Chapter 15

Averaging

For it, the mystic evolution;
Not the right only justified
– what we call evil also justified.
—Walt Whitman,
Leaves of Grass: Song of the Universal

We discuss first the necessity of studying the averages of observables in chaotic dynamics, and then cast the formulas for averages in a multiplicative form that motivates the introduction of evolution operators and further formal developments to come. The main result is that any *dynamical* average measurable in a chaotic system can be extracted from the spectrum of an appropriately constructed evolution operator. In order to keep our toes closer to the ground, in sect. 15.3 we try out the formalism on the first quantitative diagnosis that a system's got chaos, Lyapunov exponents.

15.1 Dynamical averaging

In chaotic dynamics detailed prediction is impossible, as any finitely specified initial condition, no matter how precise, will fill out the entire accessible state space. Hence for chaotic dynamics one cannot follow individual trajectories for a long time; what is attainable is a description of the geometry of the set of possible outcomes, and evaluation of long time averages. Examples of such averages are transport coefficients for chaotic dynamical flows, such as escape rate, mean drift and diffusion rate; power spectra; and a host of mathematical constructs such as generalized dimensions, entropies and Lyapunov exponents. Here we outline how such averages are evaluated within the evolution operator framework. The key idea is to replace the expectation values of observables by the expectation values of generating functionals. This associates an evolution operator with a given observable, and relates the expectation value of the observable to the leading eigenvalue of the evolution operator.

15.1.1 Time averages

Let $a = a(x)$ be any *observable*, a function that associates to each point in state space a number, a vector, or a tensor. The observable reports on a property of the dynamical system. It is a device, such as a thermometer or laser Doppler velocitometer. The device itself does not change during the measurement. The velocity field $a_i(x) = v_i(x)$ is an example of a vector observable; the length of this vector, or perhaps a temperature measured in an experiment at instant τ are examples of scalar observables. We define the *integrated observable* A^t as the time integral of the observable a evaluated along the trajectory of the initial point x_0,

$$A^t(x_0) = \int_0^t d\tau\, a(f^\tau(x_0))\,. \tag{15.1}$$

If the dynamics is given by an iterated mapping and the time is discrete, $t \to n$, the integrated observable is given by

$$A^n(x_0) = \sum_{k=0}^{n-1} a(f^k(x_0)) \tag{15.2}$$

(we suppress possible vectorial indices for the time being). For example, if the observable is the velocity, $a_i(x) = v_i(x)$, its time integral $A_i^t(x_0)$ is the trajectory $A_i^t(x_0) = x_i(t)$. Another familiar example, for Hamiltonian flows, is the action associated with a trajectory $x(t) = [q(t), p(t)]$ passing through a phase space point $x_0 = [q(0), p(0)]$ (this function will be the key to the semiclassical quantization of chapter 32):

$$A^t(x_0) = \int_0^t d\tau\, \dot{\mathbf{q}}(\tau)\cdot\mathbf{p}(\tau)\,. \tag{15.3}$$

The *time average* of the observable along a trajectory is defined by

$$\overline{a(x_0)} = \lim_{t\to\infty} \frac{1}{t} A^t(x_0)\,. \tag{15.4}$$

If a does not behave too wildly as a function of time – for example, if $a_i(x)$ is the Chicago temperature, bounded between -80^oF and $+130^oF$ for all times – $A^t(x_0)$ is expected to grow not faster than t, and the limit (15.4) exists. For an example of a time average - the Lyapunov exponent - see sect. 15.3.

The time average depends on the trajectory, but not on the initial point on that trajectory: if we start at a later state space point $f^T(x_0)$ we get a couple of extra finite contributions that vanish in the $t \to \infty$ limit:

$$\begin{aligned}
\overline{a(f^T(x_0))} &= \lim_{t\to\infty} \frac{1}{t} \int_T^{t+T} d\tau\, a(f^\tau(x_0)) \\
&= \overline{a(x_0)} - \lim_{t\to\infty} \frac{1}{t} \left(\int_0^T d\tau\, a(f^\tau(x_0)) - \int_t^{t+T} d\tau\, a(f^\tau(x_0)) \right) \\
&= \overline{a(x_0)}\,.
\end{aligned}$$

The integrated observable $A^t(x_0)$ and the time average $\overline{a(x_0)}$ take a particularly simple form when evaluated on a periodic orbit. Define

