac{1}{\tau_p} \sum_{m=0}^{\tau_p-1} x_{p,m} e^{im\omega},$$

and the Fourier transform of the r -th repeat, $t = \tau_p r$, by

$$\hat{x}_t(\omega, x) = \frac{1}{r\tau_p} \sum_{\ell=0}^{r-1} \sum_{m=0}^{\tau_p-1} x_{p,m} \exp(i(m + \tau_p \ell)\omega) = \hat{x}_p(\omega) \frac{1}{r} \sum_{\ell=0}^{r-1} \exp(i\tau_p \ell \omega). \tag{33}$$

As $\hat{x}_t(\omega, x_{p,m}) = e^{-i\omega m} \hat{x}_t(\omega, x_{p,0})$, $|\hat{x}_p(\omega)|$ is the same for all cycle points belonging to the prime cycle p , but the cycle weight depends on the initial cycle point through the phase factor $e^{-i\omega m}$. However, as the trace (32) is invariant under θ translations, this dependence can be rotated away, so the Fourier cycle weight depends only on the cycle, and not on the initial cycle point.

If the frequency is irrational, the last sum in (33) in the $t \rightarrow \infty$ limit traces out a circle in the complex plane, and averages to zero. However, for a rational frequency of form $\omega = 2\pi n/t$, $n = 0, \dots, t-1$, the sum projects out resonant periodic orbits,

$$\frac{1}{r} \sum_{\ell=0}^{r-1} e^{2\pi i n \ell / r} = \delta_{n,kr}, \quad k = 0, \dots, \tau_p - 1.$$

Here n, t can share common divisors. Thus, $\hat{x}_p(\omega)$ contributes its own value to (32)

$$|\hat{x}_t(\omega, x_{p,m})| = \begin{cases} |\hat{x}_p(\omega)| & \text{if } \tau_p | t \text{ and } \omega = 2\pi k / \tau_p \\ 0 & \text{otherwise} \end{cases}. \tag{34}$$

Integrating (32) over x yields the trace formula of Ref. [22]

$$\text{tr } \mathcal{L}^t = \sum_p \tau_p \sum_{r=1}^{\infty} \frac{\delta_{t,\tau_p r}}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} \exp(\beta t |\hat{x}_t(\omega)|)_p,$$

$$\exp(\beta t |\hat{x}_t(\omega)|)_p = \begin{cases} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{\beta r \tau_p |\hat{x}_p(\omega)| \cos \theta} = J_0(i\beta r \tau_p |\hat{x}_p(\omega)|) & \text{if } \omega = 2\pi k / \tau_p \\ 1 & \text{otherwise} \end{cases}$$

Assuming no drift, the power spectrum is given by

$$D(\omega) = \lim_{t \rightarrow \infty} \frac{t}{2} \langle |\hat{x}_t(\omega)|^2 \rangle = \frac{1}{2} \left. \frac{\partial^2 Q}{\partial \beta^2} \right|_{\beta=0}, \quad (35)$$

so the second derivative with respect to β yields the cycle averaging formula for the power spectrum

$$D(\omega) = \frac{1}{2} \frac{1}{\langle \tau \rangle_p} \sum' \frac{(-1)^{k+1}}{|A_{p_1} \cdots A_{p_k}|} (\tau_{p_1} |\hat{x}_{p_1}(\omega)| + \cdots + \tau_{p_k} |\hat{x}_{p_k}(\omega)|)^2. \quad (36)$$

Only those prime cycles p whose periods τ_p are integer multiples of the frequency $\omega = 2\pi k/n$ denominator n contribute to the numerator of the cycle expansion (36). All cycles contribute to the denominator, but the denominator is a frequency-independent normalization factor which needs to be computed only once.

A power spectrum cycle averaging formula has been checked by Pikovsky [11] for several 1D mappings, and it works well. However, it should be noted that the above formalism is inadequate for evaluation of power spectra of continuous time flows, as it hinges on the time in (28) being discrete, and picking out sets of orbits that resonate at rational frequencies. For continuous time flows, there is generally no reason to expect such resonant sets.

5. How reliable are cycle averaging formulas?

5.1. Cycle expansions vs. log-log fits

The *thermodynamic formalism* [1–3] takes the parameter β seriously, as a kind of mathematician's temperature, refers to $Q(\beta)$ as a “pressure”, “free energy” or something similarly puzzling, and studies the function $Q(\beta)$, defined implicitly by the condition (16), for ranges of β . This makes it possible to plot a variety of smooth curves which can be helpful in understanding gross features in the distribution of scales in dynamically generated Cantor sets. Various approximations to the trace formula (13) are in physics literature called the Renyi [23], the generalized dimensions [24], the “multifractal” [25] or the f -of- α formalism [26]. The idea is to stare at rectangles stretched and squeezed by the flow, and estimate, from the stability of nearby periodic orbit p or by other means, their size to be proportional to the inverse of local stretching, of order of $1/|A_p|$; for example, for large t the weight in (13) is dominated by the product of expanding eigenvalues, $\det(\mathbf{1} - \mathbf{J}_p) \rightarrow A_p$. In such approximations one replaces the *exact* trace formula (13) by

$$\text{tr } \mathcal{L}^t \simeq Z^t(\beta) = \sum_i^{(t)} \frac{1}{|A_i|} e^{\beta \cdot \Phi_i},$$

where the sum goes over all periodic points x_i of period t . (In the multifractal literature the “time” t is taken discrete, but one can also model continuous flows by introducing a “time ceiling function” [3].) The finite time t estimate of the average is then

$$\langle \phi \rangle_t = \frac{1}{t} \frac{\sum_i^{(t)} \Phi_i / |A_i|}{\sum_i^{(t)} 1 / |A_i|} = \frac{1}{t} \frac{\partial}{\partial \beta} \ln Z^t(\beta) \Big|_{\beta=0}, \quad (37)$$

which (by log-log extrapolations from the finite t data) leads to a $t \rightarrow \infty$ estimate of the expectation value $\langle \phi \rangle$. Such average is an approximate sum built by partitioning the phase space into neighborhoods of periodic points of period t . In contrast, cycle averaging formulas (21) are *exact* $t \rightarrow \infty$ sums over all prime cycles.

