Chapter 19

Transporting densities

Paulina: I'll draw the curtain:
My lord's almost so far transported that
He'll think anon it lives.
—W. Shakespeare, *The Winter's Tale*

(P. Cvitanović, R. Artuso, L. Rondoni, and E.A. Spiegel)

In chapters 2, 3, 8 and 9 we learned how to track an individual trajectory, and saw that such a trajectory can be very complicated. In chapter 4 we studied a small neighborhood of a trajectory and learned that such neighborhood can grow exponentially with time, making the concept of tracking an individual trajectory for long times a purely mathematical idealization.

While the trajectory of an individual representative point may be highly convoluted, as we shall see, the density of these points might evolve in a manner that is relatively smooth. The evolution of the density of representative points is for this reason (and other that will emerge in due course) of great interest. So are the behaviors of other properties carried by the evolving swarm of representative points.

We shall now show that the global evolution of the density of representative points is conveniently formulated in terms of linear action of evolution operators. We shall also show that the important, long-time "natural" invariant densities are unspeakably unfriendly and essentially uncomputable everywhere singular functions with support on fractal sets. Hence, in chapter 20 we rethink what is it that the theory needs to predict ("expectation values" of "observables"), relate these to the eigenvalues of evolution operators, and in chapters 21 to 23 show how to compute these without ever having to compute a "natural" invariant density ρ_0.

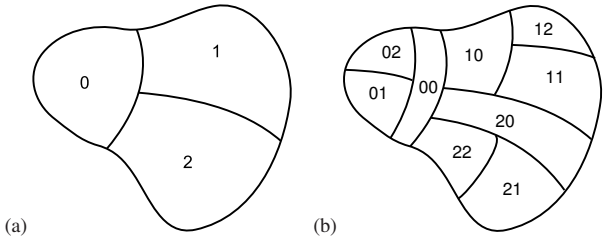


Figure 19.1: (a) First level of partitioning: A coarse partition of $\mathcal{M}$ into regions $\mathcal{M}_0$, $\mathcal{M}_1$, and $\mathcal{M}_2$. (b) $n = 2$ level of partitioning: A refinement of the above partition, with each region $\mathcal{M}_i$ subdivided into $\mathcal{M}_{i0}$, $\mathcal{M}_{i1}$, and $\mathcal{M}_{i2}$.

19.1 Measures

Do I then measure, O my God, and know not what I measure?
—St. Augustine, *The confessions of Saint Augustine*

A fundamental concept in the description of dynamics of a chaotic system is that of *measure*, which we denote by $d\mu(x) = \rho(x)dx$. An intuitive way to define and construct a physically meaningful measure is by a process of *coarse-graining*. Consider a sequence 1, 2, ..., n, ... of increasingly refined partitions of state space, figure 19.1, into 3 regions $\mathcal{M}_i$ defined by the characteristic function

$$\chi_i(x) = \begin{cases} 1 & \text{if } x \in \mathcal{M}_i\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{19.1}$$

A coarse-grained measure is obtained by assigning the "mass," or the fraction of trajectories contained in the ith region $\mathcal{M}_i \subset \mathcal{M}$ at the nth level of partitioning of the state space:

$$\Delta\mu_i = \int_{\mathcal{M}} d\mu(x)\,\chi_i(x) = \int_{\mathcal{M}_i} d\mu(x) = \int_{\mathcal{M}_i} dx\,\rho(x)\,. \tag{19.2}$$

The function $\rho(x) = \rho(x,t)$ denotes the *density* of representative points in state space at time t. This density can be (and in chaotic dynamics, often is) an arbitrarily ugly function, and it may display remarkable singularities; for instance, there may exist directions along which the measure is singular with respect to the Lebesgue measure (namely the uniform measure on the state space). We shall assume that the measure is normalized

$$\sum_i^{(n)} \Delta\mu_i = 1\,, \tag{19.3}$$

where the sum is over subregions i at the nth level of partitioning. The infinitesimal measure $\rho(x)\,dx$ can be thought of as an infinitely refined partition limit of $\Delta\mu_i = |\mathcal{M}_i|\,\rho(x_i)$, where $|\mathcal{M}_i|$ is the volume of subregion $\mathcal{M}_i$ and $x_i \in \mathcal{M}_i$; also $\rho(x)$ is normalized

$$\int_{\mathcal{M}} dx\,\rho(x) = 1\,. \tag{19.4}$$

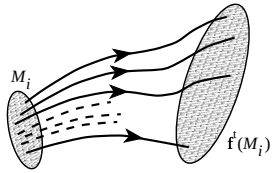


Figure 19.2: The evolution rule f^t can be used to map a region $\mathcal{M}_i$ of the state space into the region $f^t(\mathcal{M}_i)$.

Here $|\mathcal{M}_i|$ is the volume of region $\mathcal{M}_i$, and all $|\mathcal{M}_i| \to 0$ as $n \to \infty$.

So far, any arbitrary sequence of partitions will do. What are intelligent ways of partitioning state space? We already know the answer from chapter 14, but let us anyway have another look at this, in order to develop some intuition about how the dynamics transports densities. chapter 14

19.2 Perron-Frobenius operator

Given a density, the question arises as to what it might evolve into with time. Consider a swarm of representative points making up the measure contained in a region $\mathcal{M}_i$ at time $t = 0$. As the flow evolves, this region is carried into $f^t(\mathcal{M}_i)$, as in figure 19.2. No trajectory is created or destroyed, so the conservation of representative points requires that

$$\int_{f^t(\mathcal{M}_i)} dx\, \rho(x,t) = \int_{\mathcal{M}_i} dx_0\, \rho(x_0,0)\,.$$

Transform the integration variable in the expression on the left hand side to the initial points $x_0 = f^{-t}(x)$,

$$\int_{\mathcal{M}_i} dx_0\, \rho(f^t(x_0),t)\left|\det J^t(x_0)\right| = \int_{\mathcal{M}_i} dx_0\, \rho(x_0,0)\,.$$

The density changes with time as the inverse of the Jacobian (4.28)

$$\rho(x,t) = \frac{\rho(x_0,0)}{|\det J^t(x_0)|}\,, \qquad x = f^t(x_0)\,, \tag{19.5}$$

which makes sense: the density varies inversely with the infinitesimal volume occupied by the trajectories of the flow.

