

Chapter 17

Averaging

Why think when you can compute?
—Maciej Zworski

WE DISCUSS FIRST the necessity of studying the averages of observables in chaotic dynamics. A time average of an observable is computed by integrating its value along a trajectory. The integral along trajectory can be split into a sum of over integrals evaluated on trajectory segments; if exponentiated, this yields a *multiplicative* weight for successive trajectory segments. This elementary observation will enable us to recast 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. 17.3 we try out the formalism on the first quantitative diagnosis whether a system is chaotic, the Lyapunov exponent.

17.1 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 after a finite Lyapunov time (1.1). Hence for chaotic dynamics one cannot follow individual trajectories for a long time; what is attainable, however, is a description of the geometry of the set of possible outcomes, and the evaluation of long-time averages. Examples of such averages are transport coefficients for chaotic dynamical flows, such as escape rates, mean drifts and diffusion rates; 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.

17.1.1 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. The observable 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 ,

$$A^t(x_0) = \int_0^t d\tau a(x(\tau)), \quad x(t) = f^t(x_0). \quad (17.1)$$

If the dynamics are given by an iterated mapping and the time is discrete, the integrated observable after n iterations is given by

$$A^n(x_0) = \sum_{k=0}^{n-1} a(x_k), \quad x_k = f^k(x_0) \quad (17.2)$$

(we suppress vectorial indices for the time being).

Example 17.1 Integrated observables. If the observable is the velocity, $a_i(x) = v_i(x)$, its time integral $A_i^t(x_0)$ is the trajectory $A_i^t(x_0) = x_i(t)$.

For Hamiltonian flows the action associated with a trajectory $x(t) = [q(t), p(t)]$ passing through a phase-space point $x_0 = [q(0), p(0)]$ is:

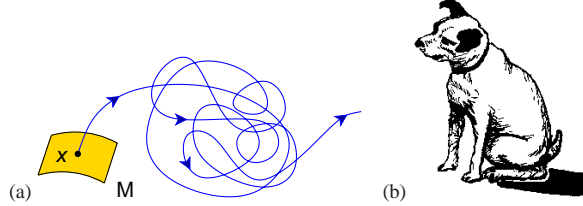
$$A^t(x_0) = \int_0^t d\tau \dot{q}(\tau) \cdot p(\tau). \quad (17.3)$$

The *time average* of the observable along an orbit is defined by

$$\overline{a(x_0)} = \lim_{t \rightarrow \infty} \frac{1}{t} A^t(x_0). \quad (17.4)$$

If a does not behave too wildly as a function of time – for example, if $a_i(x)$ is the Chicago temperature, bounded between $-80^\circ F$ and $+130^\circ F$ for all times – $A^t(x_0)$ is expected to grow no faster than t , and the limit (17.4) exists. For an example of a time average - the Lyapunov exponent - see sect. 17.3.

Figure 17.1: (a) A typical chaotic trajectory explores the state 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)



The time average is a property of the orbit, independent of the initial point on that orbit: 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 $t \rightarrow \infty$ limit:

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

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

exercise 4.6

$$A_p = \begin{cases} a_p T_p = \int_0^{T_p} d\tau a(f^\tau(x_0)) & \text{for a flow} \\ a_p n_p = \sum_{i=1}^{n_p} a(f^i(x_0)) & \text{for a map} \end{cases}, \quad x_0 \in \mathcal{M}_p, \quad (17.5)$$

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. The quantity 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 $x_0 \in \mathcal{M}_p$. (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 (17.4) therefore requires only a single traversal of the cycle:

$$a_p = A_p / T_p. \quad (17.6)$$

However, $\overline{a(x_0)}$ is in general a wild function of x_0 ; for a hyperbolic system it takes the same value $\langle a \rangle$ for almost all initial x_0 , but a different value (17.6) on any periodic orbit, i.e., on a dense set of points (figure 17.1 (b)).

Example 17.2 Deterministic diffusion. The phase space of an open system such as the Sinai gas (an infinite 2-dimensional periodic array of scattering disks, see sect. 25.1) 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 $D \propto x(t)^2/t$, (17.4) 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.