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$$\begin{aligned}
\text{flows:} \quad A_p &= a_p T_p = \int_0^{T_p} d\tau\, a\left(f^\tau(x_0)\right)\,, \qquad x_0 \in p \\
\text{maps:} \quad &= a_p n_p = \sum_{i=0}^{n_p-1} a\left(f^i(x_0)\right)\,,
\end{aligned} \tag{15.5}$$

where p is a prime cycle, T_p is its period, and n_p is its discrete time period in the case of iterated map dynamics. A_p is a loop integral of the observable along a single traversal of a prime cycle p, so it is an intrinsic property of the cycle, independent of the starting point $x_0 \in p$. (If the observable a is not a scalar but a vector or matrix we might have to be more careful in defining an average which is independent of the starting point on the cycle). If the trajectory retraces itself r times, we just obtain A_p repeated r times. Evaluation of the asymptotic time average (15.4) requires therefore only a single traversal of the cycle:

$$a_p = A_p/T_p\,. \tag{15.6}$$

However, $\overline{a(x_0)}$ is in general a wild function of x_0; for a hyperbolic system ergodic with respect to a smooth measure, it takes the same value $\langle a \rangle$ for almost all initial x_0, but a different value (15.6) on any periodic orbit, i.e., on a dense set of points (figure 15.1 (b)). For example, for an open system such as the Sinai gas of sect. 23.1 (an infinite 2-dimensional periodic array of scattering disks) the phase space is dense with initial points that correspond to periodic runaway trajectories. The mean distance squared traversed by any such trajectory grows as $x(t)^2 \sim t^2$, and its contribution to the diffusion rate $D \approx x(t)^2/t$, (15.4) evaluated with $a(x) = x(t)^2$, diverges. Seemingly there is a paradox; even though intuition says the typical motion should be diffusive, we have an infinity of ballistic trajectories.

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For chaotic dynamical systems, this paradox is resolved by robust averaging, i.e., averaging also over the initial x, and worrying about the measure of the "pathological" trajectories.

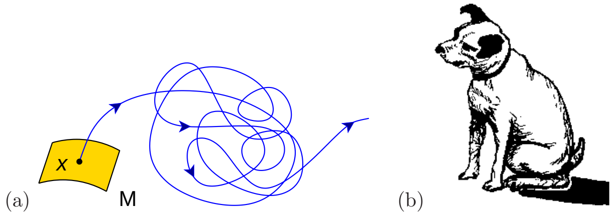

Figure 15.1: (a) A typical chaotic trajectory explores the phase space with the long time visitation frequency building up the natural measure $\rho_0(x)$. (b) time average evaluated along an atypical trajectory such as a periodic orbit fails to explore the entire accessible state space. (A. Johansen)

15.1.2 Space averages

The *space average* of a quantity a that may depend on the point x of state space $\mathcal{M}$ and on the time t is given by the d-dimensional integral over the d coordinates of the dynamical system:

$$\begin{aligned}
\langle a \rangle(t) &= \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx\, a(f^t(x)) \\
|\mathcal{M}| &= \int_{\mathcal{M}} dx = \text{volume of } \mathcal{M}\,.
\end{aligned} \tag{15.7}$$

The space $\mathcal{M}$ is assumed to have finite dimension and volume (open systems like the 3-disk game of pinball are discussed in sect. 15.1.3).

What is it we *really* do in experiments? We cannot measure the time average (15.4), as there is no way to prepare a single initial condition with infinite precision. The best we can do is to prepare some initial density $\rho(x)$ perhaps concentrated on some small (but always finite) neighborhood $\rho(x) = \rho(x, 0)$, so one should abandon the uniform space average (15.7), and consider instead

$$\langle a \rangle_\rho(t) = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx\, \rho(x) a(f^t(x))\,. \tag{15.8}$$

We do not bother to lug the initial $\rho(x)$ around, as for the ergodic and mixing systems that we shall consider here *any* smooth initial density will tend to the asymptotic natural measure $t \to \infty$ limit $\rho(x,t) \to \rho_0(x)$, so we can just as well take the initial $\rho(x) = \text{const}$. The worst we can do is to start out with $\rho(x) = \text{const.}$, as in (15.7); so let us take this case and define the *expectation value* $\langle a \rangle$ of an observable a to be the asymptotic time and space average over the state space $\mathcal{M}$

$$\langle a \rangle = \lim_{t\to\infty} \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx\, \frac{1}{t} \int_0^t d\tau\, a(f^\tau(x))\,. \tag{15.9}$$

We use the same $\langle\cdots\rangle$ notation as for the space average (15.7), and distinguish the two by the presence of the time variable in the argument: if the quantity $\langle a\rangle(t)$ being averaged depends on time, then it is a space average, if it does not, it is the expectation value $\langle a\rangle$.

The expectation value is a space average of time averages, with every $x \in \mathcal{M}$ used as a starting point of a time average. The advantage of averaging over space is that it smears over the starting points which were problematic for the time average (like the periodic points). While easy to define, the expectation value $\langle a\rangle$ turns out not to be particularly tractable in practice. Here comes a simple idea that is the basis of all that follows: Such averages are more conveniently studied by investigating instead of $\langle a\rangle$ the space averages of form

$$\left\langle e^{\beta\cdot A^t}\right\rangle = \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} dx\, e^{\beta\cdot A^t(x)}. \tag{15.10}$$

In the present context β is an auxiliary variable of no particular physical significance. In most applications β is a scalar, but if the observable is a d-dimensional vector $a_i(x) \in \mathbb{R}^d$, 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. Here we will mostly limit the considerations to scalar values of β.