The relation (19.5) is linear in ρ, so the manner in which a flow transports densities may be recast into the language of operators, by writing exercise 19.1

$$\rho(x,t) = \left(\mathcal{L}^t \circ \rho\right)(x) = \int_{\mathcal{M}} dx_0\, \delta\Big(x - f^t(x_0)\Big)\rho(x_0,0)\,. \tag{19.6}$$

Let us check this formula. As long as the zero is not smack on the border of $\partial\mathcal{M}$, integrating Dirac delta functions is easy: $\int_{\mathcal{M}} dx\, \delta(x) = 1$ if $0 \in \mathcal{M}$, zero otherwise.

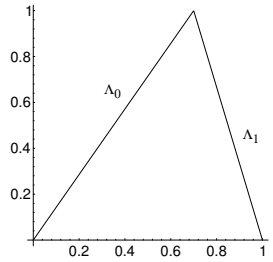
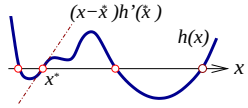


Figure 19.3: The piecewise-linear skew 'full tent map' (19.37), with $\Lambda_0 = 4/3$, $\Lambda_1 = -4$. See example 19.1.

The integral over a 1-dimensional Dirac delta function picks up the Jacobian of its argument evaluated at all of its zeros:

$$\int dx\, \delta(h(x)) = \sum_{\{x:h(x)=0\}} \frac{1}{|h'(x)|}\,, \tag{19.7}$$



and in d dimensions the denominator is replaced by

$$\int dx\, \delta(h(x)) = \sum_j \int_{\mathcal{M}_j} dx\, \delta(h(x)) = \sum_j \frac{1}{\left|\det \frac{\partial h(x_j)}{\partial x}\right|}\,, \tag{19.8}$$

where $\mathcal{M}_j$ is any open neighborhood that contains the single x_j zero of h. Now you can check that (19.6) is just a rewrite of (19.5): exercise 19.2

$$\begin{aligned}\left(\mathcal{L}^t \circ \rho\right)(x) &= \sum_{x_0 = f^{-t}(x)} \frac{\rho(x_0)}{|f^t(x_0)'|} \qquad \text{(1-dimensional)} \\ &= \sum_{x_0 = f^{-t}(x)} \frac{\rho(x_0)}{|\det J^t(x_0)|} \qquad (d\text{-dimensional})\,. \end{aligned} \tag{19.9}$$

For a deterministic, invertible flow x has only one preimage x_0; allowing for multiple preimages also takes account of noninvertible mappings such as the 'stretch & fold' maps of the interval, to be discussed briefly in example 19.1, and in more detail in sect. 14.3.

We shall refer to the integral operator with singular kernel (19.6) as the *Perron-Frobenius operator*: exercise 19.3 example 28.7

$$\mathcal{L}^t(y,x) = \delta\Big(y - f^t(x)\Big)\,. \tag{19.10}$$

The Perron-Frobenius operator assembles the density $\rho(y,t)$ at time t by going back in time to the density $\rho(x,0)$ at time $t = 0$. The family of Perron-Frobenius operators $\{\mathcal{L}^t\}_{t\in\mathbb{R}_+}$ forms a semigroup parameterized by time

(a) $\mathcal{L}^0 = I$

(b) $\mathcal{L}^t\mathcal{L}^{t'} = \mathcal{L}^{t+t'} \qquad t, t' \geq 0 \qquad$ (semigroup property) .

If you do not like the word "kernel" you might prefer to think of $\mathcal{L}^t(y, x)$ as a matrix with indices x, y, and index summation in matrix multiplication replaced by an integral over x, $(\mathcal{L}^t \circ \rho)(y) = \int dy\, \mathcal{L}^t(y, x)\rho(x)$. In example 19.1, Perron-Frobenius operator *is* a matrix, and (19.11) illustrates a matrix approximation to the Perron-Frobenius operator.

remark 22.4

example 19.1 p. 360

fast track: sect. 19.4, p. 352

19.3 Why not just leave it to a computer?

> Another subtlety in the [dynamical systems] theory is that topological and measure-theoretic concepts of genericity lead to different results.
>
> — John Guckenheimer

(R. Artuso and P. Cvitanović)

To a student with a practical bent the above Example 19.1 suggests a strategy for constructing evolution operators for smooth maps, as limits of partitions of state space into regions $\mathcal{M}_i$, with a piecewise-linear approximations f_i to the dynamics in each region, but that would be too naive; much of the physically interesting spectrum would be missed. As we shall see, the choice of function space for ρ is crucial, and the physically motivated choice is a space of smooth functions, rather than the space of piecewise constant functions.

chapter 28

All of the insight gained in this chapter and in what is to follow is nothing but an elegant way of thinking of the evolution operator, $\mathcal{L}$, as a matrix (this point of view will be further elaborated in chapter 28). There are many textbook methods of approximating an operator $\mathcal{L}$ by sequences of finite matrix approximations $\mathcal{L}$, but in what follows the great achievement will be that we shall avoid constructing any matrix approximation to $\mathcal{L}$ altogether. Why a new method? Why not just run it on a computer, as many do with such relish in diagonalizing quantum Hamiltonians?

