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*

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N 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 .

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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

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

A coarse-grained measure is obtained by assigning the "mass," or the fraction of trajectories contained in the *i*th region $\mathcal{M}_i \subset \mathcal{M}$ at the *n*th 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

$$\sum_{i}^{(n)} \Delta \mu_{i} = 1, \qquad (19.3)$$

where the sum is over subregions *i* at the *n*th 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

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

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

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

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

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

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

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

and in d dimensions the denominator is replaced by

$$\int dx \,\delta(h(x)) = \sum_{j} \int_{\mathcal{M}_{j}} dx \,\delta(h(x)) = \sum_{j} \frac{1}{\left|\det \frac{\partial h(x_{j})}{\partial x}\right|},$$
(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):

$$(\mathcal{L}^{t} \circ \rho)(x) = \sum_{x_{0}=f^{-t}(x)} \frac{\rho(x_{0})}{|f^{t}(x_{0})'|}$$
(1-dimensional)
$$= \sum_{x_{0}=f^{-t}(x)} \frac{\rho(x_{0})}{|\det J^{t}(x_{0})|}$$
(d-dimensional). (19.9)

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

$$\mathcal{L}^{t}(y,x) = \delta(y - f^{t}(x)).$$
(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) $\mathcal{L}^{t}\mathcal{L}^{t'} = \mathcal{L}^{t+t'}$ $t, t' \ge 0$ (semigroup property).

If you do not like the word "kernel" you might prefer to think of $\mathcal{L}(y, x)$ 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 the next example Perron-Frobenius operator *is* a matrix, and (19.11) illustrates a matrix approximation to the Perron-Frobenius operator.

19.4 Invariant measures

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

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

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(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:

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

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,

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

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

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

$$\overline{\rho}_{x_0}(y) = \begin{cases} \lim_{t \to \infty} \frac{1}{t} \int_0^t d\tau \,\delta(y - f^{\tau}(x_0)) & \text{flows} \\ \\ \lim_{n \to \infty} \frac{1}{n} \sum_{k=0}^{n-1} \,\delta(y - f^k(x_0)) & \text{maps} \,, \end{cases}$$
(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 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) b e a n y *observable*. In physical applications the observable a(x) is necessarily a smooth function. The observable reports on some property of the dynamical system.

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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} :

$$\langle a \rangle_{\rho} = \int_{\mathcal{M}} dx \, \rho(x) a(x)$$

$$\int (19.17)$$

By its construction, $\langle a \rangle_{\rho}$ is a function(al) of ρ . F or $\rho = \rho_0$ 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

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



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*.

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 $\Delta \rho_i$.

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*,

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

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

Reformulated this way, classical dynamics takes on a distinctly quantummechanical 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.

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 $\Lambda_1 = -\Lambda_0/(\Lambda_0 - 1) < -1$:

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

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

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

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

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 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 M_i . What we see is a typical invariant measure - a complicated, singular function concentrated on a fractal set.

Exercises

- 19.1. Integrating over Dirac delta functions. Check the delta function integrals in
 - (a) 1 dimension (19.7),

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

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

$$\int_{\mathbb{R}^d} dx \,\delta(h(x)) = \sum_j \int_{\mathcal{M}_j} dx \,\delta(h(x))$$
$$= \sum_{\{x:h(x)=0\}} \frac{1}{\left|\det \frac{\partial h(x)}{\partial x}\right|}.41)$$

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

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

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

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

These formulas are useful for computing effects of weak noise on deterministic dynamics [9].

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

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

(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 γ(*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



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

the eigenvalues are available analytically, compute the first few.

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