If the limit $\overline{a(x_0)}$ for the time average (15.4) exists for "almost all" initial x_0 and the system is ergodic and mixing (in the sense of sect. 1.3.1), we expect the time average along almost all trajectories to tend to the same value $\overline{a}$, and the integrated observable A^t to tend to $t\overline{a}$. The space average (15.10) is an integral over exponentials, and such integral also grows exponentially with time. So as $t \to \infty$ we would expect the space average of $\left\langle \exp(\beta\cdot A^t)\right\rangle$ itself to grow exponentially with time

$$\left\langle e^{\beta\cdot A^t}\right\rangle \propto e^{ts(\beta)}\,,$$

and its rate of growth to go to a limit

$$s(\beta) = \lim_{t\to\infty}\frac{1}{t}\ln\left\langle e^{\beta\cdot A^t}\right\rangle\,. \tag{15.11}$$

Now we understand one reason for why it is smarter to compute $\left\langle \exp(\beta\cdot A^t)\right\rangle$ rather than $\langle a\rangle$: the expectation value of the observable (15.9) and the moments of the integrated observable (15.1) can be computed by evaluating the derivatives of $s(\beta)$

$$\begin{aligned}
\left.\frac{\partial s}{\partial\beta}\right|_{\beta=0} &= \lim_{t\to\infty}\frac{1}{t}\left\langle A^t\right\rangle = \langle a\rangle\,,\\
\left.\frac{\partial^2 s}{\partial\beta^2}\right|_{\beta=0} &= \lim_{t\to\infty}\frac{1}{t}\left(\left\langle A^tA^t\right\rangle - \left\langle A^t\right\rangle\left\langle A^t\right\rangle\right)\\
&= \lim_{t\to\infty}\frac{1}{t}\left\langle (A^t - t\,\langle a\rangle)^2\right\rangle\,,
\end{aligned} \tag{15.12}$$

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and so forth. We have written out the formulas for a scalar observable; the vector case is worked out in the exercise 15.2. If we can compute the function $s(\beta)$, we have the desired expectation value without having to estimate any infinite time limits from finite time data.

Suppose we could evaluate $s(\beta)$ and its derivatives. What are such formulas good for? A typical application is to the problem of describing a particle scattering elastically off a 2-dimensional 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 $\left\langle x(t)^2\right\rangle \approx 4Dt$. In contrast to D estimated numerically from trajectories $x(t)$ for finite but large t, the above formulas yield the asymptotic D without any extrapolations to the $t \to \infty$ limit. For example, for $a_i = v_i$ and zero mean drift $\langle v_i\rangle = 0$, in d dimensions the diffusion constant is given by the curvature of $s(\beta)$ at $\beta = 0$,

$$D = \lim_{t\to\infty}\frac{1}{2dt}\left\langle x(t)^2\right\rangle = \frac{1}{2d}\sum_{i=1}^{d}\left.\frac{\partial^2 s}{\partial\beta_i^2}\right|_{\beta=0}\,, \tag{15.13}$$

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so if we can evaluate derivatives of $s(\beta)$, we can compute transport coefficients that characterize deterministic diffusion. As we shall see in chapter 23, periodic orbit theory yields an explicit closed form expression for D.

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15.1.3 Averaging in open systems

If the $\mathcal{M}$ is a compact region or set of regions to which the dynamics is confined for all times, (15.9) is a sensible definition of the expectation value. However, if the trajectories can exit $\mathcal{M}$ without ever returning,

$$\int_{\mathcal{M}} dy\,\delta(y - f^t(x_0)) = 0 \qquad \text{for } t > t_{exit}\,, \qquad x_0 \in \mathcal{M}\,,$$

we might be in trouble. In particular, for a repeller the trajectory $f^t(x_0)$ will eventually leave the region $\mathcal{M}$, unless the initial point x_0 is on the repeller, so the identity

$$\int_{\mathcal{M}} dy\,\delta(y - f^t(x_0)) = 1\,, \quad t > 0\,, \qquad \text{iff } x_0 \in \text{non–wandering set} \tag{15.14}$$

might apply only to a fractal subset of initial points a set of zero Lebesgue measure. Clearly, for open systems we need to modify the definition of the

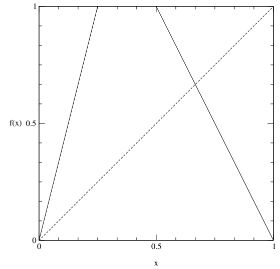

Figure 15.2: A piecewise-linear repeller (15.17): All trajectories that land in the gap between the f_0 and f_1 branches escape ($\Lambda_0 = 4$, $\Lambda_1 = -2$).

expectation value to restrict it to the dynamics on the non–wandering set, the set of trajectories which are confined for all times.