The simplest possible way of introducing a state space discretization, figure 19.4, is to partition the state space $\mathcal{M}$ with a non-overlapping collection of sets $\mathcal{M}_i$, $i = 1, \ldots, N$, and to consider densities (19.2) piecewise constant on each $\mathcal{M}_i$:

$$\rho(x) = \sum_{i=1}^{N} \rho_i \frac{\chi_i(x)}{|\mathcal{M}_i|}$$

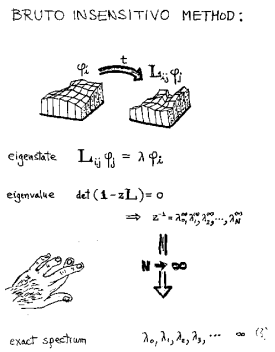


Figure 19.4: State space discretization approach to computing averages.

where $\chi_i(x)$ is the characteristic function (19.1) of the set $\mathcal{M}_i$. This piecewise constant density is a coarse grained presentation of a fine grained density $\hat{\rho}(x)$, with (19.2)

$$\rho_i = \int_{\mathcal{M}_i} dx\, \hat{\rho}(x).$$

The Perron-Frobenius operator does not preserve the piecewise constant form, but we may reapply coarse graining to the evolved measure

$$\begin{aligned} \rho'_i &= \int_{\mathcal{M}_i} dx\, (\mathcal{L} \circ \rho)(x) \\ &= \sum_{j=1}^{N} \frac{\rho_j}{|\mathcal{M}_j|} \int_{\mathcal{M}_i} dx \int_{\mathcal{M}_j} dy\, \delta(x - f(y)) \ , \end{aligned}$$

or

$$\rho'_i = \sum_{j=1}^{N} \rho_j \frac{|\mathcal{M}_j \cap f^{-1}(\mathcal{M}_i)|}{|\mathcal{M}_j|} .$$

In this way

$$\mathbf{L}_{ij} = \frac{|\mathcal{M}_i \cap f^{-1}(\mathcal{M}_j)|}{|\mathcal{M}_i|}, \quad \rho' = \rho\mathbf{L} \tag{19.11}$$

is a matrix approximation to the Perron-Frobenius operator, and its leading left eigenvector is a piecewise constant approximation to the invariant measure.

remark 19.3

The problem with such state space discretization approaches is that they are blind, the grid knows not what parts of the state space are more or less important. This observation motivated the development of the invariant partitions of chaotic systems undertaken in chapter 14, we exploited the intrinsic topology of a flow to give us both an invariant partition of the state space and a measure of the partition volumes, in the spirit of figure 15.13.

Furthermore, a piecewise constant ρ belongs to an unphysical function space, and with such approximations one is plagued by numerical artifacts such as spurious eigenvalues. In chapter 28 we shall employ a more refined approach to extracting spectra, by expanding the initial and final densities ρ, ρ' in some basis $\varphi_0, \varphi_1, \varphi_2, \cdots$ (orthogonal polynomials, let us say), and replacing $\mathcal{L}(y, x)$ by its φ_α basis representation $\mathbf{L}_{\alpha\beta} = \langle\varphi_\alpha|\mathcal{L}|\varphi_\beta\rangle$. The art is then the subtle art of finding a "good" basis for which finite truncations of $\mathbf{L}_{\alpha\beta}$ give accurate estimates of the eigenvalues of $\mathcal{L}$.

chapter 28

Regardless of how sophisticated the choice of basis might be, the basic problem cannot be avoided - as illustrated by the natural measure for the Hénon map (3.17) sketched in figure 19.5, eigenfunctions of $\mathcal{L}$ are complicated, singular functions concentrated on fractal sets, and in general cannot be represented by a nice basis set of smooth functions. We shall resort to matrix representations of $\mathcal{L}$ and the φ_α basis approach only insofar this helps us prove that the spectrum that we compute is indeed the correct one, and that finite periodic orbit truncations do converge.

in depth:
chapter 1, p. 3

19.4 Invariant measures

A *stationary* or *invariant density* is a density left unchanged by the flow

$$\rho(x, t) = \rho(x, 0) = \rho(x)\,. \tag{19.12}$$

Conversely, if such a density exists, the transformation $f^t(x)$ is said to be *measure-preserving*. As we are given deterministic dynamics and our goal is the computation of asymptotic averages of observables, our task is to identify interesting invariant measures for a given $f^t(x)$. Invariant measures remain unaffected by dynamics, so they are fixed points (in the infinite-dimensional function space of ρ densities) of the Perron-Frobenius operator (19.10), with the unit eigenvalue:

exercise 19.3

$$\mathcal{L}^t\rho(x) = \int_{\mathcal{M}} dy\, \delta(x - f^t(y))\rho(y) = \rho(x). \tag{19.13}$$

We will construct explicitly such eigenfunction for the piecewise linear map in example 20.4, with $\rho(y) = \text{const}$ and eigenvalue 1. In general, depending on the choice of $f^t(x)$ and the function space for $\rho(x)$, there may be no, one, or many solutions of the eigenfunction condition (19.13). For instance, a singular measure $d\mu(x) = \delta(x - x_q)dx$ concentrated on an equilibrium point $x_q = f^t(x_q)$, or any linear combination of such measures, each concentrated on a different equilibrium point, is stationary. There are thus infinitely many stationary measures that can be constructed. Almost all of them are unnatural in the sense that the slightest perturbation will destroy them.

From a physical point of view, there is no way to prepare initial densities which are singular, so we shall focus on measures which are limits of transformations experienced by an initial smooth distribution $\rho(x)$ under the action of f,

$$\rho_0(x) = \lim_{t\to\infty} \int_{\mathcal{M}} dy\, \delta(x - f^t(y))\rho(y, 0)\,, \qquad \int_{\mathcal{M}} dy\, \rho(y, 0) = 1\,. \tag{19.14}$$

Intuitively, the "natural" measure should be the measure that is the least sensitive to the (in practice unavoidable) external noise, no matter how weak, or round-off errors in a numerical computation.

