Lecture 12: Detailed balance and Eigenfunction methods

Readings

Recommended:

- Pavliotis [2014] 4.5-4.7 (eigenfunction methods and reversibility), 4.2-4.4 (explicit examples of eigenfunction methods)
- Gardiner [2009] 6.2-6.3 (detailed balance), 6.5 (eigenfunction methods, multi-dimensional), 5.4 (eigenfunction methods, 1-dimensional)

Optional:

- Pavliotis [2014] 4.9 (reduction to a Schrodinger equation)
- Risken [1984] has many examples of solving the Fokker-Planck equation using eigenfunction expansions.

Consider a time-homogeneous diffusion X on a domain $\Omega \subset \mathbb{R}^d$ which could be bounded or unbounded:

$$dX_t = b(X_t)dt + \sigma(X_t)dW_t. \tag{1}$$

Recall the generator and its adjoint are

$$\mathscr{L} f = b(x) \cdot \nabla f + a(x) : \nabla^2 f, \qquad \mathscr{L}^* p = -\nabla \cdot (b(x)p) + \nabla \cdot \nabla \cdot (a(x)p),$$

where $a(x) = \frac{1}{2}\sigma(x)\sigma^T(x)$. Throughout this lecture we assume that a is *uniformly elliptic*, i.e. $y^T a(x) y \geq \lambda_0 > 0$ for all $x \in \Omega$, $y \in \mathbb{R}^d$.

The Fokker-Planck equation for the evolution of probability density ρ is

$$\partial_t \rho = \mathscr{L}^* \rho = -\nabla \cdot \underline{\mathrm{j}}, \tag{2}$$

where $\underline{\mathrm{j}} = b\rho - \nabla \cdot (a\rho)$ is the flux associated with ρ, and $\mathscr{L}^*$ comes with suitable boundary conditions. A stationary density $\pi(x)$ solves

$$\nabla \cdot \underline{\mathrm{j}}_s = 0 \tag{3}$$

with probability-conserving boundary conditions (reflecting or periodic boundary conditions in a bounded domain, decay conditions at infinity in an unbounded domain), where $\underline{\mathrm{j}}_s = b\pi - \nabla \cdot (a\pi)$ is the flux associated with π. We saw in an earlier lecture that sometimes the flux vanishes in steady-state:

$$\underline{\mathrm{j}}_s = 0. \tag{4}$$

Condition (4) is stronger than (3), because it involves d equations, whereas (3) is only one equation. Therefore (4) shouldn't be expected to hold in general. When does it hold? And what does it imply or require about the physics of the process? In this lecture we will show the following:

$$\underline{\mathrm{j}}_s = 0 \quad \Longleftrightarrow \quad \mathscr{L} \text{ is symmetric in } L^2_\pi(\Omega) \quad \Longleftrightarrow \quad X \text{ satisfies detailed balance.} \tag{5}$$

Here $L^2_\pi(\Omega)$ is a weighted inner product space, which uses a locally stationary distribution π as a weight for the inner product:

$$\langle f, g \rangle_\pi = \int_\Omega f(x)g(x)\pi(x)dx. \tag{6}$$

We retain the notation $\langle f,g\rangle = \int_\Omega fg dx$ to mean the regular L^2 inner product in Ω. Hereafter we will suppress Ω in our notation, and simply write $L^2_\pi = L^2_\pi(\Omega)$, $\int \cdot dx = \int_\Omega \cdot dx$.

A *locally stationary distribution* is a bounded function solving $\mathscr{L}^*\pi = 0$ with probability-conserving boundary conditions. Sometimes π is a stationary distribution, when one exists, but when it doesn't we may still find a solution to $\mathscr{L}^*\pi = 0$ that is not normalizable (see Exercise 12.1). We know from PDE theory that $\pi(x) > 0$.

Example 12.1 Consider Brownian motion on $\mathbb{R}$. A locally stationary distribution is $\pi(x) = 1$.

We will then show that when (5) holds, we can use eigenfunction expansions of $\mathscr{L}$ to solve for quantities like the transition probability, correlation functions, and mean-first passage times.

We give a definition of detailed balance in Section 12.3, although some references take the condition $\underset{\sim}{\mathrm{j}}_s = 0$ as a definition of detailed balance. The definition we will give will be easier to generalize to systems with odd variables such as velocities; see Section 12.5.

As for Markov chains, detailed balance is equivalent to the system being time-reversible. When constructing a model of a physical system, it is important to keep in mind whether the system is time-reversible or not. Not only should the model have the correct stationary distribution, but, if the system is time-reversible, the model should also have zero flux in steady-state. Indeed, if $\underset{\sim}{\mathrm{j}}_s \neq 0$, then the steady-state flux will move, on average, and so by conservation of probability it must contain loops. If this were possible in an isolated system, then we could extract energy indefinitely out of these cycles! Therefore, when $\underset{\sim}{\mathrm{j}}_s \neq 0$, the system must be subject to *external* forcing, and furthermore, the amount of energy required to sustain the non-zero flux, must be consistent with the energy input by the forcing. Some systems where external forcing occurs and hence $\underset{\sim}{\mathrm{j}}_s \neq 0$ include active matter, such as particles that propel themselves by chemical reactions, bacteria that swim, etc, and many biological systems, like molecular motors, where energy is input via ATP consumption.