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Note by $\mathcal{M}$ a state space region that encloses all interesting initial points, say the 3-disk Poincaré section constructed from the disk boundaries and all possible incidence angles, and denote by $|\mathcal{M}|$ the volume of $\mathcal{M}$. The volume of the state space containing all trajectories which start out within the state space region $\mathcal{M}$ and recur within that region at the time t

$$|\mathcal{M}(t)| = \int_{\mathcal{M}} dxdy\, \delta\big(y - f^t(x)\big) \;\sim\; |\mathcal{M}|e^{-\gamma t} \tag{15.15}$$

is expected to decrease exponentially, with the escape rate γ. The integral over x takes care of all possible initial points; the integral over y checks whether their trajectories are still within $\mathcal{M}$ by the time t. For example, any trajectory that falls off the pinball table in figure 1.3 is gone for good.

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The non–wandering set can be very difficult object to describe; but for any finite time we can construct a normalized measure from the finite-time covering volume (15.15), by redefining the space average (15.10) as

$$\left\langle e^{\beta\cdot A^t}\right\rangle = \int_{\mathcal{M}} dx\, \frac{1}{|\mathcal{M}(t)|} e^{\beta\cdot A^t(x)} \sim \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} dx\, e^{\beta\cdot A^t(x)+\gamma t} \,. \tag{15.16}$$

in order to compensate for the exponential decrease of the number of surviving trajectories in an open system with the exponentially growing factor $e^{\gamma t}$. What does this mean? Once we have computed γ we can replenish the density lost to escaping trajectories, by pumping in $e^{\gamma t}$ in such a way that the overall measure is correctly normalized at all times, $\langle 1\rangle = 1$.

Example 15.1 A piecewise-linear repeller: *(continuation of example 14.1)* *What is gained by reformulating the dynamics in terms of "operators?" We start by considering a simple example in which the operator is a $[2\times 2]$ matrix. Assume the expanding 1-d map $f(x)$ of figure 15.2, a piecewise-linear 2–branch repeller with slopes $\Lambda_0 > 1$ and $\Lambda_1 < -1$:*

$$f(x) = \begin{cases} f_0 = \Lambda_0 x & \text{if } \; x \in \mathcal{M}_0 = [0, 1/\Lambda_0] \\ f_1 = \Lambda_1(x-1) & \text{if } \; x \in \mathcal{M}_1 = [1 + 1/\Lambda_1, 1] \end{cases} \,. \tag{15.17}$$

Both $f(\mathcal{M}_0)$ and $f(\mathcal{M}_1)$ map onto the entire unit interval $\mathcal{M} = [0,1]$. Assume a piecewise constant density

$$\rho(x) = \begin{cases} \rho_0 & \text{if } x \in \mathcal{M}_0 \\ \rho_1 & \text{if } x \in \mathcal{M}_1 \end{cases} \,. \tag{15.18}$$

There is no need to define $\rho(x)$ in the gap between $\mathcal{M}_0$ and $\mathcal{M}_1$, as any point that lands in the gap escapes.

The physical motivation for studying this kind of mapping is the pinball game: f is the simplest model for the pinball escape, figure 1.9, with f_0 and f_1 modelling its two strips of survivors.

As can be easily checked using (14.9), the Perron-Frobenius operator acts on this piecewise constant function as a [2×2] "transfer" matrix with matrix elements

$$\begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} \to \mathcal{L}\rho = \begin{pmatrix} \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \\ \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} , \tag{15.19}$$

stretching both ρ_0 and ρ_1 over the whole unit interval Λ, and decreasing the density at every iteration. In this example the density is constant after one iteration, so $\mathcal{L}$ has only one non-zero eigenvalue $e^{s_0} = 1/|\Lambda_0| + 1/|\Lambda_1|$, with constant density eigenvector $\rho_0 = \rho_1$. The quantities $1/|\Lambda_0|$, $1/|\Lambda_1|$ are, respectively, the sizes of the $|\mathcal{M}_0|$, $|\mathcal{M}_1|$ intervals, so the exact *escape rate (1.3) – the log of the fraction of survivors at each iteration for this linear repeller – is given by the sole eigenvalue of $\mathcal{L}$:*

$$\gamma = -s_0 = -\ln(1/|\Lambda_0| + 1/|\Lambda_1|) \,. \tag{15.20}$$

Voila! Here is the rationale for introducing operators – in one time step we have solved the problem of evaluating escape rates at infinite time. This simple explicit matrix representation of the Perron-Frobenius operator is a consequence of the piecewise linearity of f, and the restriction of the densities ρ to the space of piecewise constant functions. The example gives a flavor of the enterprise upon which we are about to embark in this book, but the full story is much subtler: in general, there will exist no such finite-dimensional representation for the Perron-Frobenius operator.

We now turn to the problem of evaluating $\left\langle e^{\beta\cdot A^t}\right\rangle$.