19.4.1 Natural measure

Huang: Chen-Ning, do you think ergodic theory gives us useful insight into the foundation of statistical mechanics?
Yang: I don't think so.
—Kerson Huang, *C.N. Yang interview*

In computer experiments, as the Hénon example of figure 19.5, the long time evolution of many "typical" initial conditions leads to the same asymptotic distribution. Hence the *natural* measure (also called equilibrium measure, SRB measure, Sinai-Bowen-Ruelle measure, physical measure, invariant density, natural density, or even "natural invariant") is defined as the limit

exercise 19.8
exercise 19.9

$$\overline{\rho}_{x_0}(y) \quad = \quad \begin{cases} \lim_{t\to\infty} \frac{1}{t} \int_0^t d\tau\, \delta(y - f^\tau(x_0)) & \text{flows} \\ \\ \lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} \delta\Big(y - f^k(x_0)\Big) & \text{maps}\,, \end{cases} \tag{19.15}$$

where x_0 is a generic initial point. Generated by the action of f, the natural measure satisfies the stationarity condition (19.13) and is thus invariant by construction.

Staring at an average over infinitely many Dirac deltas is not a prospect we cherish. From a computational point of view, the natural measure is the visitation frequency defined by coarse-graining, integrating (19.15) over the $\mathcal{M}_i$ region

$$\Delta\overline{\mu}_i = \lim_{t\to\infty} \frac{t_i}{t}\,, \tag{19.16}$$

where t_i is the accumulated time that a trajectory of total duration t spends in the $\mathcal{M}_i$ region, with the initial point x_0 picked from some smooth density $\rho(x)$.

Let $a = a(x)$ be any *observable*. In the mathematical literature $a(x)$ is a function belonging to some function space, for instance the space of integrable functions L^1, that associates to each point in state space a number or a set of numbers. In physical applications the observable $a(x)$ is necessarily a smooth function. The observable reports on some property of the dynamical system. Several examples will be given in sect. 20.1.

The *space average* of the observable a with respect to a measure ρ is given by the d-dimensional integral over the state space $\mathcal{M}$:

$$\langle a \rangle_\rho = \frac{1}{|\rho_\mathcal{M}|} \int_\mathcal{M} dx\, \rho(x) a(x)$$
$$|\rho_\mathcal{M}| = \int_\mathcal{M} dx\, \rho(x) = \text{mass in } \mathcal{M}\,. \tag{19.17}$$

For now we assume that the state space $\mathcal{M}$ has a finite dimension and a finite volume. By its construction, $\langle a \rangle_\rho$ is a function(al) of ρ. For $\rho = \rho_0$ natural measure we shall drop the subscript in the definition of the space average; $\langle a \rangle_\rho = \langle a \rangle$.

Inserting the right-hand-side of (19.15) into (19.17), we see that the natural measure corresponds to a *time average* of the observable a along a trajectory of the initial point x_0,

$$\overline{a_{x_0}} = \lim_{t\to\infty} \frac{1}{t} \int_0^t d\tau\, a(f^\tau(x_0))\,. \tag{19.18}$$

Analysis of the above asymptotic time limit is the central problem of ergodic theory. The *Birkhoff ergodic theorem* asserts that if an invariant measure ρ exists, the limit $\overline{a(x_0)}$ for the time average (19.18) exists for (almost) all initial x_0. Still, Birkhoff theorem says nothing about the dependence on x_0 of time averages $\overline{a_{x_0}}$ (or, equivalently, that the construction of natural measures (19.15) leads to a "single" density, independent of x_0). This leads to one of the possible definitions of *ergodic* evolution: f is ergodic if for any integrable observable a in (19.18) the limit function is constant. If a flow enjoys such a property, the time averages coincide (apart from a set of ρ measure 0) with space averages

remark 19.1
appendix A1

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t d\tau\, a(f^\tau(x_0)) = \langle a \rangle\,. \tag{19.19}$$

For future reference, we note a further property that is stronger than ergodicity: if the space average of a product of any two variables decorrelates with time,

section 27.3

$$\lim_{t\to\infty} \langle a(x) b(f^t(x)) \rangle = \langle a \rangle \langle b \rangle\,, \tag{19.20}$$

the dynamical system is said to be *mixing*. The terminology may be understood better once we consider as the pair of observables in (19.20) characteristic functions of two sets $\mathcal{A}$ and $\mathcal{B}$: then (19.20) may be written as

$$\lim_{t\to\infty} \frac{\mu(\mathcal{A} \cap f^t(\mathcal{B}))}{\mu(\mathcal{A})} = \mu(\mathcal{B})$$

so that the set $\mathcal{B}$ spreads "uniformly" over the whole state space as t increases. Mixing is a fundamental notion in characterizing statistical behavior for dynamical systems: suppose we start with an arbitrary smooth nonequilibrium distribution $\rho(x)\nu(x)$: the after time t the average of an observable a is given by

$$\int_\mathcal{M} dx\, \rho(x) \nu(f^t(x)) a(x)$$

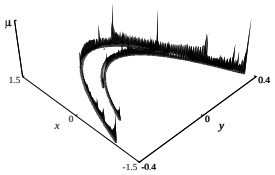


Figure 19.5: Natural measure (19.16) for the Hénon map (3.17) strange attractor at parameter values $(a, b) = (1.4, 0.3)$. See figure 3.6 for a sketch of the attractor without the natural measure binning. See example 19.2. (Courtesy of J.-P. Eckmann)

and this tends to the equilibrium average $\langle a \rangle_\rho$ if f is mixing.

example 19.2
p. 361
remark A1.2

If an invariant measure is quite singular –for instance a Dirac δ concentrated on a fixed point or a cycle– it is most likely of no physical import. No smooth initial density will converge to this measure if its neighborhood is repelling. In practice the average (19.15) is problematic and often hard to control, as generic dynamical systems are neither uniformly hyperbolic nor structurally stable: it is not known whether even the simplest model of a strange attractor, the Hénon attractor of figure 19.5, is "strange," or merely a transient to a very long stable cycle.

exercise 6.3

19.4.2 Determinism vs. stochasticity

While dynamics can lead to very singular ρ's, in any physical setting we cannot do better than to measure ρ averaged over some region $\mathcal{M}_i$; the coarse-graining is not an approximation but a physical necessity. One is free to think of a measure as a probability density, as long as one keeps in mind the distinction between deterministic and stochastic flows. In deterministic evolution the evolution kernels are not probabilistic; the density of trajectories is transported *deterministically*. What this distinction means will became apparent later: for deterministic flows our trace and determinant formulas will be *exact*, while for quantum and stochastic flows they will only be the leading saddle point (stationary phase, steepest descent) approximations.

chapter 22

Clearly, while deceptively easy to define, measures spell trouble. The good news is that if you hang on, you will *never need to compute them*, at least not in this book. How so? The evolution operators to which we next turn, and the trace and determinant formulas to which they will lead us, will assign the correct weights to desired averages without recourse to any explicit computation of the coarse-grained measure $\Delta\rho_i$.

