Averaging

ChaosBook Chapter 20

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The big picture

Local v.s. **global** way of thinking

Key idea: Replace expectation values of observables with that of exponential generating functions

Any dynamical average can be extracted from the spectrum of an appropriately constructed evolution operator

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Dynamical averaging

Why?

Detailed prediction impossible in chaotic dynamics

Any initial condition will fill whole state space after finite Lyapunov time

Hence we cannot follow them for a long time

Examples of averages:

- transport coefficients: escape rates, mean drifts, diffusion rates
- entropies
- power spectra
- Lyapunov exponents

Observables

Observable: a function that associates to each point in state space a number, a vector or a tensor

Observables report on a property of the dynamical system

e.g. velocity field $a_i(x) = v_i(x)$

We can also define an **integrated observable:**

$$A(x_0, t) = \int_0^t \mathrm{d}\tau \, a(x(\tau)), \qquad x(t) = f^t(x_0) \tag{1}$$

Exercise: What is the integrated observable of the velocity field?

Example 20.1

(a) If the observable is the velocity, $a_i(x) = v_i(x)$, its time integral $A(x_0, t_i)$ is the trajectory $A(x_0, t_i) = x_i(t)$

(b) For Hamiltonian flows, the action associated with trajectory x(t)=[q(t),p(t)] is an integrated observable:

$$A(x_0, t) = \int_0^t \mathrm{d}\tau \, \dot{\mathsf{q}}(\tau) \cdot \mathsf{p}(\tau) \tag{2}$$

Discrete time

If dynamics are given by an iterated mapping the integrated observable after n iterations is given by:

$$A(x_0, n) = \sum_{k=0}^{n-1} a(x_k), \qquad x_k = f^k(x_0) \tag{3}$$

Time averages

We define the **time average** of the observable along an orbit:

$$\overline{a(x_0)} = \lim_{t \to \infty} \frac{1}{t} A(x_0, t) \tag{4}$$

If a is not too wild this limit should exist.

Exercise: What is $\overline{a\left(f^T(x_0)\right)}$?

Exercise

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

Key result: Time averages are properties of the orbit.

Periodic Orbits

Define

$$A_p = \begin{cases} a_p T_p = \int_0^{T_p} \mathrm{d}\tau\, a(x(\tau)) & \text{for a flow} \\ a_p n_p = \sum_{i=1}^{n_p} a(x_i) & \text{for a map} \end{cases} \tag{5}$$

A_p is a loop integral of the observable alone a single traversal of the prime cycle p

This implies $\overline{a(x_0)}$ is in general a wild function of x_0 e.g. for a hyperbolic system it takes a different value on (almost) every periodic orbit

Spatial averages

The **space average** is defined by a d-dimensional integral:

$$\langle a \rangle (t) = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} \mathrm{d}x_0 a(x(t)), \qquad x(t) = f^t(x_0) \tag{6}$$

where $|\mathcal{M}|$ is the (finite) volume of $\mathcal{M}$

In experiments, we can't prepare an initial condition, but we can prepare an initial density, so define the **weighed spatial average**:

$$\langle a \rangle_\rho (t) = \frac{1}{|\mathcal{M}_\rho|} \int_{\mathcal{M}} \mathrm{d}x_0 \rho(x_0) a(x(t)), \quad |\mathcal{M}_\rho| = \int_{\mathcal{M}} \mathrm{d}x \rho(x) \tag{7}$$

Expectation value

For ergodic mixing systems, any smooth initial density will tend to the asymptotic natural measure in the $t \to \infty$ limit

So, we can take any smooth initial $\rho(x)$ and define the **expectation value**:

$$\langle a \rangle = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} \mathrm{d}x \, \overline{a(x)} = \lim_{t \to \infty} \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} \mathrm{d}x_0 \, \frac{1}{t} \int_0^t \mathrm{d}\tau \, a(x(t)) \tag{8}$$

Advantage: smears the starting points of the time average that were troublesome (e.g. periodic points)

Unfortunately, not very tractable in practice.

Exponential generating functions

Instead, let's consider the following spatial average:

$$\left\langle e^{\beta\cdot A}\right\rangle = \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} \mathrm{d}x\, e^{\beta\cdot A(x,t)} \tag{9}$$

where in this context β is an auxiliary variable with no physical significant.

Exercise: How can we recover the desired space average $\langle A_i\rangle$ from $\left\langle e^{\beta\cdot A}\right\rangle$?

Exercise

$$\langle A_i \rangle = \frac{\partial}{\partial \beta_i} \left\langle e^{\beta \cdot A} \right\rangle \Big|_{\beta=0}$$

Generating function with time

If $\overline{a(x_0)}$ exists for almost all x_0 and system is ergodic and mixing, we expect $\overline{a(x_0)} \to \bar{a}$ for all x_0 and hence $A \to t\bar{a}$

So, as $t \to \infty$ we expect:

$$\left\langle e^{\beta A} \right\rangle \to (\text{const})e^{ts(\beta)}$$

where its rate of growth characteristic state function is given by:

$$s(\beta) = \lim_{t \to \infty} \frac{1}{t} \ln \left\langle e^{\beta A} \right\rangle \tag{10}$$

Exercise: How can we calculate $\langle a \rangle$?