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. (continued in example 17.3)

17.1.2 Space averages

The space average of a quantity a evaluated over all state space trajectories $x(t)$ at time t is given by the d -dimensional integral over the d coordinates of the dynamical system:

$$\begin{aligned} \langle a \rangle(t) &= \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx_0 a(f^t(x)), \quad x(t) = f^t(x_0) \\ |\mathcal{M}| &= \int_{\mathcal{M}} dx = \text{volume of } \mathcal{M}. \end{aligned} \quad (17.7)$$

The space \mathcal{M} is assumed to have finite volume - open systems like the 3-disk game of pinball are discussed in sect. 17.3.3.

What is it we really do in experiments? We cannot measure the time average (17.4), as there is no way to prepare a single initial condition with infinite precision. The best we can do is prepare an initial density $\rho(x)$, perhaps concentrated on some small (but always finite) neighborhood. Then we can abandon the uniform space average (17.7) and consider instead

$$\langle a \rangle_\rho(t) = \frac{1}{|\mathcal{M}_\rho|} \int_{\mathcal{M}} dx_0 \rho(x_0) a(x(t)), \quad |\mathcal{M}_\rho| = \int_{\mathcal{M}} dx \rho(x). \quad (17.8)$$

For ergodic mixing systems, any smooth initial density will tend to the asymptotic natural measure in the $t \rightarrow \infty$ limit $\rho(x, t) \rightarrow \rho_0(x)$. This allows us to take any smooth initial $\rho(x)$ and define the expectation value $\langle a \rangle$ of an observable a as the asymptotic time and space average over the state space \mathcal{M}

$$\langle a \rangle = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx \overline{a(x)} = \lim_{t \rightarrow \infty} \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx \frac{1}{t} \int_0^t d\tau a(f^\tau(x)). \quad (17.9)$$

We use the same $\langle \cdot \cdot \rangle$ notation as for the space average (17.7) 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 is the infinite time limit, 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

$$\langle e^{\beta \cdot A^t} \rangle = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx e^{\beta \cdot A^t(x)}. \tag{17.10}$$

In the present context β is an auxiliary variable of no physical significance whose role is to enable us to recover the desired space average by differentiation,

$$\langle A^t \rangle = \frac{\partial}{\partial \beta} \langle e^{\beta \cdot A^t} \rangle \Big|_{\beta=0}.$$

In most applications β is a scalar, but if the observable is a d -dimensional vector $a(x) \in \mathbb{R}^d$, then $\beta \in \mathbb{R}^d$; 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 β .

If the limit $\overline{a(x_0)}$ for the time average (17.4) 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 \bar{a} , and the integrated observable A^t to tend to $t\bar{a}$. The space average (17.10) is an integral over exponentials, and such integral also grows exponentially with time. So as $t \rightarrow \infty$ we would expect the space average of $\exp(\beta \cdot A^t(x))$ to grow exponentially with time

$$\langle e^{\beta \cdot A^t} \rangle \rightarrow (\text{const}) e^{ts(\beta)},$$

and its rate of growth to be given by the limit

$$s(\beta) = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \langle e^{\beta \cdot A^t} \rangle. \tag{17.11}$$

Now we understand one reason for why it is smarter to compute $\langle \exp(\beta \cdot A^t) \rangle$ rather than $\langle a \rangle$: the expectation value of the observable (17.9) and the moments of the integrated observable (17.1) can be computed by evaluating the derivatives of $s(\beta)$

$$\begin{aligned} \frac{\partial s}{\partial \beta} \Big|_{\beta=0} &= \lim_{t \rightarrow \infty} \frac{1}{t} \langle A^t \rangle = \langle a \rangle, \\ \frac{\partial^2 s}{\partial \beta^2} \Big|_{\beta=0} &= \lim_{t \rightarrow \infty} \frac{1}{t} (\langle A^t A^t \rangle - \langle A^t \rangle \langle A^t \rangle) \\ &= \lim_{t \rightarrow \infty} \frac{1}{t} \langle (A^t - t \langle a \rangle)^2 \rangle, \end{aligned} \tag{17.12}$$

and so forth. We have written out the formulas for a scalar observable; the vector case is worked out in the exercise 17.2. 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 determining transport coefficients from underlying deterministic dynamics.