15.2 Evolution operators

The above simple shift of focus, from studying $\langle a\rangle$ to studying $\left\langle \exp\left(\beta\cdot A^t\right)\right\rangle$ is the key to all that follows. Make the dependence on the flow explicit by rewriting this quantity as

$$\left\langle e^{\beta\cdot A^t}\right\rangle = \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} dx \int_{\mathcal{M}} dy\; \delta\big(y - f^t(x)\big)\, e^{\beta\cdot A^t(x)} \,. \tag{15.21}$$

Here $\delta\big(y - f^t(x)\big)$ is the Dirac delta function: for a deterministic flow an initial point x maps into a unique point y at time t. Formally, all we have done above is to insert the identity

$$1 = \int_{\mathcal{M}} dy\; \delta\big(y - f^t(x)\big) \;, \tag{15.22}$$

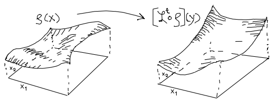

Figure 15.3: Space averaging pieces together the time average computed along the $t \to \infty$ trajectory of figure 15.1 by a space average over infinitely many short t trajectory segments starting at all initial points at once. (A. Johansen)

into (15.10) to make explicit the fact that we are averaging only over the trajectories that remain in $\mathcal{M}$ for all times. However, having made this substitution we have replaced the study of individual trajectories $f^t(x)$ by the study of the evolution of density of *the totality* of initial conditions. Instead of trying to extract a temporal average from an arbitrarily long trajectory which explores the phase space ergodically, we can now probe the entire state space with short (and controllable) finite time pieces of trajectories originating from every point in $\mathcal{M}$.

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As a matter of fact (and that is why we went to the trouble of defining the generator (14.27) of infinitesimal transformations of densities) *infinitesimally* short time evolution can suffice to determine the spectrum and eigenvalues of $\mathcal{L}^t$.

We shall refer to the kernel of the operation (15.21) as $\mathcal{L}^t(y,x)$.

$$\mathcal{L}^t(y,x) \;=\; \delta\big(y - f^t(x)\big)\; e^{\beta\cdot A^t(x)} \,. \tag{15.23}$$

The evolution operator acts on scalar functions $\phi(x)$ as

$$(y) = \int_{\mathcal{M}} dx\, \delta\big(y - f^t(x)\big)\, e^{\beta\cdot A^t(x)} \phi(x) \,. \tag{15.24}$$

In terms of the evolution operator, the space average of the generating function (15.21) is given by

$$\left\langle e^{\beta\cdot A^t} \right\rangle = \langle\rangle \;,$$

and, if the spectrum of the linear operator $\mathcal{L}^t$ can be described, by (15.11) this limit

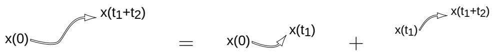
$$s(\beta) = \lim_{t\to\infty} \frac{1}{t} \ln \left\langle \mathcal{L}^t \right\rangle \,.$$

yields the leading eigenvalue of $s_0(\beta)$, and, through it, all desired expectation values (15.12).

The evolution operator is different for different observables, as its definition depends on the choice of the integrated observable A^t in the exponential.

Its job is deliver to us the expectation value of a, but before showing that it accomplishes that, we need to verify the semigroup property of evolution operators.

By its definition, the integral over the observable a is additive along the trajectory



$$\begin{aligned} A^{t_1+t_2}(x_0) &= \int_0^{t_1} d\tau \;+\; \int_{t_1}^{t_1+t_2} d\tau \\ &= A^{t_1}(x_0) \;+\; A^{t_2}(f^{t_1}(x_0)) \,. \end{aligned}$$

If $A^t(x)$ is additive along the trajectory, the evolution operator generates a semigroup

$$\mathcal{L}^{t_1+t_2}(y,x) = \int_{\mathcal{M}} dz\, \mathcal{L}^{t_2}(y,z)\mathcal{L}^{t_1}(z,x) \,, \tag{15.25}$$

as is easily checked by substitution

$$\mathcal{L}^{t_2}\mathcal{L}^{t_1}a(y) = \int_{\mathcal{M}} dx\, \delta(y - f^{t_2}(x)) e^{\beta\cdot A^{t_2}(x)} (\mathcal{L}^{t_1}a)(x) = \mathcal{L}^{t_1+t_2}a(y) \,.$$

This semigroup property is the main reason why (15.21) is preferable to (15.9) as a starting point for evaluation of dynamical averages: it recasts averaging in form of operators multiplicative along the flow.

15.3 Lyapunov exponents

(J. Mathiesen and P. Cvitanović)

Let us apply the newly acquired tools to the fundamental diagnostics in this subject: Is a given system "chaotic"? And if so, how chaotic? If all points in a neighborhood of a trajectory converge toward the same trajectory, the attractor is a fixed point or a limit cycle. However, if the attractor is strange, two trajectories

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$$x(t) = f^t(x_0) \quad \text{and} \quad x(t) + \delta x(t) = f^t(x_0 + \delta x(0)) \tag{15.26}$$

that start out very close to each other separate exponentially with time, and in a finite time their separation attains the size of the accessible state space. This *sensitivity to initial conditions* can be quantified as

$$|\delta x(t)| \approx e^{\lambda t} |\delta x(0)| \tag{15.27}$$

where λ, the mean rate of separation of trajectories of the system, is called the *Lyapunov exponent*.