Calculating moments

We can use derivatives of $s(\beta)$ to calculate the expectation value of the observable, the (generalized) diffusion tensor, and higher moments of the integrated observable.

For example,

$$\left.\frac{\partial s}{\partial \beta_j}\right|_{\beta=0} = \lim_{t\to\infty} \frac{1}{t} \langle A_j \rangle = \langle a_j \rangle \tag{11}$$

Evolution operators

Evolution operator

We can make the dependence on the flow explicit by writing:

$$\left\langle e^{\beta A} \right\rangle = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} \mathrm{d}x \underbrace{\int_{\mathcal{M}} \mathrm{d}x \, \delta\left(y - f^{t}(x)\right)}_{=1} e^{\beta A(x,t)} \tag{12}$$

This makes it explicit that we are averaging only over trajectories that remain in $\mathcal{M}$ for all times.

We are now studying evolution of the density of the **totality** of initial conditions

Evolution operator

The kernel of this operation is the **evolution operator**:

$$\mathcal{L}^t(y,x) = \delta\left(y - f^t(x)\right) e^{\beta A(x,t)} \tag{13}$$

When $\beta = 0$ we have the **Perron-Frobenius operator**.

The action of the evolution operator on a function ϕ is:

$$\left[\mathcal{L}^t \phi\right](y) = \int_{\mathcal{M}} \mathrm{d}x \, \delta\left(y - f^t(x)\right) e^{\beta A(x,t)} \phi(x) \tag{14}$$

Semigroup property

A, which is an integral over observable a. is additive by definition:

$$A(x_0, t_1 + t_2) = \int_0^{t_1} \mathrm{d}\tau\, a\left(f^\tau(x)\right) + \int_{t_1}^{t_1+t_2} \mathrm{d}\tau\, a\left(f^\tau(x)\right) \tag{15}$$

so the evolution operator generates a semigroup

$$\mathcal{L}^{t_1+t_2}(y, x) = \int_{\mathcal{M}} \mathrm{d}x\, \mathcal{L}^{t_2}(y, z)\mathcal{L}^{t_1}(z, x) \tag{16}$$

Evolution operator

In terms of the evolution operator,

$$\left\langle e^{\beta A}\right\rangle = \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} \mathrm{d}x \int_{\mathcal{M}} \mathrm{d}y\, \phi(y)\mathcal{L}^t(y,x)\phi(x) \tag{17}$$

where $\phi(x) = 1$.

If we think of $\mathcal{L}^t$ as a matrix, higher powers of it will be dominated by its fastest growing matrix elements and hence

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

yields the leading eigenvalue $s_0(\beta)$, from which we can calculate the desired expectation values

How do we find these eigenvalues?

Spectrum of an evolution operator

A linear operator has a spectrum of eigenvalues and eigenfunctions

$$\left[\mathcal{L}^t \varphi_\alpha\right](y) = e^{s_\alpha t} \varphi_\alpha(x), \qquad \alpha = 0, 1, 2, \ldots \tag{18}$$

where we assume that $\mathrm{Re}\, s_\alpha \geq \mathrm{Re}\, s_{\alpha+1}$.

Hence the $t \to \infty$ limit will be dominated by $s_0 = s(\beta)$

$$\left[\mathcal{L}^t \rho_\beta\right](y) = \int_{\mathcal{M}} \mathrm{d}x \, \delta\left(y - f^t(x)\right) e^{\beta A(x,t) \rho_\beta(x)} = e^{ts(\beta)} \rho_\beta(y) \tag{19}$$

Exercise: Are these operators local or global?

Evolution for infinitesimal times

For infinitesimal time δt,

$$\begin{aligned}\rho(y,\delta t) &= \int \mathrm{d}x\, e^{\beta A(x,\delta t)} \delta(y - f^{\delta t}(x))\rho(x,0) \\ &= \int \mathrm{d}x\, e^{\beta a(x)\delta t} \delta(y - x - \delta t\, v(x))\rho(x,0) \\ &= (1 + \delta t \beta a(y)) \frac{\rho(y,0) - \delta t\, v \cdot \frac{\partial}{\partial x}\rho(y,0)}{1 + \delta t \frac{\partial v}{\partial x}}\end{aligned}$$

Which gives rise to the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(v_i \rho) = \beta a \rho \tag{20}$$

Evolution generator

Recall that the **time-evolution generator** is defined as

$$\mathcal{A} = -\partial \cdot v - \sum_{i}^{d} v_i(x)\partial_i \tag{21}$$

From the continuity equation,the evolution generator eigenfunctions now satisfy

$$(s(\beta) - \mathcal{A})\rho(x, \beta) = \beta a(x)\rho(x, \beta) \tag{22}$$

Resolvent of $\mathcal{L}$

Perron-Frobenius operator $\mathcal{L}$ acts multiplicatively in time, so reasonable to assume $\left\|\mathcal{L}^t\right\| \leq Me^{ts_0}$.