These developments generalized our results for Markov chains. Recall that for Markov chains that satisfy detailed balance, we symmetrized the transition matrix by the similarity transformation $D^{1/2}PD^{-1/2}$, where $D_{ij} = \pi_i\delta_{ij}$ is the matrix with the stationary distribution on its diagonal. We used this to argue that P has real eigenvalues and a complete orthonormal basis of eigenvectors, and then we expanded many quantities of interest in terms of these eigenvectors. We will follow the same path here, which is more involved because we are working in infinite-dimensional vector spaces, so instead of linear algebra, the conclusions follow from functional analysis.

Remark. We will only show that $\mathscr{L}$ is symmetric, not self-adjoint. In our examples it will be true that it is self-adjoint, but this is harder to show. A *symmetric* operator is one such that $\langle \mathscr{L}f, g\rangle = \langle f, \mathscr{L}g\rangle$ for all f,g in the domain of $\mathscr{L}$, and it is *self-adjoint*, roughly, if the domains of the operator and its adjoint are the same.

12.1 Flux in steady-state

We start by asking what conditions on $b(x), a(x)$ are required for $\underset{\sim}{\mathrm{j}}_s = 0$ to hold. First consider a one-dimensional process $X \in \mathbb{R}$. Equation (3) implies that $\underset{\sim}{\mathrm{j}}_s = cst$. Consider different possibilities for Ω.

- If $\Omega = [a,b]$ and the boundaries are reflecting, then $\underset{\sim}{\mathrm{j}}_s = 0$ since it's zero at the boundary.

- If $\Omega = \mathbb{R}$ then the probability and flux must decay at $\pm\infty$, so similarly $\underset{\sim}{j}_s = 0$.
- If $\Omega = [a,b]$ and the boundaries are periodic, then it is possible to have $\underset{\sim}{j}_s \neq 0$.

Therefore $\underset{\sim}{j}_s = 0$ should hold for reflecting boundary conditions, but for periodic boundary conditions it doesn't necessarily have to hold.

***Exercise* 12.1.** Find conditions on the drift and diffusion that ensure $\underset{\sim}{j}_s = 0$ for periodic boundary conditions.

Now consider a higher-dimensional process $X \in \mathbb{R}^d$. Suppose the stationary distribution satisfies $\underset{\sim}{j}_s = 0$. Rewriting this equation gives

$$a(x)\,\nabla\pi(x) = \pi(x)(b(x) - \nabla\cdot a(x))\,. \tag{7}$$

Since $a(x)$ is uniformly elliptic it is invertible, so

$$\nabla \log \pi(x) = Q(x)\,, \qquad \text{where} \quad Q(x) = a^{-1}(x)(b(x) - \nabla\cdot a(x))\,. \tag{8}$$

In components, $Q_i = \sum_k a^{-1}_{ik}(2b_k - \sum_j \frac{\partial}{\partial x_j} a_{kj})$. Notice that this implies Q is a perfect gradient: $Q(x) = -\nabla\Phi(x)$ for some scalar function $\Phi : \Omega \to \mathbb{R}$. A necessary and sufficient condition for Q to be a perfect gradient is that its curl is zero:

$$\frac{\partial Q_i}{\partial x_j} - \frac{\partial Q_j}{\partial x_i} = 0 \qquad \text{for all } i \neq j.$$

Given a, b but not π, one can compute the curl to verify whether $\underset{\sim}{j}_s = 0$. T

We can express π in terms of Φ as

$$\pi(x) = Z^{-1} e^{-\Phi(x)}, \qquad \text{with} \quad \Phi(x) = -\int_{x_0}^{x} Q(x')dx'. \tag{9}$$

Here Z is a normalizing constant (which could be absorbed into the definition of Φ), and x_0 is some arbitrary, fixed point; changing it changes $\Phi(x)$ by a constant. Note that it doesn't matter which path is taken in the integral since $Q(x)$ is a gradient.

Equation (9) gives a general expression for the stationary density when $\underset{\sim}{j}_s = 0$. This expression is similar to the Boltzmann distribution $e^{-U(x)}$ we considered in the last lecture, showing that Φ plays the role of a potential energy; it is sometimes called a generalized potential.

Example 12.2 Suppose the diffusivity is constant: $a_{ij}(x) = A_{ij}$, where A_{ij} are constants and $A_{ij} = A_{ji}$. Then $\nabla\cdot a(x) = 0$, so $A^{-1}b(x) = \nabla\Phi$ or equivalently,

$$b(x) = \nabla\phi(x)$$

for some scalar function ϕ. This is an important result: given constant diffusivity, the flux in steady-state vanishes if and only if the drift is a perfect gradient. If the drift has any curl component, the flux cannot vanish in steady-state.