Example 17.3 Deterministic diffusion. (continued from example 17.2) Consider a point particle scattering elastically off a d -dimensional array of scatterers. If the scatterers 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 $\langle x(t)^2 \rangle \approx 4Dt$. 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 $t \rightarrow \infty$ 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 $\beta = 0$, section 25.1

$$D = \lim_{t \rightarrow \infty} \frac{1}{2dt} \langle x(t)^2 \rangle = \frac{1}{2d} \sum_{i=1}^d \frac{\partial^2 s}{\partial \beta_i^2} \Big|_{\beta=0}, \tag{17.13}$$

so if we can evaluate derivatives of $s(\beta)$, we can compute transport coefficients that characterize deterministic diffusion. As we shall see in chapter 25, periodic orbit theory yields an exact and explicit closed form expression for D .



fast track:
sect. 17.2, p. 353

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

17.2 Evolution operators

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

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

$$\langle e^{\beta \cdot A^t} \rangle = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx \int_{\mathcal{M}} dy \delta(y - f^t(x)) e^{\beta \cdot A^t(x)}. \tag{17.14}$$

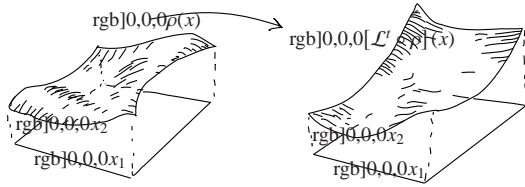


Figure 17.2: Space averaging pieces together the time average computed along the $t \rightarrow \infty$ orbit of figure 17.1 by a space average over infinitely many short t trajectory segments starting at all initial points at once.

Here $\delta(y - f^t(x))$ 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

$$1 = \int_{\mathcal{M}} dy \delta(y - f^t(x)), \tag{17.15}$$

into (17.10) 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 state 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} .

As a matter of fact (and that is why we went to the trouble of defining the generator (16.27) of infinitesimal transformations of densities) *infinitesimally* short time evolution induced by the generator \mathcal{A} of (16.27) suffices to determine the spectrum and eigenvalues of \mathcal{L}^t .

We shall refer to the kernel of the operation (17.14) as the *evolution operator*

$$\mathcal{L}^t(y, x) = \delta(y - f^t(x)) e^{\beta \mathcal{A}^t(x)}. \tag{17.16}$$

The simplest example is the $\beta = 0$ case, i.e., the Perron-Frobenius operator introduced in sect. 16.2. Another example - designed to deliver the Lyapunov exponent - will be the evolution operator (17.30) discussed below. The action of the evolution operator on a function ϕ is given by

$$(\mathcal{L}^t \phi)(y) = \int_{\mathcal{M}} dx \delta(y - f^t(x)) e^{\beta \mathcal{A}^t(x)} \phi(x). \tag{17.17}$$

In terms of the evolution operator, the space average of the generating function (17.14) is given by

$$\langle e^{\beta \mathcal{A}^t} \rangle = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx \int_{\mathcal{M}} dy \phi(y) \mathcal{L}^t(y, x) \phi(x).$$

where $\phi(x)$ is the constant function $\phi(x) = 1$. If the linear operator \mathcal{L}^t can be thought of as a matrix, high powers of a matrix are dominated by its fastest growing matrix elements, and the limit (17.11)

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

yields the leading eigenvalue of $s_0(\beta)$, and, through it, all desired expectation values (17.12).

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

$$\begin{aligned} \int_{x(0)}^{x(t_1+t_2)} a(f^\tau(x)) d\tau &= \int_{x(0)}^{x(t_1)} a(f^\tau(x)) d\tau + \int_{x(t_1)}^{x(t_1+t_2)} a(f^\tau(x)) d\tau \\ A^{t_1+t_2}(x_0) &= A^{t_1}(x_0) + A^{t_2}(f^{t_1}(x_0)). \end{aligned}$$

exercise 16.3

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

section 16.5

$$\mathcal{L}^{t_1+t_2}(y, x) = \int_{\mathcal{M}} dz \mathcal{L}^{t_2}(y, z) \mathcal{L}^{t_1}(z, x), \tag{17.18}$$

as is easily checked by substitution

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

This semigroup property is the main reason why (17.14) is preferable to (17.9) as a starting point for evaluation of dynamical averages: it recasts averaging in form of operators multiplicative along the flow.

17.2.1 Resolvent of \mathcal{L}

Here we limit ourselves to a brief remark about the notion of the “spectrum” of a linear operator.