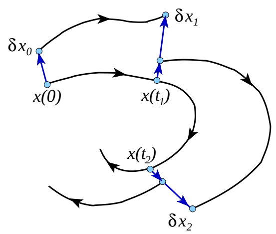

Figure 15.4: A long-time numerical calculation of the leading Lyapunov exponent requires rescaling the distance in order to keep the nearby trajectory separation within the linearized flow range.

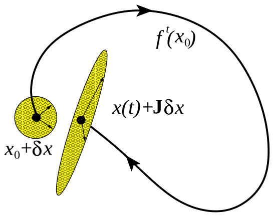

Figure 15.5: The symmetric matrix $\left(J^t\right)^T J^t$ maps a swarm of initial points in an infinitesimal spherical neighborhood of x_0 into a cigar-shaped neighborhood finite time t later, with semiaxes determined by the local stretching/shrinking $|\Lambda_1|$, but local individual trajectory rotations by the complex phase of J^t ignored.

15.3.1 Lyapunov exponent as a time average

We can start out with a small δx and try to estimate λ from (15.27), but now that we have quantified the notion of linear stability in chapter 4 and defined the dynamical time averages in sect. 15.1.1, we can do better. The problem with measuring the growth rate of the distance between two points is that as the points separate, the measurement is less and less a local measurement. In study of experimental time series this might be the only option, but if we have the equations of motion, a better way is to measure the growth rate of vectors transverse to a given orbit.

The mean growth rate of the distance $|\delta x(t)|/|\delta x(0)|$ between neighboring trajectories (15.27) is given by the *Lyapunov exponent*

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \ln |\delta x(t)|/|\delta x(0)| \tag{15.28}$$

(For notational brevity we shall often suppress the dependence of quantities such as $\lambda = \lambda(x_0)$, $\delta x(t) = \delta x(x_0, t)$ on the initial point x_0 and the time t). One can take (15.28) as is, take a small initial separation $\delta x(0)$, track distance between two nearby trajectories until $|\delta x(t_1)|$ gets significantly bigger, then record $t_1\lambda_1 = \ln(|\delta x(t_1)|/|\delta x(0)|)$, rescale $\delta x(t_1)$ by factor $|\delta x(0)|/|\delta x(t_1)|$, and continue add infinitum, with the leading Lyapunov exponent given by

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \sum_i t_i \lambda_i \,. \tag{15.29}$$

However, we can do better. Given the equations of motion and baring numerical problems (such as evaluating the fundamental matrix (4.43) for

high-dimensional flows), for infinitesimal δx we know the $\delta x_i(t)/\delta x_j(0)$ ratio exactly, as this is by definition the fundamental matrix (4.43)

$$\lim_{\delta x\to 0} \frac{\delta x_i(t)}{\delta x_j(0)} = \frac{\partial x_i(t)}{\partial x_j(0)} = J^t_{ij}(x_0)\,,$$

so the leading Lyapunov exponent can be computed from the linear approximation (4.28)

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \ln \frac{\left|J^t(x_0)\delta x(0)\right|}{|\delta x(0)|} = \lim_{t\to\infty} \frac{1}{2t} \ln \left| \hat{n}^T (J^t)^T J^t \hat{n} \right| \,. \tag{15.30}$$

In this formula the scale of the initial separation drops out, only its orientation given by the initial orientation unit vector $\hat{n} = \delta x/|\delta x|$ matters. The eigenvalues of J are either real or come in complex conjugate pairs. As J is in general not symmetric and not diagonalizable, it is more convenient to work with the symmetric and diagonalizable matrix $\mathbf{J} = (J^t)^T J^t$, with real positive eigenvalues $\{|\Lambda_1|^2 \geq \ldots \geq |\Lambda_d|^2\}$, and a complete orthonormal set of eigenvectors of $\{u_1, \ldots, u_d\}$. Expanding the initial orientation $\hat{n} = \sum(\hat{n}\cdot u_i)u_i$ in the $\mathbf{J}u_i = u_i$ eigenbasis, we have

$$\hat{n}^T \mathbf{J} \hat{n} = \sum_{i=1}^{d} (\hat{n}\cdot u_i)^2 |\Lambda_i|^2 = (\hat{n}\cdot u_1)^2 e^{2\lambda_1 t} \left(1 + O(e^{-2(\lambda_1-\lambda_2)t})\right), \tag{15.31}$$

where $t\lambda_i = \ln|\Lambda_i(x_0,t)|$, with exponents ordered by $\lambda_1 > \lambda_2 \geq \lambda_3 \cdots$. For long times the largest Lyapunov exponent dominates exponentially (15.30), provided the orientation $\hat{n}$ of the initial separation was not chosen perpendicular to the dominant expanding eigendirection u_1. The Lyapunov exponent is the time average

$$\begin{aligned} \overline{\lambda(x_0)} &= \lim_{t\to\infty} \frac{1}{t} \left\{ \ln|\hat{n}\cdot u_1| + \ln|\Lambda_1(x_0,t)| + O(e^{-2(\lambda_1-\lambda_2)t}) \right\} \\ &= \lim_{t\to\infty} \frac{1}{t} \ln|\Lambda_1(x_0,t)|\,, \end{aligned} \tag{15.32}$$

where $\Lambda_1(x_0,t)$ is the leading eigenvalue of $J^t(x_0)$. By choosing the initial displacement such that $\hat{n}$ is normal to the first (i-1) eigendirections we can define not only the leading, but all Lyapunov exponents as well:

$$\overline{\lambda_i(x_0)} = \lim_{t\to\infty} \frac{1}{t} \ln|\Lambda_i(x_0,t)|\,, \qquad i = 1, 2, \cdots, d\,. \tag{15.33}$$