Example 12.3 If $a(x) \neq cst$, then using (7) we solve for the drift in terms of a, Φ, as $b = -a\nabla\Phi + \nabla\cdot a$, and obtain

$$\mathscr{L}^*\rho = -\nabla\cdot(-a\nabla\Phi\,\rho + \nabla\cdot a\,\rho - \nabla\cdot(a\rho))\,. \tag{10}$$

This corresponds to an SDE

$$dX_t = -a\nabla\Phi\,dt + \nabla\cdot a\,dt + \sqrt{2a}\,dW_t \tag{11}$$

where $\sqrt{2a}$ means any matrix σ such that $\sigma\sigma^T = 2a$. This shows the dynamics of a diffusion with zero flux in steady-state are fully prescribed by two ingredients: the generalized potential Φ, and the diffusivity tensor a.

Equation (11) is the most general form of the overdamped Langevin equation. Compared to the overdamped Langevin equation from Lecture 10, we have introduced a varying friction or diffusivity matrix, and an additional drift $\nabla\cdot a$. The addition drift compensates for the non-constant diffusivity matrix, pushing the system back to regions of high diffusivity (see Exercise 12.2). One of the uses of this equation is to model a collection of N particles in a $d-$dimensional fluid, $x\in\mathbb{R}^{Nd}$, which interact with potential energy $\Phi(x)$ (nondimensionalized by k_BT) and via hydrodynamic interactions. The effect of the hydrodynamic interactions is not to change the stationary distribution, which is constrained by the laws of statistical mechanics to be the Boltzmann distribution $e^{-\Phi(x)}$, but rather to change the particles' dynamics. If the dynamics are given by a time-reversible SDE, then our calculations showed the only way to change the particles' dynamics is to change their diffusivity tensor, $a(x)$. For example, for a pair of microspheres close to each other, $a(x)$ will be smaller for motions v that push spheres normal to each other's surfaces (meaning $v^T a(x)v$ is small), because this requires squeezing fluid in or out of the small gap, and larger for motions where the spheres move in the tangential direction.

***Exercise* 12.2.** Consider the one-dimensional diffusion $dX_t = (\sin X_t + 2)dW_t$ with periodic boundary conditions on $[-\pi,\pi]$. Solve for the stationary distribution and show it is larger in regions with low diffusivity, and smaller in regions with high diffusivity. Work out the drift one would have to add, to ensure the stationary distribution is constant.

***Exercise* 12.3.** Show that if $\underset{\sim}{\mathrm{j}}_s = 0$, then $\mathscr{L}^*$ and its adjoint can be written as

$$\mathscr{L}^*\rho = \nabla\cdot\left(\pi a\nabla\cdot\left(\rho\pi^{-1}\right)\right), \qquad \mathscr{L}f = \pi^{-1}\nabla\cdot(\pi a\nabla f).$$

where $\pi = Z^{-1}e^{\Phi}$ is the stationary distribution.

12.2 Symmetry of $\mathscr{L}$

In this section we'll consider the symmetry of the generator, and show that $\mathscr{L}$ is symmetric in L^2_π (see (6)) if and only if $\underset{\sim}{\mathrm{j}}_s = 0$.

Lemma. *Let π be a locally stationary distribution, and let $\underset{\sim}{j}_s = b\pi - \nabla\cdot(a\pi)$ be the associated steady-state flux. Then*

$$\langle\mathscr{L}f,g\rangle_\pi = -\langle a\nabla f,\nabla g\rangle_\pi - \langle f,\pi^{-1}\nabla g\cdot\underset{\sim}{j}_s\rangle_\pi \tag{12}$$

for all $f,g\in L^2_\pi$ satisfying boundary conditions consistent with the relation $\langle\mathscr{L}f,g\rangle = \langle f,\mathscr{L}^*g\rangle$.

The boundary conditions could include reflecting or absorbing boundary conditions, for example.

Proof. This follows from multiple integration by parts. In detail,

$$\langle \mathscr{L} f, g\rangle_\pi = \int b\cdot\nabla f g\pi + \int (a:\nabla^2 f) g\pi.$$

Consider each of the terms on the right-hand side separately. We have

$$\int b\cdot\nabla f g\pi = \int \underbrace{\nabla\cdot(fg\pi b)}_{\text{boundary}} - \int \underbrace{f\pi b\cdot\nabla g}_{A} - \int \underbrace{fg\nabla\cdot(b\pi)}_{B}.$$

We also have

$$\begin{aligned}\int (a:\nabla^2 f) g\pi &= \int \nabla\cdot(a\nabla f g\pi) - \int a\nabla f\cdot\nabla g\pi - \int (\nabla f g)\cdot\nabla\cdot(a\pi)\\ &= \int \underbrace{\nabla\cdot(a\nabla f g\pi)}_{\text{boundary}} - \langle a\nabla f,\nabla g\rangle_\pi - \int \underbrace{\nabla\cdot(fg\nabla\cdot(a\pi))}_{\text{boundary}} + \int \underbrace{f\nabla g\cdot\nabla\cdot(a\pi)}_{A} + \int \underbrace{fg\nabla\cdot\nabla\cdot(a\pi)}_{B}.\end{aligned}$$

The terms labelled 'A' combine to give $-\int f\nabla g\cdot \underline{\mathrm{j}}_s = -\langle f, \pi^{-1}\nabla g\cdot\underline{\mathrm{j}}_s\rangle_\pi$.