The Perron-Frobenius operator \mathcal{L} acts multiplicatively in time, so it is reasonable to suppose that there exist constants $M > 0, \beta \geq 0$ such that $\|\mathcal{L}^t\| \leq M e^{t\beta}$

for all $t \geq 0$. What does that mean? The operator norm is defined in the same spirit in which one defines matrix norms: We are assuming that no value of $\mathcal{L}^t \rho(x)$ grows faster than exponentially for any choice of function $\rho(x)$, so that the fastest possible growth can be bounded by $e^{t\beta}$, a reasonable expectation in the light of the simplest example studied so far, the exact escape rate (17.35). If that is so, multiplying \mathcal{L}^t by $e^{-t\beta}$ we construct a new operator $e^{-t\beta} \mathcal{L}^t = e^{t(\mathcal{A}-\beta)}$ which decays exponentially for large t , $\|e^{t(\mathcal{A}-\beta)}\| \leq M$. We say that $e^{-t\beta} \mathcal{L}^t$ is an element of a bounded semigroup with generator $\mathcal{A} - \beta I$. Given this bound, it follows by the Laplace transform

$$\int_0^\infty dt e^{-st} \mathcal{L}^t = \frac{1}{s - \mathcal{A}}, \quad \text{Re } s > \beta, \quad (17.19)$$

that the *resolvent* operator $(s - \mathcal{A})^{-1}$ is bounded (“resolvent” = able to cause separation into constituents)

$$\left\| \frac{1}{s - \mathcal{A}} \right\| \leq \int_0^\infty dt e^{-st} M e^{t\beta} = \frac{M}{s - \beta}.$$

If one is interested in the spectrum of \mathcal{L} , as we will be, the resolvent operator is a natural object to study; it has no time dependence, and it is bounded. The main lesson of this brief aside is that for continuous time flows, the Laplace transform is the tool that brings down the generator in (16.29) into the resolvent form (17.19) and enables us to study its spectrum.

17.3 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, any two trajectories

example 2.3
section 1.3.1

$$x(t) = f^t(x_0) \quad \text{and} \quad x(t) + \delta x(t) = f^t(x_0 + \delta x_0) \quad (17.20)$$

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

$$|\delta x(t)| \approx e^{\lambda t} |\delta x_0| \quad (17.21)$$

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

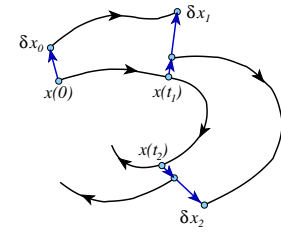


Figure 17.3: A long-time numerical calculation of the leading Lyapunov exponent requires rescaling the distance in order to keep the nearby trajectory separation within the linearized flow range.

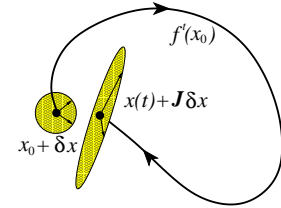


Figure 17.4: The symmetric matrix $\mathbf{J} = (J^t)^T J$ maps a swarm of initial points in an infinitesimal spherical neighborhood of x_0 into a cigar-shaped neighborhood finite time t later, with semiaxes determined by the local stretching/shrinking $|\Lambda_i|$, but local individual trajectory rotations by the complex phase of J^t ignored.

17.3.1 Lyapunov exponent as a time average

We can start out with a small δx and try to estimate λ from (17.21), but now that we have quantified the notion of linear stability in chapter 4 and defined the dynamical time averages in sect. 17.1.1, 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 (17.21) is given by the *Lyapunov exponent*

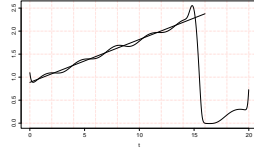
$$\lambda = \lim_{t \rightarrow \infty} \frac{1}{t} \ln |\delta x(t)|/|\delta x_0| \quad (17.22)$$

(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/or the time t). One can take (17.22) as is, take a small initial separation δx_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, as in figure 17.3, with the leading Lyapunov exponent given by

$$\lambda = \lim_{t \rightarrow \infty} \frac{1}{t} \sum_i t_i \lambda_i. \quad (17.23)$$