19.5 Density evolution for infinitesimal times

Consider the evolution of a smooth density $\rho(x) = \rho(x,0)$ under an infinitesimal step $\delta\tau$, by expanding the action of $\mathcal{L}^{\delta\tau}$ to linear order in $\delta\tau$:

$$\begin{aligned}
\mathcal{L}^{\delta\tau}\rho(y) &= \int_{\mathcal{M}} dx\, \delta\Big(y - f^{\delta\tau}(x)\Big)\rho(x) \\
&= \int_{\mathcal{M}} dx\, \delta(y - x - \delta\tau v(x))\,\rho(x) \\
&= \frac{\rho(y - \delta\tau v(y))}{\left|\det\left(1 + \delta\tau \frac{\partial v(y)}{\partial x}\right)\right|} = \frac{\rho(y) - \delta\tau v_i(y)\partial_i\rho(y)}{1 + \delta\tau \sum_{i=1}^{d} \partial_i v_i(y)} \\
\rho(x,\delta\tau) &= \rho(x,0) - \delta\tau \frac{\partial}{\partial x}(v(x)\rho(x,0))\,. \qquad (19.21)
\end{aligned}$$

Here we have used the infinitesimal form of the flow (2.7), the Dirac delta Jacobian (19.9), and the ln det = tr ln relation. By the Einstein summation convention, repeated indices imply summation, $v_i(y)\partial_i = \sum_{i=1}^{d} v_i(y)\partial_i$. Moving $\rho(y,0)$ to the left hand side and dividing by $\delta\tau$, we discover that the rate of the deformation of ρ under the infinitesimal action of the Perron-Frobenius operator is nothing but the *continuity equation* for the density:

exercise 4.1

$$\partial_t\rho + \partial\cdot(\rho v) = 0\,. \qquad (19.22)$$

From (19.21), time evolution by an infinitesimal step $\delta\tau$ forward in time is generated by

$$\mathcal{A}\rho(x) = +\lim_{\delta\tau\to 0^+} \frac{1}{\delta\tau}\Big(\mathcal{L}^{\delta\tau} - I\Big)\rho(x) = -\partial_i(v_i(x)\rho(x))\,. \qquad (19.23)$$

We shall refer to

$$\mathcal{A} = -\partial\cdot v - \sum_{i}^{d} v_i(x)\partial_i \qquad (19.24)$$

as the time-evolution *generator*. If the flow is finite-dimensional and invertible, $\mathcal{A}$ is a generator of a full-fledged group. The left hand side of (19.23) is the definition of time derivative, so the evolution equation for $\rho(x)$ is

$$\left(\frac{\partial}{\partial t} - \mathcal{A}\right)\rho(x) = 0\,. \qquad (19.25)$$

The finite time Perron-Frobenius operator (19.10) can be formally expressed by exponentiating the time evolution generator $\mathcal{A}$ as

$$\mathcal{L}^t = e^{t\mathcal{A}}\,. \qquad (19.26)$$

The generator $\mathcal{A}$ is reminiscent of the generator of translations. Indeed, for a constant velocity field dynamical evolution is nothing but a translation by (time $\times$ velocity):

exercise 19.10

$$e^{-tv\frac{\partial}{\partial x}}a(x) = a(x - tv)\,. \qquad (19.27)$$

19.6 Liouville operator

A case of special interest is the Hamiltonian or symplectic flow defined by Hamilton's equations of motion (8.1). A reader versed in quantum mechanics will have observed by now that with replacement $\mathcal{A} \to -\frac{i}{\hbar}\hat{H}$, where $\hat{H}$ is the quantum Hamiltonian operator, (19.25) looks rather like the time dependent Schrödinger equation, so this is the right moment to figure out what all this means for Hamiltonian flows.

The Hamilton's evolution equations (8.1) for any time-independent quantity $Q = Q(q,p)$ are given by

$$\frac{dQ}{dt} = \frac{\partial Q}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial Q}{\partial p_i}\frac{dp_i}{dt} = \frac{\partial H}{\partial p_i}\frac{\partial Q}{\partial q_i} - \frac{\partial Q}{\partial p_i}\frac{\partial H}{\partial q_i}\,, \qquad (19.28)$$

where (p_i, q_i) span the full state space, which for Hamiltonian flows we shall refer to as the *phase space*. As equations with this structure arise frequently for symplectic flows, it is convenient to introduce a notation for them, the *Poisson bracket*

remark 19.4

$$\{A,B\} = \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} - \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i}\,. \qquad (19.29)$$

In terms of Poisson brackets the time-evolution equation (19.28) takes the compact form

$$\frac{dQ}{dt} = \{H, Q\}\,. \qquad (19.30)$$

The discussion of sect. 19.5 applies to any deterministic flow. The full phase space flow velocity is $\dot{x} = v = (\dot{q}, \dot{p})$, where the dot signifies time derivative.

section 32.1

If the density itself is a material invariant, combining

$$\partial_t I + v\cdot\partial I = 0\,.$$

and (19.22) we conclude that $\partial_i v_i = 0$ and $\det J^t(x_0) = 1$. An example of such incompressible flow is the Hamiltonian flow. For incompressible flows the continuity equation (19.22) becomes a statement of conservation of the phase space volume (see sect. 8.3), or the *Liouville theorem*

$$\partial_t\rho + v_i\partial_i\rho = 0\,. \qquad (19.31)$$

The symplectic structure of Hamilton's equations (8.1) implies that the flow is incompressible, $\partial_i v_i = 0$, so for Hamiltonian flows the equation for ρ reduces to the *continuity equation* for the phase-space density:

$$\partial_t\rho + \partial_i(\rho v_i) = 0\,, \qquad i = 1, 2\ldots, D\,. \qquad (19.32)$$