The terms labelled 'B' combine to give $-\int fg\nabla\cdot\underline{\mathrm{j}}_s = 0$.

The terms labelled 'boundary' vanish, by assumption. We are left with (12). □

Proposition. $\underline{j}_s = 0$ *if and only if* $\mathscr{L}$ *is symmetric in* L^2_π.

Proof. Suppose $\underline{\mathrm{j}}_s = 0$. Then by the Lemma above,

$$\langle \mathscr{L} f, g\rangle_\pi = \langle a\nabla f,\nabla g\rangle_\pi \quad \text{and} \quad \langle f, \mathscr{L} g\rangle_\pi = \langle a\nabla g,\nabla f\rangle_\pi = \langle a\nabla f,\nabla g\rangle_\pi$$

so $\langle \mathscr{L} f, g\rangle_\pi = \langle f, \mathscr{L} g\rangle_\pi$.

Now suppose $\mathscr{L}$ is symmetric in L^2_π. Then from the Lemma above,

$$\int f\nabla g\cdot\underline{\mathrm{j}}_s - g\nabla f\cdot\underline{\mathrm{j}}_s = 0$$

or all $f, g \in L^2_\pi$ satisfying suitable boundary conditions. This is only possible if $\underline{\mathrm{j}}_s = 0$ (for example, take $f = cst$). □

Here is another useful relationship when $\underline{\mathrm{j}}_s = 0$ or equivalently (7) holds.

Lemma. *If* $\underline{j}_s = 0$*, then for* $g \in L^2_\pi$,

$$\mathscr{L}^*(g\pi) = \pi\mathscr{L} g\,. \tag{13}$$

This holds no matter what the boundary conditions on $\mathscr{L}, \mathscr{L}^*$ are.

Proof. Calculate:

$$\begin{aligned}\mathscr{L}^*(g\pi) &= -\nabla\cdot(bg\pi) + \nabla\cdot\nabla\cdot(ag\pi)\\ &= -\nabla\cdot(bg\pi) + \nabla\cdot(g(\nabla\cdot a)\pi + ga\nabla\pi + \pi a\nabla g) && \text{expanding } \nabla\cdot\\ &= -\nabla\cdot(bg\pi) + \nabla\cdot(bg\pi + \pi a\nabla g) && \text{using (7)}\\ &= \nabla\cdot(\pi a\nabla g)\,.\end{aligned}$$

This representation is useful in itself (see Exercise 12.3). Continue expanding this expression:

$$\begin{aligned}\mathscr{L}^*(g\pi) &= a\nabla\pi\cdot\nabla g + \pi\nabla\cdot a\nabla g + \pi a : \nabla^2 g \\ &= \pi b\cdot\nabla g + \pi a : \nabla^2 g \qquad \text{using (7)} \\ &= \pi\mathscr{L}g\,.\end{aligned}$$

□

***Exercise* 12.4.** Derive the symmetry of $\mathscr{L}$, using the result of the Lemma above .

***Exercise* 12.5.** Let the probability density be $\rho(x,t) = g(x,t)\pi(x)$, so that g is the density of ρ with respect to π. Use the Lemma above to show that if $\underset{\sim}{\mathrm{j}}_s = 0$ and ρ solves the forward equation, then g solves the backward equation.

12.3 Detailed balance

Our goal is to show that

$$\mathscr{L} \text{ is symmetric in } L^2_\pi \quad \Longleftrightarrow \quad X_t \text{ satisfies detailed balance.} \tag{14}$$

Recall that a Markov Chain satisfies detailed balance if $\pi_i p_{ij} = \pi_j p_{ji}$. Advancing this equation by n steps in time, shows that $\pi_i P^{(n)}_{ij} = \pi_j P^{(n)}_{ji}$ for all n, where $P^{(n)}$ is the n-step transition matrix. The condition can be interpreted in terms of flux: $\pi_i p_{ij}$ is the flux of probability from edge $i \to j$ in steady-state, and $\pi_j p_{ji}$ is the flux of probability from edge $j \to i$ in steady-state, so the net flux of probability across each edge is 0 in steady-state.

We generalize these ideas to a continuous Markov process.

Definition. A continuous Markov process is *reversible* or satisfies *detailed balance* if, for all $x, y \in \Omega$ and all $s < t$,

$$\pi(x)p(y,t|x,s) = \pi(y)p(x,t|y,s)\,. \tag{15}$$

One can show that detailed balance is equivalent to the process $(X_t)_{0\le t\le T}$ with $X_0 \sim \pi$ and the time-reversed process $(X_{T-t})_{0\le t\le T}$ having the same law; including the same finite-dimensional distributions; see Pavliotis [2014], Section 4.6 Theorem 4.5.