As shown in the Ref. [4], the prefactors $(-1)^k$ enforce the curvature (shadowing) cancelations (18), and accelerate the convergence of finite cycle length truncations of cycle expansions.

As for dynamical systems evaluation of the exact trace (21) and the approximate trace (37) requires the same amount of labor, nothing is gained by the approximation. The utility of the f -of- α formalism lies not in its applications to the deterministic dynamical systems (where the original Bowen-Sinai-Ruelle theory is much more powerful), but in its applications to numerical evaluations of averages over random objects, such as fractal aggregates and noisy experimental data, where no dynamical theory exists.

5.2. Convergence

When the dynamical system’s symbolic dynamics does not have a finite grammar, and we are not able to arrange its cycle expansion into curvature combinations (18), the series is truncated by including all pseudocycles such that $|A_{p_1} \cdots A_{p_k}| \leq |A_P|$, where P is the most unstable prime cycle included into truncation. The truncation error should then be of order $O(e^{h\tau_P} \tau_P / |A_P|)$, with h the topological entropy, and $e^{h\tau_P}$ roughly the number of pseudocycles of stability $\approx |A_P|$. In this case the cycle averaging formulas do not converge significantly better [16,21] than the approximations such as the trace formula (37). Even that is not the worst case scenario; generic dynamical systems are plagued by intermittency and other nonhyperbolic effects, and methods that go beyond cycle expansions need to be developed [27]. However, for smooth hyperbolic flows with finite symbolic dynamics grammar the convergence as function of the cycle length truncation can be dramatically better, even faster than exponential [28,5].

Numerical results (see for example the plots of the accuracy of the cycle expansion truncations for the Hénon map in Ref. [12]) indicate that the truncation error of most averages tracks closely the fluctuations due to the irregular growth in the number of cycles. It is not known whether one can exploit the sum rules such as the probability conservation (23) to improve the accuracy of dynamical averaging.

5.3. Mathematical caveats

The periodic orbit theory is learned in stages. At first glance, it seems totally impenetrable. After basic exercises are gone through, it seems totally trivial; in practice all that is at stake are elementary manipulations with traces, determinants, derivatives. Still, from the mathematical point of view, the theory is full of perils.

Birkhoff’s 1931 ergodic theorem [29] states that the time average (3) exists almost everywhere, and, if the flow is ergodic, it implies that $\langle \phi(x) \rangle = \langle \phi \rangle$ is a constant for almost all x . The problem is that the above cycle averaging formulas implicitly rely on ergodic hypothesis: they are strictly correct only if the dynamical system is locally hyperbolic and globally mixing. If one takes a β derivative of both sides of (9)

$$\rho_\beta(y) e^{tQ(\beta)} = \int_M dx \delta(y - f^t(x)) e^{\beta \cdot \Phi^t(x)} \rho_\beta(x),$$

and integrates over y

$$\int_M dy \left. \frac{\partial}{\partial \beta} \rho_\beta(y) \right|_{\beta=0} + t \left. \frac{\partial Q}{\partial \beta} \right|_{\beta=0} \int_M dy \rho_0(y) = \int_M dx \Phi^t(x) \rho_0(x) + \int_M dx \left. \frac{\partial}{\partial \beta} \rho_\beta(x) \right|_{\beta=0},$$

one obtains

$$\left. \frac{\partial Q}{\partial \beta} \right|_{\beta=0} = \int_M dy \rho_0(x) \langle \phi(x) \rangle. \tag{38}$$

This is the expectation value (10) only if the time average (3) equals the space average (4) $\langle \phi(x) \rangle = \langle \phi \rangle$ for all x except a subset $x \in M$ of zero measure; if the phase space is foliated into non-communicating subspaces $M = M_1 + M_2$ of finite measure such that $f^t(M_1) \cap M_2 = \emptyset$ for all t , this fails. In other words, we have tacitly assumed ergodicity. We have also glossed over the nature of the “phase space” M . For example, if the dynamical system is open, such as the 3-disk pinball, M in the expectation value integral (6) is a Cantor set, the closure of the union of all periodic orbits. Alternatively, x can be considered continuous, but then the measure ρ_0 in (38) is highly singular. The beauty of the periodic theory is that instead of using an arbitrary coordinatization $x \in M$ it partitions the phase space by the intrinsic topology of the dynamical flow and builds the correct measure from cycle invariants, the stability eigenvalues of periodic orbits.

Were we to restrict the applications of the formalism only to systems which have been rigorously proven to be ergodic, we would not have much to do. For example, even for something as simple as the Hénon mapping we do not know whether the asymptotic time attractor is strange or periodic. Physics applications require a more pragmatic attitude. In the cycle expansions approach we construct the invariant set of the given dynamical system as a closure of the union of periodic orbits, and investigate how robust are the averages computed on this set. This turns out to depend very much on the observable being averaged over; dynamical averages exhibit “phase transitions” [30], and the above cycle averaging formulas apply in a “hyperbolic phase” where the average is dominated by exponentially many exponentially small contributions, but fail in a phase dominated by few marginally stable orbits.

Still, in spite of all the caveats, periodic orbit theory is a beautiful theory, and the cycle averaging formulas are the most elegant and powerful tool available today for evaluation of dynamical averages for low dimensional chaotic deterministic systems.

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