However, we can do better. Given the equations of motion, for infinitesimal δx we know the $\delta x_i(t)/\delta x_j(0)$ ratio exactly, as this is by definition the Jacobian matrix

Figure 17.5: A numerical estimate of the leading Lyapunov exponent for the Rössler flow (2.17) from the dominant expanding eigenvalue formula (17.24). The leading Lyapunov exponent $\lambda \approx 0.09$ is positive, so numerics supports the hypothesis that the Rössler attractor is strange. (J. Mathiesen)



(4.38)

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

so the leading Lyapunov exponent can be computed from the linear approximation (4.23)

$$\overline{\lambda(x_0)} = \lim_{t \rightarrow \infty} \frac{1}{t} \ln \frac{|J^t(x_0)\delta x_0|}{|\delta x_0|} = \lim_{t \rightarrow \infty} \frac{1}{2t} \ln (\hat{n}^T (J^t)^T J^t \hat{n}). \quad (17.24)$$

In this formula the scale of the initial separation drops out, only its orientation given by the initial orientation unit vector $\hat{n} = \delta x_0/|\delta x_0|$ 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 $\mathbf{M} = (J^t)^T J^t$, with real positive eigenvalues $\{|\Lambda_1|^2 \geq \dots \geq |\Lambda_d|^2\}$, and a complete orthonormal set of eigenvectors $\{u_1, \dots, u_d\}$. Expanding the initial orientation $\hat{n} = \sum (\hat{n} \cdot u_i)u_i$ in the $\mathbf{M}u_i = |\Lambda_i|^2 u_i$ eigenbasis, we have

$$\hat{n}^T \mathbf{M} \hat{n} = \sum_{i=1}^d (\hat{n} \cdot u_i)^2 |\Lambda_i|^2 = (\hat{n} \cdot u_1)^2 e^{2\mu_1 t} (1 + O(e^{-2(\mu_1 - \mu_2)t})), \quad (17.25)$$

where $\ln |\Lambda_i(x_0, t)| = t\mu_i$, with real parts of characteristic exponents (4.18) ordered by $\mu_1 > \mu_2 \geq \mu_3 \dots$. For long times the largest Lyapunov exponent dominates exponentially (17.24), provided the orientation \hat{n} of the initial separation was not chosen perpendicular to the dominant expanding eigen-direction u_1 . The Lyapunov exponent is the time average

$$\begin{aligned} \overline{\lambda(x_0)} &= \lim_{t \rightarrow \infty} \frac{1}{t} \left\{ \ln |\hat{n} \cdot u_1| + \ln |\Lambda_1(x_0, t)| + O(e^{-2(\lambda_1 - \lambda_2)t}) \right\} \\ &= \lim_{t \rightarrow \infty} \frac{1}{t} \ln |\Lambda_1(x_0, t)|, \end{aligned} \quad (17.26)$$

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 $(i-1)$ eigen-directions we can define not only the leading, but all Lyapunov exponents as well:

$$\overline{\lambda_i(x_0)} = \lim_{t \rightarrow \infty} \frac{1}{t} \ln |\Lambda_i(x_0, t)|, \quad i = 1, 2, \dots, d. \quad (17.27)$$

The leading Lyapunov exponent now follows from the Jacobian matrix by numerical integration of (4.9). The equations can be integrated accurately for a finite time, hence the infinite time limit of (17.24) can be only estimated from plots of $\frac{1}{2} \ln(\hat{n}^T \mathbf{M} \hat{n})$ as function of time, such as figure 17.5 for the Rössler flow (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 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 (17.26) 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 , $\bar{\lambda}$ 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 captured in the neighborhood of an elliptic island every so often 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 $\bar{\lambda}$ might be dead wrong.

exercise 17.1

17.3.2 Evolution operator evaluation of Lyapunov exponents

A solution to these problems was proposed in sect. 17.2 - replace time averaging along a single orbit by action of a multiplicative evolution operator on the entire state space, and extract average of the Lyapunov exponent from its leading eigenvalue. from finite length cycles. 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 a non-wandering set, will characterize the chaotic transient; this is actually what any experiment would measure, as even a very small amount of external noise will suffice to destabilize a long stable cycle with a minute immediate basin of attraction. The main idea - what is the Lyapunov ‘observable’ - can be illustrated by the dynamics of a 1-dimensional map.