Our arguments to show (14) will be purely formal [Pavliotis, 2014, Section 4.6]. In particular, we'll make frequent use of the operator $e^{\mathscr{L}t} = I + \mathscr{L}t + \frac{1}{2}\mathscr{L}^2t^2 + \cdots$, which is such that if $u(x,t)$ solves the PDE $\partial_t u = \mathscr{L}u$, $u(x,0) = f(x)$, then $u(x,t) = e^{\mathscr{L}t}f(x)$. In particular, we have the representation

$$p(y,t|x,s) = e^{\mathscr{L}^*_y(t-s)}\delta(x-y). \tag{16}$$

One can show that the adjoint of $e^{\mathscr{L}t}$ is $e^{\mathscr{L}^*t}$, and similarly that $\mathscr{L}$ is symmetric in a given inner product space, if and only if $e^{\mathscr{L}t}$ is too.

Multiply both sides of (15) by test functions $f(x), g(y)$ and integrate over x, y. The left-hand side becomes

$$\begin{aligned}\int \pi(x)f(x)g(y)p(y,t|x,s)dxdy &= \int \pi(x)f(x)g(y)e^{\mathscr{L}_y^*(t-s)}\delta(x-y)dxdy \\ &= \int \pi(x)f(x)\delta(x-y)e^{\mathscr{L}_y(t-s)}g(y)dxdy \\ &= \int \pi(y)f(y)e^{\mathscr{L}_y(t-s)}g(y)dy \\ &= \langle f, e^{\mathscr{L}_y(t-s)}g\rangle_\pi.\end{aligned}$$

This quantity has stochastic interpretation $\mathbb{E}[f(X_s)g(X_t)|X_s \sim \pi] = \mathbb{E}^\pi[f(X_0)g(X_T)]$ for $T = t-s$.

The right-hand side becomes

$$\begin{aligned}\int \pi(y)f(x)g(y)p(x,t|y,s)dxdy &= \int \pi(x)f(y)g(x)p(y,t|x,s)dxdy \\ &= \int \pi(x)f(y)g(x)e^{\mathscr{L}_y^*(t-s)}\delta(x-y)dxdy \\ &= \int \pi(x)g(x)\delta(x-y)e^{\mathscr{L}_y(t-s)}f(y)dxdy \\ &= \int \pi(y)g(y)e^{\mathscr{L}_y(t-s)}f(y)dy \\ &= \langle g, e^{\mathscr{L}_y(t-s)}f\rangle_\pi.\end{aligned}$$

This quantity has stochastic interpretation $\mathbb{E}[f(X_t)g(X_s)|X_s \sim \pi] = \mathbb{E}^\pi[f(X_T)g(X_0)]$.

Now suppose that (15) holds. Putting together the pieces above shows that

$$\langle f, e^{\mathscr{L}_y(t-s)}g\rangle_\pi = \langle g, e^{\mathscr{L}_y(t-s)}f\rangle_\pi. \tag{17}$$

Therefore $e^{\mathscr{L}t}$ is symmetric in L^2_π; differentiate in t to show that $\mathscr{L}$ is symmetric in L^2_π.

Conversely, suppose that $\mathscr{L}$ is symmetric in L^2_π. Then (17) holds, so working backwards,

$$\int \pi(x)f(x)g(y)p(y,t|x,s)dxdy = \int \pi(y)f(x)g(y)p(x,t|y,s)dxdy.$$

This holds for all test functions f, g, so (15) holds.

12.4 Eigenfunction methods

When $\mathscr{L}$ is symmetric in L^2_π, its eigenvalues are real, countable, and its eigenfunctions are orthonormal in L^2_π:

$$\int \phi_i \psi_j \pi dx = \delta_{ij},$$

where δ is the Kronecker delta. To expand the transition probability using eigenfunctions, we need to know the eigenfunctions are *complete*, i.e. they span L^2_π. This is a question in functional analysis ; see [Pavliotis,

2014, Chapter 4] for a discussion of some conditions that imply completeness of the eigenfunctions, particularly for the overdamped Langevin equation. Henceforth we will assume that the eigenfunctions of $\mathscr{L}$ are complete for the examples we study, and solve for various quantities of interest in terms of eigenfunctions.

Let us write $\{\lambda_i\}_{i=1}^\infty$ for the eigenvalues of $\mathscr{L}$ and $\mathscr{L}^*$, $\{\phi_i\}_{i=1}^\infty$ for the eigenfunctions of $\mathscr{L}$, and $\{\psi_i\}_{i=1}^\infty$ for the eigenfunctions of $\mathscr{L}^*$. The eigenfuctions and eigenvalues must satisfy the same boundary conditions imposed on the operators they are associated with; note that changing the boundary conditions will change both the eigenvalues and eigenfunctions.

Here are some facts about the eigenvalues and eigenfunctions, assuming throughout that $\mathscr{L}$ is symmetric in L^2_π and $a(x)$ is uniformly elliptic.

(1) $\mathscr{L}$ is negative semi-definite, so the eigenvalues of $\mathscr{L}$ are nonpositive, $\lambda_i \le 0$.

(In fact, it can be shown that $\lambda_i \to -\infty$ as $i \to \infty$.)

