LECTURE 2

Mathematical tools from potential theory:
capacities, harmonic functions, variational principles.

§ SETTING

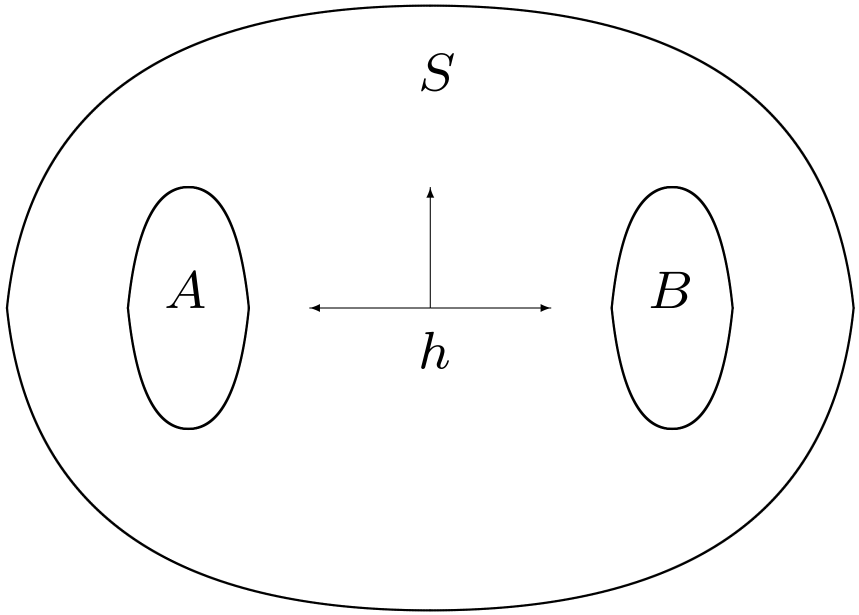
We place ourselves in the setting of a discrete-time Markov process $X = (X_n)_{n\in\mathbb{N}_0}$ on a countable state space S with a transition kernel

$$P = (p(x,y))_{x,y\in S}$$

and a generator $L = P - \mathbb{I}$. We assume that X is irreducible.

1. The first fundamental object in potential theory is the following. Let $A, B \subset S$ be two non-empty disjoint subsets. Consider the Dirichlet problem

$$\begin{aligned}
(-Lh)(x) &= 0, & \forall\, x \in S\backslash(A \cup B),\\
h(x) &= 1, & \forall\, x \in A,\\
h(x) &= 0, & \forall\, x \in B.
\end{aligned}$$



Dirichlet problem for $h\colon\ S \to [0,1]$ with boundary conditions $h \equiv 1$ on A ('target set') and $h \equiv 0$ on B ('killing set').

If S is finite, then the Dirichlet problem always has a unique solution. This solution, which is harmonic on $S\backslash(A\cup B)$, is denoted by $h_{A,B}(x)$ and is called the equilibrium potential.

2. The following representation holds:

$$h_{A,B}(x) = \mathbb{P}_x\left(\tau_A < \tau_B\right), \quad x \in S\backslash(A\cup B).$$

Here, $\tau_C = \inf\{n\in\mathbb{N}\colon\ X_n \in C\}$, where X_0 is ignored.

REMARK: For $x \in A\cup B$, we can write

$$\begin{aligned}
\mathbb{P}_x\left(\tau_A < \tau_B\right) &= \sum_{y\in S\backslash(A\cup B)} p(x,y)\mathbb{P}_y\left(\tau_A < \tau_B\right) + \sum_{y\in A} p(x,y) \\
&= \sum_{y\in S} p(x,y) h_{A,B}(y) = (P h_{A,B})(x) \\
&= (L h_{A,B})(x) + h_{A,B}(x).
\end{aligned}$$

Hence

$$x \in A: \quad (-Lh_{A,B})(x) = \mathbb{P}_x\left(\tau_B < \tau_A\right),$$
$$x \in B: \quad (Lh_{A,B})(x) = \mathbb{P}_x\left(\tau_A < \tau_B\right).$$

The quantity

$$e_{A,B}(x) \equiv (-Lh_{A,B})(x), \qquad x \in A,$$

is called the equilibrium measure on A, and is the second fundamental object. We know that $e_{A,B}(x) = 0$ for all $x \in S \setminus (A \cup B)$.