If this is true, we can construct a new operator $e^{-ts_0}\mathcal{L}^t = e^{t(\mathcal{A}-s_0)}$ which decays exponentially and is bounded $\left\|e^{t(\mathcal{A}-s_0)}\right\| \leq M$

[Recall: $\mathcal{L}^t = e^{t\mathcal{A}}$]

We say $e^{-ts_0}\mathcal{L}^t$ is an element of a **bounded** semigroup with generator $\mathcal{A} - s_0 I$

Resolvent of $\mathcal{L}$

It follows by the Laplace transform

$$\int_0^\infty \mathrm{d}t\, e^{-st}\mathcal{L}^t = \frac{1}{s-\mathcal{A}}, \qquad \mathrm{Re}\, s > s_0 \tag{23}$$

that the **resolvent** operator $(s-\mathcal{A})^{-1}$ is bounded

$$\left\|\frac{1}{s-\mathcal{A}}\right\| \leq \int_0^\infty \mathrm{d}t\, e^{-st} M e^{ts_0} = \frac{M}{s-s_0} \tag{24}$$

No time dependence, bounded

It separates spectrum of $\mathcal{L}$ into individual constituents, one for each spectral 'line'.

Averaging in open systems

Open systems

A **repeller** is a dynamical system for which a trajectory eventually leaves $\mathcal{M}$ unless the initial point is on the repeller, so the identity

$$\int_{\mathcal{M}} \mathrm{d}y \, \delta\left(y - f^t(x_0)\right) = 1, \qquad t > 0, \qquad \text{iff } x_0 \in \text{non-wandering set} \tag{25}$$

only applies to a fractal subset of initial points.

We need to modify the definition of expectation value to restrict it to the dynamics of the non-wandering set

Averaging in open systems

Volume of state space containing all of the trajectories which start out within $\mathcal{M}$ and recur within that region at time t given by:

$$|\mathcal{M}(t)| = \int_{\mathcal{M}} \mathrm{d}x\mathrm{d}y\, \delta\left(y - f^t(x)\right) \sim |\mathcal{M}|e^{-\gamma t} \tag{26}$$

Escape rate γ

The integral over x takes care of all possible initial points, integral over y checks whether their trajectories are still within $\mathcal{M}$ by the time t

Averaging in open systems

The fraction of trapped trajectories decays as

$$\Gamma_{\mathcal{M}}(t) = \frac{\int_{\mathcal{M}} \mathrm{d}x\, [\mathcal{L}^t \rho](x)}{\int_{\mathcal{M}} \mathrm{d}x\, \rho(x)} = \sum_{\alpha} e^{s_\alpha t} a_\alpha \frac{\int_{\mathcal{M}} \mathrm{d}x\, \varphi_\alpha(x)}{\int_{\mathcal{M}} \mathrm{d}x\, \rho(x)}$$
$$= e^{s_0 t} \left((\mathrm{const}) + O(e^{(s_1 - s_0)t}) \right) \tag{27}$$

Escape rate $\gamma = -s_0$ is intrinsic property of repelling set

The leading eigenvalue of $\mathcal{L}^t$ dominates $\Gamma_{\mathcal{M}}(t)$ and yields escape rate, a measurable property

Averaging in open systems

We can redefine the space average

$$\left\langle e^{\beta A}\right\rangle = \int_{\mathcal{M}} \mathrm{d}x \, \frac{1}{|\mathcal{M}(t)|} e^{\beta A(x,t)} \sim \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} \mathrm{d}x \, e^{\beta A(x,t)+\gamma t} \qquad (28)$$

to compensate for the exponential decrease of number of surviving trajectories.

We replenish density lost to escaping trajectories by pumping in $e^{\gamma t}$ new trajectories

This ensures the overall measure is correctly normalized at all times.

Evaluation of Lyapunov exponents

Evaluation of Lyapunov exponents

Construction of the evolution operator for the evaluation of the Lyapunov spectra for a *d*-dimensional flow: we need 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

$$\lambda = \langle \ln |f'(x)| \rangle = \left. \frac{\partial s(\beta)}{\partial \beta} \right|_{\beta=0} = s'(0) \tag{29}$$

How?

Recap of big picture ideas

Since detailed prediction is impossible in chaotic dynamics, averages are useful to describe the system.

The key idea is to replace expectation values of observables with that of exponential generating functions. Averages (and higher moments) of observables are found by taking derivatives.

We can construct a multiplicative evolution operator which as $t \to \infty$ is dominated by its largest eigenvalue.

Dynamical averages can then be extracted from the spectrum of an appropriately constructed evolution operator.

Questions?