Proof. Since $\underset{\sim}{\mathrm{j}}_s = 0$, (12) implies that

$$\langle \mathscr{L} f, f\rangle_\pi = \int \pi f \mathscr{L} f = -\int \pi (\nabla f)^T a \nabla f \;\le\; -\lambda_0 \|\nabla f\|_\pi \;\le\; 0.$$

□

(2) If $\mathscr{L}$ has reflecting boundary conditions, then its null space is one-dimensional and contains only constants. Therefore the largest eigenvalue is $\lambda_1 = 0$ with multiplicity 1, and the corresponding eigenfunctions are $\phi_0 = 1$, $\psi_0 = \pi$.

Proof. Suppose $\mathscr{L} f = 0$. By the calculations above,

$$0 = \langle \mathscr{L} f, f\rangle_\pi \le -\lambda_0 \|\nabla f\|_\pi \le 0.$$

The only way this is possible is if $\nabla f = 0$, so $f = cst$. Notice that this one-dimensional space of solutions does satisfy the reflecting boundary condition. □

(3) If $\mathscr{L}$ has absorbing boundary conditions, then all eigenvalues are strictly negative.

Proof. This follows from the calculations above, because there is no nontrivial solution satisfying $f|_{\partial\Omega} = 0$. □

(4) The left and right eigenfunctions are related by a factor of π:

$$\psi_i(x) = \pi(x)\phi_i(x). \tag{18}$$

Recall this same relation was true for Markov chains.

Proof. Calculate, using (13) for an eigenfunction ϕ_i,

$$\mathscr{L}^*(\pi\phi_i) = \pi \mathscr{L}\phi_i = \lambda_i \pi \phi_i.$$

Therefore if ϕ_i is an eigenfunction of $\mathscr{L}$ with eigenvalue λ_i, then $\pi\phi_i$ is an eigenfunction of $\mathscr{L}^*$ with the same eigenvalue. □

(5) ϕ_i, ψ_i form a bi-orthogonal set in L^2:

$$\langle \phi_i, \psi_j \rangle = \delta_{ij}\,, \tag{19}$$

where δ is the Kronecker delta.

Proof. This follows from the orthonormality of $\{\phi_i\}$ in L^2_π. □

Many quantities can be expressed using eigenfunctions.

Example 12.4 (Transition probability) Let's solve for the transition probability using separation of variables. Make the ansatz

$$p(x,t|y,0) = \sum_{i=1}^{\infty} a_i g_i(t)\psi_i(x)$$

where $a_i \in \mathbb{R}$ are unknown coefficients and g_i are unknown functions. Substitute into the forward equation to find

$$p_t = \mathscr{L}_x^* p \qquad \Rightarrow \qquad \sum_{i=1}^{\infty} a_i g_i'(t)\psi_i(x) = \sum_{i=1}^{\infty} a_i g_i(t)\lambda_i\psi_i(x)\,.$$

Projecting onto ϕ_i and using (19) shows that $g_i(t) = e^{\lambda_i t}$. To find the coefficients a_i use the initial condition $p(x,0|y,0) = \delta(x-y)$ and take the L^2 inner product of $p(x,0|y,0)$ with ϕ_i to get

$$a_i = \langle p(x,0|y,0), \phi_i(x)\rangle = \langle \delta(x-y), \phi_i(x)\rangle = \phi_i(y).$$

Putting this all together shows the transition probability can be written as

$$p(x,t|y,0) = \sum_{i=1}^{\infty} \phi_i(y)\psi_i(x)e^{\lambda_i t}\,. \tag{20}$$

Example 12.5 (Stationary covariance matrix) We derive an expression for the covariance matrix of a stationary process when $\mathbb{E}^\pi X_t = 0$; calculations with $\mathbb{E}^\pi X_t \neq 0$ give the same result and are left as an exercise. Note that the process must have reflecting or probability-conserving boundary conditions, in order to be stationary. The stationary covariance matrix is

$$\begin{aligned}
C(t) = \mathbb{E}^\pi X_t X_0^T &= \iint xy^T p(x,t|y,0)\pi(y)dxdy \\
&= \iint xy^T \pi(y) \sum_{k=1}^{\infty} \phi_k(y)\psi_k(x)e^{\lambda_k t}dxdy \\
&= \sum_{k=1}^{\infty} \left(\int x\psi_k(x)dx\right)\left(\int x\psi_k(x)dx\right)^T e^{\lambda_k t} \qquad \text{using(18)} \\
&= \sum_{k=2}^{\infty} C^{(k)} e^{\lambda_k t}\,.
\end{aligned} \tag{21}$$

Here $C^{(k)}$ is a matrix constructed as

$$C^{(k)} = \bar{x}^{(k)} \otimes \bar{x}^{(k)} = \bar{x}^{(k)}\,(\bar{x}^{(k)})^T\,, \qquad \text{with} \quad \bar{x}^{(k)} = \int x\psi_k(x)dx.$$

That is, it has ijth element $C_{ij}^{(k)} = (\int x_i\psi_k(x)dx)(\int x_j\psi_k(x)dx)$. Notice that the sum in (21) starts at $i=2$ since $\int x\psi_1(x)dx = \int x\pi(x)dx = \mathbb{E}^\pi X_t = 0$. The covariance function is therefore a sum of decaying exponentials, with a decay rate governed by $|\lambda_2|$.