3. The Green function of X killed at B is defined as

$$G_B(x,y) = \mathbb{E}_x\left[\sum_{n=0}^{\tau_B-1} 1_{\{X_n=y\}}\right], \qquad x,y \notin B,$$

and is the third fundamental object.

4. The equilibrium potential $h_{A,B}$ satisfies the following inhomogeneous Dirichlet problem

$$\begin{array}{rcll} (-Lh)(x) & = & e_{A,B}(x), & \qquad \forall\, x \in S\backslash B, \\ h(x) & = & 0, & \qquad \forall\, x \in B. \end{array}$$

THEOREM 2.1

$$h_{A,B}(x) = \sum_{y\in A} G_B(x,y)e_{A,B}(y), \qquad x \in S.$$

THEOREM 2.1, whose proof is straightforward, allows us to express the Green function in terms of the equilibrium potential and the equilibrium measure: simply choose $A = \{a\}$, to get

$$G_B(x,a) = \frac{h_{a,B}(x)}{e_{a,B}(a)}, \qquad x \in S.$$

Note that

$$e_{a,B}(a) = \mathbb{P}_a(\tau_B < \tau_a)$$

has the meaning of an escape probability from $a \in A$ to B.

§ DIRICHLET FORM

Henceforth we restrict to reversible Markov processes.

DEFINITION 2.2

A Markov process with countable state space S and with transition kernel $P = (p(x,y))_{x,y \in S}$ is called reversible if there exists $\mu\colon\ S \to [0,\infty)$ such that

$$\mu(x)p(x,y) = \mu(y)p(y,x) \qquad \forall\, x,y \in S.$$

The function μ is called the reversible measure of the Markov process, and is easy to compute except for the normalisation.

The function space $L^2(S,\mu)$ is a natural space to work on when the Markov process is reversible with respect to μ.

LEMMA 2.3

(a) If μ is a reversible measure for P, then μ is an invariant measure for P.

(b) If μ is an invariant measure for P, then $Pf \in L^2(S,\mu)$ for all $f \in L^2(S,\mu)$.

DEFINITION 2.4

Let L be the generator of a Markov process with reversible measure μ. Then L defines a quadratic form

$$\mathcal{E}(f,g) \equiv \sum_{x\in S} \mu(x) f(x)(-Lg)(x), \qquad f,g \in L^2(S,\mu),$$

called the Dirichlet form, which is non-negative-definite.

In the discrete case it is easy to write out $\mathcal{E}(f,g)$ explicitly. Namely, by reversibility,

$$\mathcal{E}(f,g) = \sum_{x,y\in S} \mu(x)p(x,y)f(x)[g(x)-g(y)]$$
$$= \sum_{x,y\in S} \mu(x)p(x,y)f(y)[g(y)-g(x)].$$

Symmetrising between the first and the second expression, we get

$$\begin{aligned}\mathcal{E}(f,g) &= \frac{1}{2}\sum_{x,y\in S} \mu(x)p(x,y) \\ &\qquad \times \Big\{ f(x)[g(x)-g(y)] + f(y)[g(y)-g(x)] \Big\} \\ &= \frac{1}{2}\sum_{x,y\in S} \mu(x)p(x,y) \\ &\qquad \times [f(x)-f(y)][g(x)-g(y)].\end{aligned}$$

THEOREM 2.5

If P is reversible with respect to μ, then for all non-empty disjoint sets $A, B \subset S$,

$$h_{A,B}(x) = \sum_{y \in A} \frac{\mu(y)}{\mu(x)} G_B(y,x)\, e_{A,B}(y), \qquad x \in S.$$

In particular, if f given g is a solution of the inhomogeneous Dirichlet problem

$$\begin{aligned} (-Lf)(x) &= g(x), \qquad && \forall\, x \in S \setminus B, \\ f(x) &= 0, && \forall\, x \in B, \end{aligned}$$

then

$$\sum_{y \in A} \nu_{A,B}(y) f(y) = \frac{1}{\mathrm{cap}(A,B)} \sum_{x \in S} \mu(x) h_{A,B}(x) g(x),$$

where $\nu_{A,B}$ is the probability measure on A given by

$$\nu_{A,B}(y) = \frac{\mu(y) e_{A,B}(y)}{\mathrm{cap}(A,B)}, \qquad y \in A,$$

with normalisation factor the capacity

$$\text{cap}(A,B) \equiv \sum_{x\in A} \mu(x) e_{A,B}(x).$$

PROOF:

By reversibility,

$$\mu(x)G_B(x,y) = \mu(y)G_B(y,x), \qquad x,y \in S,$$

which yields the formula for $h_{A,B}$ via THEOREM 2.1.