The leading Lyapunov exponent now follows from the fundamental matrix by numerical integration of (4.9).

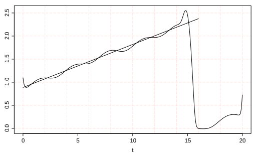

Figure 15.6: A numerical estimate of the leading Lyapunov exponent for the Rössler system (2.17) from the dominant expanding eigenvalue formula (15.30). The leading Lyapunov exponent $\lambda \approx 0.09$ is positive, so numerics supports the hypothesis that the Rössler attractor is strange. (J. Mathiesen)

The equations can be integrated accurately for a finite time, hence the infinite time limit of (15.30) can be only estimated from plots of $\frac{1}{2}\ln|\hat{n}^T\mathbf{J}\hat{n}|$ as function of time, such as the figure 15.6 for the Rössler system (2.17).

As the local expansion and contraction rates vary along the flow, the temporal dependence exhibits small and large humps. The sudden fall to a low level is caused by a close passage to a folding point of the attractor, an illustration of why numerical evaluation of the Lyapunov exponents, and proving the very existence of a strange attractor is a very difficult problem. The approximately monotone part of the curve can be used (at your own peril) to estimate the leading Lyapunov exponent by a straight line fit.

As we can already see, we are courting difficulties if we try to calculate the Lyapunov exponent by using the definition (15.32) directly. First of all, the state space is dense with atypical trajectories; for example, if x_0 happened to lie on a periodic orbit p, $\overline{\lambda}$ would be simply $\ln|\Lambda_p|/T_p$, a local property of cycle p, not a global property of the dynamical system. Furthermore, even if x_0 happens to be a "generic" state space point, it is still not obvious that $\ln|\Lambda(x_0,t)|/t$ should be converging to anything in particular. In a Hamiltonian system with coexisting elliptic islands and chaotic regions, a chaotic trajectory gets every so often captured in the neighborhood of an elliptic island and can stay there for arbitrarily long time; as there the orbit is nearly stable, during such episode $\ln|\Lambda(x_0,t)|/t$ can dip arbitrarily close to 0^+. For state space volume non-preserving flows the trajectory can traverse locally contracting regions, and $\ln|\Lambda(x_0,t)|/t$ can occasionally go negative; even worse, one never knows whether the asymptotic attractor is periodic or "strange", so any finite estimate of $\overline{\lambda}$ might be dead wrong.

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15.3.2 Evolution operator evaluation of Lyapunov exponents

A cure to these problems was offered in sect. 15.2. We shall now replace time averaging along a single trajectory by action of a multiplicative evolution operator on the entire state space, and extract the Lyapunov exponent from its leading eigenvalue. If the chaotic motion fills the whole state space, we are indeed computing the asymptotic Lyapunov exponent. If the chaotic motion is transient, leading eventually to some long attractive cycle, our Lyapunov exponent, computed on nonwandering set, will characterize the chaotic transient; this is actually what any experiment would measure, as even very small amount of external noise will suffice to destabilize a long stable cycle with a minute immediate basin of attraction.

Due to the chain rule (4.51) for the derivative of an iterated map, the stability of a 1-d mapping is multiplicative along the flow, so the integral (15.1) of the observable $a(x) = \ln|f'(x)|$, the local trajectory divergence rate, evaluated along the trajectory of x_0 is additive:

$$A^n(x_0) = \ln\left|f^{n\prime}(x_0)\right| = \sum_{k=0}^{n-1} \ln\left|f'(x_k)\right| . \tag{15.34}$$

The Lyapunov exponent is then the expectation value (15.9) given by a spatial integral (15.8) weighted by the natural measure

$$\lambda = \left\langle \ln|f'(x)|\right\rangle = \int_{\mathcal{M}} dx\, \rho_0(x) \ln|f'(x)| . \tag{15.35}$$

The associated (discrete time) evolution operator (15.23) is

appendix G.1

$$\mathcal{L}(y,x) \;=\; \delta(y - f(x))\; e^{\beta \ln|f'(x)|} . \tag{15.36}$$

Here we have restricted our considerations to $1-d$ maps, as for higher-dimensional flows only the fundamental matrices are multiplicative, not the individual eigenvalues. Construction of the evolution operator for evaluation of the Lyapunov spectra in the general case requires more cleverness than warranted at this stage in the narrative: an extension of the evolution equations to a flow in the tangent space.

in depth:
appendix G.1, p. 755

All that remains is to determine the value of the Lyapunov exponent

$$\lambda = \left\langle \ln|f'(x)|\right\rangle = \left.\frac{\partial s(\beta)}{\partial \beta}\right|_{\beta=1} = s'(1) \tag{15.37}$$

example 18.1

from (15.12), the derivative of the leading eigenvalue $s_0(\beta)$ of the evolution operator (15.36).