***Exercise* 12.6.** Consider Brownian motion on an interval $[0,1]$ with reflecting boundary conditions. Calculate the eigenvalues and eigenfunctions. Suppose you start the process with initial condition $\rho(x,0) = 2\cdot 1_{x\in[0,\frac{1}{2}]}$. Write down an expression for the probability density $\rho(x,t)$ at time t. Estimate how quickly this decays to the stationary distribution.

Example 12.6 (Ornstein-Uhlenbeck process, 1D) The generator and its adjoint are

$$\mathscr{L}f = -\alpha x f_x + \frac{1}{2}\sigma^2 f_{xx}\,, \qquad \mathscr{L}^* p = \partial_x(\alpha x p) + \frac{1}{2}\sigma^2 \partial_{xx} p\,.$$

The eigenfunctions of the generator solve

$$\phi_\lambda'' - \frac{2\alpha x}{\sigma^2}\phi_\lambda' - \frac{2\lambda}{\sigma^2}\phi_\lambda = 0$$

with appropriate decay conditions at $\pm\infty$. Let $y = x\sqrt{\frac{2\alpha}{\sigma^2}}$. The eigenfunction equation becomes

$$\phi_\lambda'' - y\phi_\lambda' - \frac{\lambda}{\alpha}\phi_\lambda = 0.$$

This is the eigenvalue equation for the Hermite polynomials[1] (with eigenvalues scaled by α), which are defined as:

$$H_n(x) = (-1)^n e^{x^2/2}\frac{d^n}{dx^n}e^{-x^2/2}, \qquad H_n = \{1, x, x^2-1, x^3-3x, x^4-6x^2+3, \ldots\}$$

Therefore, with normalizing constants chosen so that $\|\phi_n\|_\pi = 1$, we have

$$\phi_n(x) = (n!)^{-1/2}H_n(x\sqrt{2\alpha/\sigma^2}), \qquad \lambda_n = -n\alpha, \quad n = 0,1,\ldots.$$

The probability density at time t is

$$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma^2/2\alpha}}e^{-\frac{x^2\alpha}{\sigma^2}}\sum_n (n!)^{-1/2}A_n H_n(x\sqrt{2\alpha/\sigma^2})e^{-n\alpha t}$$

where the coefficients are

$$A_n = \frac{1}{\sqrt{n!}}\langle \rho_0(x), H_n(x\sqrt{2\alpha/\sigma^2})\rangle\,.$$

The probability density relaxes to the stationary probability exponentially quickly, with a rate governed by the smallest non-zero eigenvalue $\lambda_1 = \alpha$.

Let's calculate the stationary covariance function. Using our earlier calculations,

$$C(t) = \sum_{n=0}^{\infty} c_n^2 e^{-n\alpha t}, \qquad \text{where } c_n = \langle x, \psi_n\rangle_{L^2}\,.$$

Note that $x = \sqrt{\sigma^2/2\alpha}\phi_1(x)$, and $\langle \phi_1, \psi_j\rangle = 0$ if $j \neq 1$. Therefore $c_1 = \sqrt{\sigma^2/2\alpha}$, and $c_n = 0$ for $n \neq 1$. Putting this together gives

$$C(t) = \frac{\sigma^2}{2\alpha}e^{-\alpha t}.$$

The covariance function is just a single exponential, because x itself is an eigenfunction of the generator!

[1] This is the "probabilist's" definition of Hermite polynomials. You may also encounter the "physicist's" definition: $H_n^p(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}$, which differs from the probabilist's definition by a rescaling: $H_n^p(x) = 2^{n/2}H_n(\sqrt{2}x)$.

Example 12.7 (Mean first passage time) Let's calculate the $T(x)$, the mean first passage time to ∂D from $x \in D$, using an eigenfunction expansion. Expand the mfpt as

$$T(x) = \sum_{i=1}^{\infty} a_i \phi_i(x)\,,$$

where ϕ_i are eigenfunctions for the problem with absorbing boundary conditions. Then, substituting into the equation for the mfpt and taking the inner product with ψ_i, gives

$$\mathscr{L}T = -1 \quad \Rightarrow \quad \sum_{i=1}^{\infty} a_i \lambda_i \phi_i(x) = -1 \quad \Rightarrow \quad a_i \lambda_i = \langle -1, \psi_i \rangle\,.$$

Therefore

$$T(x) = \sum_i \frac{1}{|\lambda_i|} \phi_i(x) \int \psi_i(y) dy\,.$$

Suppose the smallest eigenvalue (in absolute value) is a lot smaller than all the others: $|\lambda_1| \ll |\lambda_i|$ for $i > 1$. Then the series above can be approximated by its first term. Then $\mathscr{L}\phi_1 = \lambda_1 \phi_1 \approx 0$, since $|\lambda_1|$ is small. Therefore $\phi_1 \approx K$, a constant, so $1 = \int \psi_1(x)\phi_1(x) \approx K \int \psi_1(x)$. We obtain the approximation

$$T(x) \approx \frac{1}{|\lambda_1|}\,.$$

That is, the smallest absolute eigenvalue gives the inverse timescale for reaching the boundary. These approximations can be made more systematic using asymptotic methods, see [Gardiner, 2009, Section 6.6.1, p.166] and [Gardiner, 2009, Chapter 14].