Example 17.4 Lyapunov exponent, discrete time 1-dimensional dynamics. Due to the chain rule (4.47) for the derivative of an iterated map, the stability of a 1 - dimensional mapping is multiplicative along the flow, so the integral (17.1) of the observable $a(x) = \ln |f'(x)|$, the local trajectory divergence rate, evaluated along the trajectory

of x_0 is additive:

$$A^n(x_0) = \ln |f^{n'}(x_0)| = \sum_{k=0}^{n-1} \ln |f'(x_k)|. \tag{17.28}$$

The Lyapunov exponent is then the expectation value (17.9) given by a spatial integral (17.8) weighted by the natural measure

$$\lambda = \langle \ln |f'(x)| \rangle = \int_{\mathcal{M}} dx \rho_0(x) \ln |f'(x)|. \tag{17.29}$$

The associated (discrete time) evolution operator (17.16) is

$$\mathcal{L}(y, x) = \delta(y - f(x)) e^{\beta \ln |f'(x)|}. \tag{17.30}$$

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

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

$$\lambda = \langle \ln |f'(x)| \rangle = \left. \frac{\partial s(\beta)}{\partial \beta} \right|_{\beta=0} = s'(0) \tag{17.31}$$

from (17.12), the derivative of the leading eigenvalue $s_0(\beta)$ of the evolution operator (17.30).

example 20.1

The only question is: how? (By chapter 20 you will know.)

17.3.3 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, (17.9) is a sensible definition of the expectation value. However, if the trajectories can exit \mathcal{M} without ever returning,

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

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

$$\int_{\mathcal{M}} dy \delta(y - f^t(x_0)) = 1, \quad t > 0, \quad \text{iff } x_0 \in \text{non-wandering set} \tag{17.32}$$

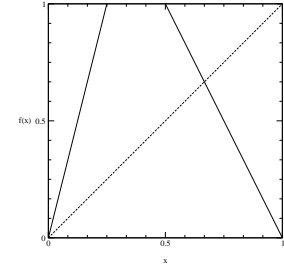


Figure 17.6: A piecewise-linear repeller (16.11): All trajectories that land in the gap between the f_0 and f_1 branches escape ($\Lambda_0 = 4$, $\Lambda_1 = -2$).

might apply only to a fractal subset of initial points of zero Lebesgue measure (non-wandering sets defined in sect. 2.1.1). Clearly, for open systems we need to modify the definition of the expectation value to restrict it to the dynamics on the non-wandering set, the set of trajectories which are confined for all times.

Denote 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 ,

$$|\mathcal{M}(t)| = \int_{\mathcal{M}} dx dy \delta(y - f^t(x)) \sim |\mathcal{M}| e^{-\gamma t} \tag{17.33}$$

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 1.1 is gone for good.

section 1.4.3

section 22.1

The non-wandering set can be very difficult to describe; but for any finite time we can construct a normalized measure from the finite-time covering volume (17.33), by redefining the space average (17.10) as

$$\langle e^{\beta \cdot A^t} \rangle = \int_{\mathcal{M}} dx \frac{1}{|\mathcal{M}(t)|} e^{\beta \cdot A^t(x)} \sim \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} dx e^{\beta \cdot A^t(x) + \gamma t}. \tag{17.34}$$

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 $e^{\gamma t}$ of new trajectories in such a way that the overall measure is correctly normalized at all times, $\langle 1 \rangle = 1$.

Example 17.5 Escape rate for a piecewise-linear repeller: (continuation of example 16.1) 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 – dimensional map $f(x)$ of figure 17.6, a piecewise-linear 2–branch repeller (16.11). Assume a piecewise constant density (16.12). There is no need to define $\rho(x)$ in the gap between M_0 and 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 1.8, with f_0 and f_1 modelling its two strips of survivors.