The only question is: how?

Résumé

The expectation value $\langle a\rangle$ of an observable $a(x)$ measured $A^t(x) = \int_0^t d\tau a(x(\tau))$ and averaged along the flow $x \to f^t(x)$ is given by the derivative

$$\langle a\rangle = \left.\frac{\partial s}{\partial \beta}\right|_{\beta=0}$$

of the leading eigenvalue $e^{ts(\beta)}$ of the corresponding evolution operator $\mathcal{L}^t$.

Instead of using the Perron-Frobenius operator (14.10) whose leading eigenfunction, the natural measure, once computed, yields expectation value (14.20) of any observable $a(x)$, we construct a specific, hand-tailored evolution operator $\mathcal{L}$ for each and every observable. However, by time we arrive to chapter 18, the scaffolding will be removed, both $\mathcal{L}$'s and their eigenfunctions will be gone, and only the explicit and exact periodic orbit formulas for expectation values of observables will remain.

chapter 18

The next question is: how do we evaluate the eigenvalues of $\mathcal{L}$? We saw in example 15.1, in the case of piecewise-linear dynamical systems, that these operators reduce to finite matrices, but for generic smooth flows, they are infinite-dimensional linear operators, and finding smart ways of computing their eigenvalues requires some thought. In chapter 10 we undertook the first step, and replaced the *ad hoc* partitioning (14.14) by the intrinsic, topologically invariant partitioning. In chapter 13 we applied this information to our first application of the evolution operator formalism, evaluation of the topological entropy, the growth rate of the number of topologically distinct orbits. This small victory will be refashioned in chapters 16 and 17 into a systematic method for computing eigenvalues of evolution operators in terms of periodic orbits.

Commentary

Remark 15.1 "Pressure". The quantity $\langle \exp(\beta \cdot A^t) \rangle$ is called a "partition function" by Ruelle [17.1]. Mathematicians decorate it with considerably more Greek and Gothic letters than is the case in this treatise. Ruelle [17.2] and Bowen [15.1] had given name "pressure" $P(a)$ to $s(\beta)$ (where a is the observable introduced here in sect. 15.1.1), defined by the "large system" limit (15.11). As we shall apply the theory also to computation of the physical gas pressure exerted on the walls of a container by a bouncing particle, we prefer to refer to $s(\beta)$ as simply the leading eigenvalue of the evolution operator introduced in sect. 14.5. The "convexity" properties such as $P(a) \leq P(|a|)$ will be pretty obvious consequence of the definition (15.11). In the case that $\mathcal{L}$ is the Perron-Frobenius operator (14.10), the eigenvalues $\{s_0(\beta), s_1(\beta), \cdots\}$ are called the *Ruelle-Pollicott resonances* [15.2, 15.3, 15.4], with the leading one, $s(\beta) = s_0(\beta)$ being the one of main physical interest. In order to aid the reader in digesting the mathematics literature, we shall try to point out the notational correspondences whenever appropriate. The rigorous formalism is replete with lims, sups, infs, Ω-sets which are not really essential to understanding the physical applications of the theory, and are avoided in this presentation.

Remark 15.2 Microcanonical ensemble. In statistical mechanics the space average (15.7) performed over the Hamiltonian system constant energy surface invariant measure $\rho(x)dx = dqdp\,\delta(H(q,p)-E)$ of volume $\omega(E) = \int_{\mathcal{M}} dqdp\,\delta(H(q,p)-E)$

$$\langle a(t) \rangle = \frac{1}{\omega(E)} \int_{\mathcal{M}} dqdp\,\delta(H(q,p)-E) a(q,p,t) \qquad (15.38)$$

is called the *microcanonical ensemble average*.

Remark 15.3 Lyapunov exponents. The Multiplicative Ergodic Theorem of Oseledec [15.5] states that the limits (15.30–15.33) exist for almost all points x_0 and all tangent vectors $\hat{n}$. There are at most d distinct values of λ as we let $\hat{n}$ range over the tangent space. These are the Lyapunov exponents [15.7] $\lambda_i(x_0)$.

There is much literature on numerical computation of the Lyapunov exponents, see for example refs. [**?**, 15.13, 15.14, 15.15].

Remark 15.4 State space discretization. Ref. [15.16] discusses numerical discretizatons of state space, and construction of Perron-Frobenius operators as stochastic matrices, or directed weighted graphs, as coarse-grained models of the global dynamics, with transport rates between state space partitions computed using this matrix of transition probabilities; a rigorous discussion of some of the former features is included in Ref. [15.17].

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