Example 12.8 (Two-dimensional Brownian motion in a square) [From Gardiner, 2009, section 6.6.1, p.166] Consider a two-dimensional Brownian motion with constant diffusivity D in a square E with corners $(0,0),(0,1),(1,0),(1,1)$, and let $T(x)$ be the mean first passage time to the boundary, ∂E. T solves

$$\frac{D}{2}(\partial_{xx}T + \partial_{yy}T) = -1, \qquad T(\partial E) = 0\,.$$

The eigenfunctions and eigenvalues for this problem are

$$\psi_{n,m}(x,y) = \sin(n\pi x)\sin(m\pi y), \quad \phi_{n,m}(x,y) = 4\sin(n\pi x)\sin(m,\pi y)\,, \quad \lambda_{n,m} = \frac{\pi^2 D}{2}(n^2+m^2)\,,$$

with $n,m = 1,2,\ldots$. One can work out that $a_{n,m} = 0$ if either of n,m are even, and $a_{n,m} = \frac{4}{mn\pi^2}$ if both n,m are odd. Therefore

$$T(x,y) = \frac{1}{D} \sum_{n,m \text{ odd}} \frac{32}{\pi^2 nm(m^2+n^2)} \sin(n\pi x)\sin(m\pi y)\,.$$

12.5 Even versus Odd variables*

Our discussion so far applies to physical systems where all variables are *even*: they "look" the same forward and backward in time. For example, if you watch a movie of a car driving down the road, and you stop the movie halfway through and start playing it backwards, the car's position doesn't change the instant you

start playing the movie backwards. If you only observe the car's position instantaneously, you can't tell if the movie is playing forwards or backwards – position is an even variable. However, the car's velocity *does* change when you play the movie backwards – the velocity reverses sign. Based on the instantaneous velocity, you can tell whether the movie is playing forward or backward in time. Velocity is an example of an *odd* variable – it changes sign, if time starts going backward.

In general, each physical variable x_i is classified as either *even* or *odd*, depending on how it transforms under time reversal. We have $x_i \to \varepsilon_i x_i$, with $\varepsilon_i = +1(-1)$ for an even (odd) variable respectively. Examples of even variables include position, acceleration, force, voltage, energy, electric polarization. Examples of odd variables include velocity, angular and linear momentum, magnetic field, density of electric current, etc.

The previous results that link reversibility to a zero steady-state flux, do not apply to systems with odd variables. For example, you saw in a previous homework that in the Langevin equations, which contain velocities, the steady-state flux is not zero. These equations are used to model equilibrium systems all the time. How then should the concept of reversibility be generalized to such systems?

As an example, consider a gas of particles with positions contained in vector x and velocities contained in vector v, and remember that $\frac{dx}{dt} = v$. Suppose the system moves from state $(x,v) \to (x',v')$ in some time interval of length Δt. This is *not* the same as moving from $(x',v') \to (x,v)$ backwards in time, because if you change the direction of time, then the velocities of each particle must change sign. What it *is* physically equivalent to is moving from $(x',-v') \to (x,-v)$ in the same time interval Δt. Indeed, to go from $x \to x'$ in a small time Δt requires $v \approx (x'-x)/\Delta t$, and to go from $x' \to x$ requires $v' \approx (x-x')/\Delta t = -v$.

Therefore, for this gas of particles, detailed balance or time-reversibility should be written as

$$p(r',v',\tau|r,v,0)\pi(r,v) = p(r,-v,\tau|r',-v',0)\pi(r',v') \; .$$

The most general principle of detailed balance requires that

$$P(x \to y, \text{ forward in time}) = P(y \to x, \text{ backward in time}), \qquad \text{in steady-state,} \tag{22}$$

i.e. the probability of making some transition forward in time, equals the probability of making the reverse transition, backward in time, when the system is in steady-state, and where all variables change sign in the appropriate way. This principle comes from microscopic reversibility: Newton's laws are time-reversible, so if we coarse-grain them, we want the stochastic system to preserve the same property. More precisely,

Definition. A Markov process is *reversible* or satisfies *detailed balance* if

$$p(y,t|x,s)\pi(x) = p(\varepsilon x,t|\varepsilon y)\pi(y). \tag{23}$$

Conditions on the coefficients $b(x), a(x)$ of a time-homogeneous SDE that are both necessary and sufficient for detailed balance to be satisfied are [Gardiner, 2009, Section 6.3.5]

(i) $\varepsilon_i b_i(\varepsilon x)\pi(x) = -b_i(x)\pi(x) + \sum_j \partial_j(2a_{ij}(x)\pi(x))$

(ii) $\varepsilon_i \varepsilon_j a_{ij}(\varepsilon x) = a_{ij}(x)$.

Notice that these are formulated in terms of $\pi(x)$, so you need to know this first in order to check the conditions. When all variables are even, these conditions reduce to $\underline{j}_s = 0$.

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