Multiplying this formula by $\mu(x)g(x)$, summing over $x \in S$, and noting that $\sum_{x\in S} G_B(y,x)g(x) = f(y)$, we get the formula for $\sum_{y\in A} \nu_{A,B}(y)f(y)$, apart from the normalisation factor $\text{cap}(A,B)$. $\square$

Here, $\nu_{A,B}$ is called the last-exit biased distribution on A for the transition from A to B, while $\mathrm{cap}(A,B)$ is called the capacity of the pair (A,B).

The following corollary of THEOREM 2.5, obtained by picking $g=1$ on $S \setminus B$, offers a formula for mean hitting times that plays a crucial role in our study of metastability.

COROLLARY 2.6

Let $A, B \subset S$ be non-empty and disjoint. For reversible Markov processes,

$$\sum_{x \in A} \nu_{A,B}(x)\, \mathbb{E}_x[\tau_B] = \frac{1}{\mathrm{cap}(A,B)} \sum_{y \in S} \mu(y) h_{A,B}(y).$$

In particular, for $A = \{x\}$,

$$\mathbb{E}_x[\tau_B] = \frac{1}{\mathrm{cap}(x,B)} \sum_{y \in S} \mu(y) h_{x,B}(y).$$

LEMMA 2.7

Let $A, B \subset S$ *be non-empty and disjoint. Then* $\text{cap}(A, B)$ *can be expressed as*

$$\text{cap}(A, B) = \mathcal{E}(h_{A,B}, h_{A,B}).$$

PROOF:

This is obvious from the definition of the Dirichlet form, the equilibrium potential, the equilibrium measure, and the capacity. $\square$

Note that LEMMA 2.7 becomes particularly useful through the alternative representation of the Dirichlet form as a quadratic form.

§ DIRICHLET PRINCIPLE

The capacity of A, B is given by the Dirichlet Principle

$$\boxed{\mathrm{cap}(A,B) = \inf_{\phi \in \Phi_{A,B}} \mathcal{E}(\phi,\phi)}$$

where

$$\Phi_{A,B} = \{\phi\colon\ S \to [0,1]\colon\ \phi(A) = 1,\ \phi(B) = 0\}$$

and

$$\mathcal{E}(\phi,\phi) = \sum_{x,y \in S} \mu(x)p(x,y)[\phi(y) - \phi(x)]^2$$

is the Dirichlet form associated with the Markov dynamics.

§ THOMSON PRINCIPLE

A unit flow from B to A is a map $u\colon S \times S \to \mathbb{R}$ such that the flows into and out of nodes in $S \setminus \{A, B\}$ equal 0, while the flow out of B and into A equal 1.

The Thomson Principle reads

$$\boxed{\mathrm{cap}(A,B) = \sup_{u \in \mathcal{U}_{A,B}} \frac{1}{\mathcal{D}(u,u)}}$$

where $\mathcal{U}_{A,B}$ is the set of unit flows from B to A, and

$$\mathcal{D}(u,u) = \sum_{x,y \in S} \frac{1}{\mu(x)p(x,y)} u(x,y)^2$$

is a dual of the Dirichlet form.

The infimum in the Dirichlet Principle is uniquely taken at the equilibrium potential

$$\phi(x) = h_{A,B}(x),$$

while the supremum in the Thomson Principle is uniquely taken at the equilibrium flow u given by

$$u(x,y) = \frac{\mu(x)p(x,y)\left[h_{A,B}(y) - h_{A,B}(x)\right]_+}{\mathrm{cap}(A,B)}.$$

§ CAPACITY ESTIMATES

The estimation of capacity proceeds via

- Dirichlet principle
  $\text{cap}(A, B) \leq \mathcal{E}(\phi, \phi)$,
- Thomson principle
  $\text{cap}(A, B) \geq 1/\mathcal{D}(u, u)$,

where ϕ, u are properly chosen test functions and test flows that live in the vicinity of the critical droplet.

The choice of ϕ, u requires physical insight into what drives the metastable crossover.