Consider the evolution of the phase-space density ρ of an ensemble of noninteracting particles; the particles are conserved, so

$$\frac{d}{dt}\rho(q,p,t) = \left(\frac{\partial}{\partial t} + \dot{q}_i\frac{\partial}{\partial q_i} + \dot{p}_i\frac{\partial}{\partial p_i}\right)\rho(q,p,t) = 0\,.$$

Inserting Hamilton's equations (8.1) we obtain the *Liouville equation*, a special case of (19.25):

remark 19.4

$$\frac{\partial}{\partial t}\rho(q,p,t) = -\mathcal{A}\rho(q,p,t) = \{H,\rho(q,p,t)\}\,, \tag{19.33}$$

where $\{\ ,\ \}$ is the Poisson bracket (19.29). The generator of the flow (19.24) is in this case a generator of infinitesimal symplectic transformations,

$$\mathcal{A} = \dot{q}_i\frac{\partial}{\partial q_i} + \dot{p}_i\frac{\partial}{\partial p_i} = \frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i}\,. \tag{19.34}$$

For example, for separable Hamiltonians of form $H = p^2/2m+V(q)$, the equations of motion are

$$\dot{q}_i = \frac{p_i}{m}\,, \qquad \dot{p}_i = -\frac{\partial V(q)}{\partial q_i}\,. \tag{19.35}$$

and the action of the generator

exercise 19.11

$$\mathcal{A} = -\frac{p_i}{m}\frac{\partial}{\partial q_i} + \partial_i V(q)\frac{\partial}{\partial p_i}\,. \tag{19.36}$$

Looking back at (19.27) we see that the first term generates a translation in the configuration space, $f(q,p) \to f(q - dt\,\dot{q}, p)$, and the second generates acceleration by force $\partial V(q)$ in the momentum space. They do not commute, hence the time integration is not trivial.

The time-evolution generator (19.24) for the case of symplectic flows is called the *Liouville operator*. You might have encountered it in statistical mechanics, while discussing what ergodicity means for $6.02214129 \times 10^{23}$ hard balls. Here its action will be very tangible; we shall apply the Liouville operator to systems as small as 1 or 2 hard balls and to our surprise learn that this suffices to already get a bit of a grip on foundations of the nonequilibrium statistical mechanics.

Résumé

In physically realistic settings the initial state of a system can be specified only to a finite precision. If the dynamics is chaotic, it is not possible to calculate the long time trajectory of a given initial point. Depending on the desired precision, and given a deterministic law of evolution, the state of the system can then be tracked for a finite time only.

The study of long-time dynamics thus requires trading in the evolution of a single state space point for the evolution of a *measure*, or the *density* of representative points in state space, acted upon by an *evolution operator*. Essentially this means trading in *nonlinear* dynamical equations on a finite dimensional space $x = (x_1, x_2 \cdots x_d)$ for a *linear* equation on an infinite dimensional vector space of density functions $\rho(x)$. For finite times and for maps such densities are evolved by the *Perron-Frobenius operator*,

$$\rho(x,t) = \left(\mathcal{L}^t \circ \rho\right)(x)\,,$$

and in a differential formulation they satisfy the *continuity equation*:

$$\partial_t\rho + \partial\cdot(\rho v) \;=\; 0\,.$$

The most physical of stationary measures is the natural measure, a measure robust under perturbations by weak noise.

For long times the dynamics is described in terms of stationary measures, i.e., fixed points of the appropriate evolution operators. Reformulated this way, classical dynamics takes on a distinctly quantum-mechanical flavor. If the Lyapunov time (1.1), the time after which the notion of an individual deterministic trajectory loses meaning, is much shorter than the observation time, the "sharp" observables are those dual to time, the eigenvalues of evolution operators. This is very much the same situation as in quantum mechanics; as atomic time scales are so short, what is measured is the energy, the quantum-mechanical observable dual to the time. Both in classical and quantum mechanics one has a choice of implementing dynamical evolution on densities ("Schrödinger picture," sect. 19.5) or on observables ("Heisenberg picture," sect. 20.3 and chapter 21).

In what follows we shall find the second formulation more convenient, but the alternative is worth keeping in mind when posing and solving invariant density problems. However, as classical evolution operators are not unitary, their eigenfunctions can be quite singular and difficult to work with. In what follows we shall learn how to avoid dealing with these eigenstates altogether. As a matter of fact, what follows will be a labor of radical deconstruction; after having argued so strenuously here that only smooth measures are "natural," we shall merrily proceed to erect the whole edifice of our theory on periodic orbits, i.e., objects that are δ-functions in state space. The trick is that each comes with an interval, its neighborhood – periodic points only serve to pin these intervals, just as millimeter markings on a measuring rod are used to partition a continuum into intervals.

Commentary

Remark 19.1 Ergodic theory: An overview of ergodic theory is outside the scope of this book: the interested reader may find it useful to consult refs. [19.1, 28.15, 19.4, 19.5]. The existence of time average (19.18) is the basic result of ergodic theory, known as the Birkhoff theorem, see for example refs. [19.1, 19.25], or the statement of theorem 7.3.1 in ref. [19.12]. The natural measure (19.16) of sect. 19.4.1 is often referred to as the SRB or Sinai-Ruelle-Bowen measure [A39.1, A1.70, A39.14].

There is much literature on explicit form of natural measure for special classes of 1-dimensional maps [1.19, 19.14, 19.15] - J. M. Aguirregabiria [A2.12], for example, discusses several families of maps with known smooth measure, and behavior of measure under smooth conjugacies. As no such explicit formulas exist for higher dimensions and general dynamical systems, we do not discuss such measures here.