As can be easily checked using (16.9), the Perron-Frobenius operator acts on this piecewise constant function as a [2x2] “transfer” matrix (16.13) exercise 16.1
exercise 16.5

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

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 $e^{s_0} = 1/|\Lambda_0| + 1/|\Lambda_1| \leq 1$, with constant density eigenvector $\rho_0 = \rho_1$. The quantities $1/|\Lambda_0|, 1/|\Lambda_1|$ are, respectively, the sizes of the $|M_0|, |M_1|$ 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} :

$$\gamma = -s_0 = -\ln(1/|\Lambda_0| + 1/|\Lambda_1|). \tag{17.35}$$

Voila! Here is the rationale for introducing operators – in one time step we have solved the problem of evaluating escape rates at infinite time. (continued in example 23.5)

Résumé

The expectation value $\langle a \rangle$ of an observable $a(x)$ integrated, $A^t(x) = \int_0^t d\tau a(x(\tau))$, and time averaged, A^t/t , over the trajectory $x \rightarrow x(t)$ is given by the derivative

$$\langle a \rangle = \frac{\partial s}{\partial \beta} \Big|_{\beta=0}$$

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

By computing the leading eigenfunction of the Perron-Frobenius operator (16.10), one obtains the expectation value (16.20) of any observable $a(x)$. Thus we can construct a specific, hand-tailored evolution operator \mathcal{L} for each and every observable. The good news is that, by time we arrive to chapter 20, 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 20

The next question is: how do we evaluate the eigenvalues of \mathcal{L} ? In example 17.5, we saw a piecewise-linear example where these operators reduce to finite matrices \mathbf{L} , but for generic smooth flows, they are infinite-dimensional linear

operators, and finding smart ways of computing their eigenvalues requires some thought. In chapter 11 we undertook the first step, and replaced the *ad hoc* partitioning (16.14) by the intrinsic, topologically invariant partitioning. In chapter 15 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 18 and 19 into a systematic method for computing eigenvalues of evolution operators in terms of periodic orbits.

Commentary

Remark 17.1 ‘Pressure’. The quantity $\langle \exp(\beta \cdot A^t) \rangle$ is called a “partition function” by Ruelle [19.1]. Mathematicians decorate it with considerably more Greek and Gothic letters than is the case in this treatise. Ruelle [17.1] and Bowen [17.2] had given name “pressure” $P(a)$ to $s(\beta)$ (where a is the observable introduced here in sect. 17.1.1), defined by the “large system” limit (17.11). 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. 16.5. The “convexity” properties such as $P(a) \leq P(|a|)$ will be pretty obvious consequence of the definition (17.11). In the case that \mathcal{L} is the Perron-Frobenius operator (16.10), the eigenvalues $\{s_0(\beta), s_1(\beta), \dots\}$ are called the *Ruelle-Pollicott resonances* [17.3, 17.4, 17.5], 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 of the theory, and are avoided in this book.

Remark 17.2 Microcanonical ensemble. In statistical mechanics the space average (17.7) performed over the Hamiltonian system constant energy surface invariant measure $\rho(x)dx = dqdp \delta(H(q, p) - E)$ of volume $\omega(E) = \int_{\mathcal{M}} dqdp \delta(H(q, p) - E)$

$$\langle a(t) \rangle = \frac{1}{\omega(E)} \int_{\mathcal{M}} dqdp \delta(H(q, p) - E) a(q, p, t) \tag{17.36}$$

is called the *microcanonical ensemble average*.

Remark 17.3 Lyapunov exponents. The Multiplicative Ergodic Theorem of Oseledec [17.6] states that the limits (17.24–17.27) 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 [17.8] $\lambda_i(x_0)$.

We are doubtful of the utility of Lyapunov exponents as means of predicting any observables of physical significance, but that is the minority position - in the literature one encounters many provocative speculations, especially in the context of foundations of statistical mechanics (“hydrodynamic” modes) and the existence of a Lyapunov spectrum in the thermodynamic limit of spatiotemporal chaotic systems.

There is much literature on numerical computation of the Lyapunov exponents, see for example refs. [17.14, 17.15, 17.17]. For early numerical methods to compute Lyapunov vectors, see refs. [17.16, 17.17]. The drawback of the Gram-Schmidt method is that the vectors so constructed are orthogonal by fiat, whereas the stable / unstable eigenvectors of the Jacobian matrix are in general not orthogonal. Hence the Gram-Schmidt vectors are not covariant, i.e., the linearized dynamics does not transport them into the eigenvectors of the Jacobian matrix computed further downstream. For computation of covariant Lyapunov vectors, see refs. [17.18, 17.20].

Remark 17.4 State space discretization. Ref. [17.21] discusses numerical discretizations 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. [17.22].