GUIDING PRINCIPLE:

The formula relating metastable crossover time to capacity effectively links non-equilibrium to equilibrium. The inverse of the capacity plays the role of effective resistance.

ASYMPTOTICS:

The Dirichlet Principle and Thomson Principle allow for the derivation of upper and lower bounds on capacity. With care, these can be made to match asymptotically.

REDUCTION:

In metastable regimes the high-dimensional Dirichlet form and dual Dirichlet form are largely controlled by the low-dimensional set of critical droplets.

§ RANDOM WALKS

For later use, in Lecture 4, we compute relevant quantities for nearest-neighbour random walk on an interval $[a,b] \subset \mathbb{Z}$.

- The Dirichlet problem reads

$$\begin{aligned} &p(x,x+1)[h(x+1)-h(x)] \\ &\qquad\qquad + p(x,x-1)[h(x-1)-h(x)] = 0, \qquad a<x<b, \\ &h(a) = 0, \\ &h(b) = 1. \end{aligned}$$

This is a recursion relation for the differences $h(x)-h(x-1)$, and a straightforward computation leads to expression (swap the roles of a and b)

$$h_{b,a}(x) = \mathbb{P}_x(\tau_b < \tau_a) = \frac{R(a,x)}{R(a,b)}, \qquad a<x<b,$$

with (use reversibility to bring in μ)

$$R(u,v) = \sum_{y=u+1}^{v} \frac{1}{\mu(y)} \frac{1}{p(y,y-1)}, \qquad u < v.$$

- The equilibrium measure is given by the formula

$$\begin{aligned} &e_{a,b}(a) \\ &\quad = p(a,a+1) h_{b,a}(a+1) + p(a,a-1) h_{b,a}(a-1) \\ &\quad = p(a,a+1) h_{b,a}(a+1), \end{aligned}$$

where we use that $h_{b,a}(a-1) = 0$. Inserting the formula for $h_{b,a}$ derived above, we get

$$\begin{aligned} e_{a,b}(a) &= p(a,a+1) \frac{R(a,a+1)}{R(a,b)} \\ &= \frac{\frac{p(a,a+1)}{\mu(a+1)p(a+1,a)}}{R(a,b)} = \frac{1}{\mu(a)R(a,b)}. \end{aligned}$$

Consequently, for the capacity we get

$$\text{cap}(a,b) = \frac{1}{R(a,b)}.$$

• Inserting the expressions for $h_{a,b}$ and $\text{cap}(a,b)$ into the formula for $\mathbb{E}_x[\tau_a]$ in COROLLARY 2.6 (with $A = \{x\}$ and $B = \{a\}$), we get

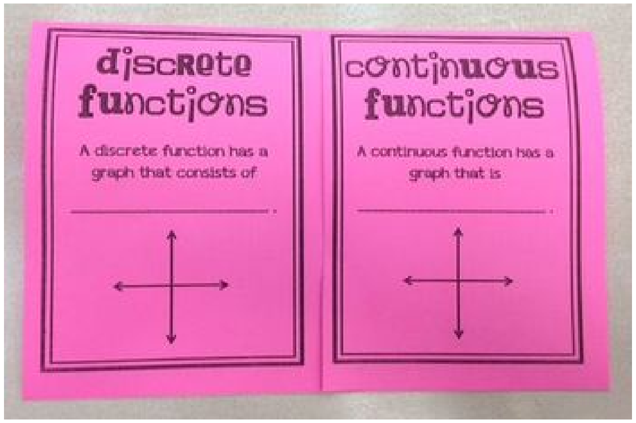
$$\mathbb{E}_x[\tau_a] = R(a,x) \left(\sum_{y=a+1}^{x-1} \mu(y) \frac{R(a,y)}{R(a,x)} + \sum_{y=x}^{\infty} \mu(y) \right), \quad a < x.$$

This formula will be needed in Lecture 4 to compute the average metastable crossover time for a mean-field model called the Curie-Weiss model. The latter will be shown to link up with the Kramers formula for Brownian motion in a double-well potential, hinted at in Lecture 1.

§ DICRETE VERSUS CONTINUOUS

Definitions and computations become more involved when the state space is infinite discrete or continuous.

Often A and B are not single configurations but are sets of configurations with an interesting geometric structure.



We will see examples in Lectures 9-12.

LITERATURE:

Chapter 7 of Bovier and den Hollander 2015, and references therein.