Remark 19.2 Time evolution as a Lie group: Time evolution of sect. 19.5 is an example of a 1-parameter Lie group. Consult, for example, chapter 2. of ref. [19.13] for a

clear and pedagogical introduction to Lie groups of transformations. For a discussion of the bounded semigroups of page 375 see, for example, Marsden and Hughes [19.6].

Remark 19.3 Discretization of the Perron-Frobenius operator operator It is an old idea of Ulam [19.18] that such an approximation for the Perron-Frobenius operator is a meaningful one. The piecewise-linear approximation of the Perron-Frobenius operator (19.11) has been shown to reproduce the spectrum for expanding maps, once finer and finer Markov partitions are used [19.19, 19.23, 19.20]. The subtle point of choosing a state space partitioning for a "generic case" is discussed in ref. [19.21, 28.22].

Remark 19.4 The sign convention of the Poisson bracket: The Poisson bracket is antisymmetric in its arguments and there is a freedom to define it with either sign convention. When such freedom exists, it is certain that both conventions are in use and this is no exception. In some texts [A1.65, 19.7] you will see the right hand side of (19.29) defined as $\{B, A\}$ so that (19.30) is $\frac{dQ}{dt} = \{Q, H\}$. Other equally reputable texts [19.24] employ the convention used here. Landau and Lifshitz [38.2] denote a Poisson bracket by $[A, B]$, notation that we reserve here for the quantum-mechanical commutator. As long as one is consistent, there should be no problem.

Remark 19.5 "Anon it lives"? "Anon it lives" refers to a statue of King Leontes's wife, Hermione, who died in a fit of grief after he unjustly accused her of infidelity. Twenty years later, the servant Paulina shows Leontes this statue of Hermione. When he repents, the statue comes to life. Or perhaps Hermione actually lived and Paulina has kept her hidden all these years. The text of the play seems deliberately ambiguous. It is probably a parable for the resurrection of Christ. (John F. Gibson)

19.7 Examples

Example 19.1 ***Perron-Frobenius operator for a piecewise-linear map:*** *Consider the expanding 1-dimensional map $f(x)$ of figure 19.3, a piecewise-linear 2–branch map with slopes $\Lambda_0 > 1$ and $\Lambda_1 = -\Lambda_0/(\Lambda_0 - 1) < -1$:* exercise 19.7

$$f(x) = \begin{cases} f_0(x) = \Lambda_0 x\,, & x \in \mathcal{M}_0 = [0, 1/\Lambda_0) \\ f_1(x) = \Lambda_1(1-x)\,, & x \in \mathcal{M}_1 = (1/\Lambda_0, 1]\,. \end{cases} \tag{19.37}$$

Both $f(\mathcal{M}_0)$ and $f(\mathcal{M}_1)$ map onto the entire unit interval $\mathcal{M} = [0, 1]$. We shall refer to any unimodal map whose critical point maps onto the "left" unstable fixed point x_0 as the "Ulam" map. Assume a piecewise constant density

$$\rho(x) = \begin{cases} \rho_0 & \text{if } x \in \mathcal{M}_0 \\ \rho_1 & \text{if } x \in \mathcal{M}_1 \end{cases}\,. \tag{19.38}$$

As can be easily checked using (19.9), the Perron-Frobenius operator acts on this piecewise constant function as a [2×2] Markov matrix $\mathbf{L}$ with matrix elements exercise 19.1 exercise 19.5

$$\begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} \to \mathbf{L}\rho = \begin{bmatrix} \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \\ \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \end{bmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix}, \tag{19.39}$$

stretching both ρ_0 and ρ_1 over the whole unit interval Λ. In this example the density is constant after one iteration, so $\mathbf{L}$ has only a unit eigenvalue $e^{s_0} = 1/|\Lambda_0| + 1/|\Lambda_1| = 1$, with constant density eigenvector $\rho_0 = \rho_1$. The quantities $1/|\Lambda_0|$, $1/|\Lambda_1|$ are, respectively, the fractions of state space taken up by the $|\mathcal{M}_0|$, $|\mathcal{M}_1|$ intervals. 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 enterprize 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. (continued in example 20.4) click to return: p. **??**

Example 19.2 ***The Hénon attractor natural measure:*** *A numerical calculation of the natural measure (19.16) for the Hénon attractor (3.17) is given by the histogram in figure 19.5. The state space is partitioned into many equal-size areas $\mathcal{M}_i$, and the coarse grained measure (19.16) is computed by a long-time iteration of the Hénon map, and represented by the height of the column over area $\mathcal{M}_i$. What we see is a typical invariant measure - a complicated, singular function concentrated on a fractal set.* click to return: p. **??**

Exercises

19.1. **Integrating over Dirac delta functions.** Check the delta function integrals in

(a) 1 dimension (19.7),

$$\int dx\,\delta(h(x)) = \sum_{\{x:h(x)=0\}} \frac{1}{|h'(x)|}\,, \tag{19.40}$$

(b) and in d dimensions (19.8), $h : \mathbb{R}^d \to \mathbb{R}^d$,

$$\begin{aligned} \int_{\mathbb{R}^d} dx\,\delta(h(x)) &= \sum_j \int_{\mathcal{M}_j} dx\,\delta(h(x)) \\ &= \sum_{\{x:h(x)=0\}} \frac{1}{\left|\det \frac{\partial h(x)}{\partial x}\right|} \end{aligned} \tag{19.41}$$

where $\mathcal{M}_j$ are arbitrarily small regions enclosing the zeros x_j (with x_j not on the boundary $\partial\mathcal{M}_j$). For a refresher on Jacobian determinants, read, for example, Stone and Goldbart Sect. 12.2.2.

(c) The delta function can be approximated by a sequence of Gaussians

$$\int dx\,\delta(x) f(x) = \lim_{\sigma\to 0} \int dx\,\frac{e^{-\frac{x^2}{2\sigma}}}{\sqrt{2\pi\sigma}} f(x)\,.$$

Use this approximation to see whether the formal expression

$$\int_{\mathbb{R}} dx\,\delta(x^2)$$

makes sense.