Exercises

17.1. How unstable is the Hénon attractor?

- (a) Evaluate numerically the Lyapunov exponent λ by iterating some 100,000 times or so the Hénon map

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} 1 - ax^2 + y \\ bx \end{bmatrix}$$

for $a = 1.4, b = 0.3$.

- (b) Would you describe the result as a 'strange attractor'? Why?
- (c) How robust is the Lyapunov exponent for the Hénon attractor? Evaluate numerically the Lyapunov exponent by iterating the Hénon map for $a = 1.39945219, b = 0.3$. How much do you trust now your result for the part (a) of this exercise?
- (d) Re-examine this computation by plotting the iterates, and erasing the plotted points every 1000 iterates or so. Keep at it until the 'strange' attractor vanishes like the smile of the Cheshire cat. What replaces it? Do a few numerical experiments to estimate the length of typical transient before the dynamics settles into this long-time attractor.
- (e) Use your Newton search routine to confirm existence of this attractor. Compute its Lyapunov exponent, compare with your numerical result from above. What is the itinerary of the attractor.
- (f) Would you describe the result as a 'strange attractor'? Do you still have confidence in claims such as the one made for the part (b) of this exercise?

17.2. Expectation value of a vector observable.

Check and extend the expectation value formulas (17.12) by evaluating the derivatives of $s(\beta)$ up to 4-th order for the space average $\langle \exp(\beta \cdot A^t) \rangle$ with a_i a vector quantity:

- (a)

$$\left. \frac{\partial s}{\partial \beta_i} \right|_{\beta=0} = \lim_{t \rightarrow \infty} \frac{1}{t} \langle A_i^t \rangle = \langle a_i \rangle, \quad (17.37)$$

- (b)

$$\begin{aligned} \left. \frac{\partial^2 s}{\partial \beta_i \partial \beta_j} \right|_{\beta=0} &= \lim_{t \rightarrow \infty} \frac{1}{t} \left(\langle A_i^t A_j^t \rangle - \langle A_i^t \rangle \langle A_j^t \rangle \right) \\ &= \lim_{t \rightarrow \infty} \frac{1}{t} \langle (A_i^t - t \langle a_i \rangle)(A_j^t - t \langle a_j \rangle) \rangle. \end{aligned}$$

Note that the formalism is smart: it automatically yields the *variance* from the mean, rather than simply the 2nd moment $\langle a^2 \rangle$.

- (c) compute the third derivative of $s(\beta)$.
- (d) compute the fourth derivative assuming that the mean in (17.37) vanishes, $\langle a_i \rangle = 0$. The 4-th order moment formula

$$K(t) = \frac{\langle x^4(t) \rangle}{\langle x^2(t) \rangle^2} - 3 \quad (17.38)$$

that you have derived is known as *kurtosis*: it measures a deviation from what the 4-th order moment would be were the distribution a pure Gaussian (see (25.22) for a concrete example). If the observable is a vector, the kurtosis $K(t)$ is given by

$$\frac{\sum_{ij} \left[\langle A_i A_j A_j A_i \rangle + 2 \langle A_i A_j \rangle \langle A_j A_i \rangle - \langle A_i A_i \rangle \langle A_j A_j \rangle \right]}{(\sum_i \langle A_i A_i \rangle)^2}$$

17.3. Pinball escape rate from numerical simulation*.

Estimate the escape rate for $R : a = 6$ 3-disk pinball by shooting 100,000 randomly initiated pinballs into the 3-disk system and plotting the logarithm of the number of trapped orbits as function of time. For comparison, a numerical simulation of ref. [8.3] yields $\gamma = .410 \dots$

17.4. Rössler attractor Lyapunov exponents.

- (a) Evaluate numerically the expanding Lyapunov exponent λ_e of the Rössler attractor (2.17).
- (b) Plot your own version of figure 17.5. Do not worry if it looks different, as long as you understand why your plot looks the way it does. (Remember the nonuniform contraction/expansion of figure 4.3.)
- (c) Give your best estimate of λ_e . The literature gives surprisingly inaccurate estimates - see whether you can do better.
- (d) Estimate the contracting Lyapunov exponent λ_c . Even though it is much smaller than λ_e , a glance at the stability matrix (4.4) suggests that you can probably get it by integrating the infinitesimal volume along a long-time trajectory, as in (4.42).

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