19.2. **Derivatives of Dirac delta functions.** Consider $\delta^{(k)}(x) = \frac{\partial^k}{\partial x^k}\delta(x)$.

Using integration by parts, determine the value of

$$\int_{\mathbb{R}} dx\,\delta'(y) \quad , \qquad \text{where } y = f(x) - x \tag{19.42}$$

$$\int dx\,\delta^{(2)}(y) = \sum_{\{x:y(x)=0\}} \frac{1}{|y'|}\left\{3\frac{(y'')^2}{(y')^4} - \frac{y'''}{(y')^3}\right\} \tag{19.43}$$

$$\begin{aligned} \int dx\,b(x)\delta^{(2)}(y) &= \sum_{\{x:y(x)=0\}} \frac{1}{|y'|}\left\{\frac{b''}{(y')^2} - \frac{b'y''}{(y')^3}\right. \\ &\quad \left. + b\left(3\frac{(y'')^2}{(y')^4} - \frac{y'''}{(y')^3}\right)\right\} \end{aligned} \tag{19.44}$$

These formulas are useful for computing effects of weak noise on deterministic dynamics [19.9].

19.3. **$\mathcal{L}^t$ generates a semigroup.** Check that the Perron-Frobenius operator has the semigroup property,

$$\int_M dz\,\mathcal{L}^{t_2}(y,z)\,\mathcal{L}^{t_1}(z,x) = \mathcal{L}^{t_2+t_1}(y,x)\,, \qquad t_1, t_2 \geq 0\,.$$

(19.45)

As the flows in which we tend to be interested are invertible, the $\mathcal{L}$'s that we will use often do form a group, with $t_1, t_2 \in \mathbb{R}$.

19.4. **Escape rate of the tent map.**

(a) Calculate by numerical experimentation the log of the fraction of trajectories remaining trapped in the interval $[0, 1]$ for the tent map

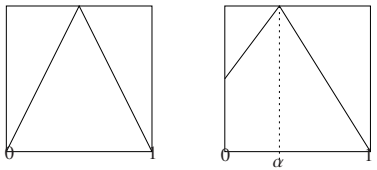
$$f(x) = a(1 - 2|x - 0.5|)$$

for several values of a.

(b) Determine analytically the a dependence of the escape rate $\gamma(a)$.

(c) Compare your results for (a) and (b).

19.5. **Invariant measure.** We will compute the invariant measure for two different piecewise linear maps.



(a) Verify the matrix $\mathcal{L}$ representation (19.39).

(b) The maximum value of the first map is 1. Compute an invariant measure for this map.

(c) Compute the leading eigenvalue of $\mathcal{L}$ for this map.

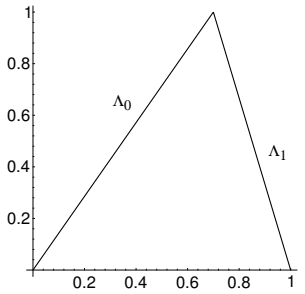
(d) For this map there is an infinite number of invariant measures, but only one of them will be found when one carries out a numerical simulation. Determine that measure, and explain why your choice is the natural measure for this map.

(e) In the second map the maximum occurs at $\alpha = (3 - \sqrt{5})/2$ and the slopes are $\pm(\sqrt{5} + 1)/2$. Find the natural measure for this map. Show that it is piecewise linear and that the ratio of its two values is $(\sqrt{5} + 1)/2$.

(medium difficulty)

19.6. **Escape rate for a flow conserving map.** Adjust Λ_0, Λ_1 in (19.37) so that the gap between the intervals $\mathcal{M}_0$, $\mathcal{M}_1$ vanishes. Show that the escape rate equals zero in this situation.

19.7. **Eigenvalues of the Perron-Frobenius operator for the skew full tent map.** Show that for the skew full tent map



$$f(x) = \begin{cases} f_0(x) = \Lambda_0 x\,, & x \in \mathcal{M}_0 = [0, 1/\Lambda_0) \\ f_1(x) = \frac{\Lambda_0}{\Lambda_0 - 1}(1 - x)\,, & x \in \mathcal{M}_1 = (1/\Lambda_0, 1]\,. \end{cases} \tag{19.46}$$

the eigenvalues are available analytically, compute the first few.

19.8. **"Kissing disks"*** (continuation of exercises 9.1 and 9.2) Close off the escape by setting $R = 2$, and look in real time at the density of the Poincaré section iterates for a trajectory with a randomly chosen initial condition. Does it look uniform? Should it be uniform? (Hint - phase-space volumes are preserved for Hamiltonian flows by the Liouville theorem). Do you notice the trajectories that loiter near special regions of phase space for long times? These exemplify "intermittency," a bit of unpleasantness to which we shall return in chapter 29.

19.9. **Invariant measure for the Gauss map.** Consider the Gauss map:

$$f(x) = \begin{cases} \frac{1}{x} - \left[\frac{1}{x}\right] & x \neq 0 \\ 0 & x = 0 \end{cases} \tag{19.47}$$

where [ ] denotes the integer part.

(a) Verify that the density

$$\rho(x) = \frac{1}{\log 2}\frac{1}{1 + x}$$

is an invariant measure for the map.

(b) Is it the natural measure?

19.10. $\mathcal{A}$ **as a generator of translations.** Verify that for a constant velocity field the evolution generator $\mathcal{A}$ in (19.27) is the generator of translations,

$$e^{tv\frac{\partial}{\partial x}} a(x) = a(x + tv)\,.$$

19.11. **Incompressible flows.** Show that (19.9) implies that $\rho_0(x) = 1$ is an eigenfunction of a volume-preserving flow with eigenvalue $s_0 = 0$. In particular, this implies that the natural measure of hyperbolic and mixing Hamiltonian flows is uniform. Compare this results with the numerical experiment of exercise 19.8.

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