LECTURE 3

Characterisation of metastability.
Towards Interacting Particle Systems.

§ CHARACTERISATION OF METASTABILITY

Consider a Markov process $X = (X_n)_{n\in\mathbb{N}_0}$ with discrete state space S in discrete time. Let $\mathbb{P}_x$ denote the law of X given $X_0 = x$. We assume that X is uniquely ergodic with reversible invariant measure μ.

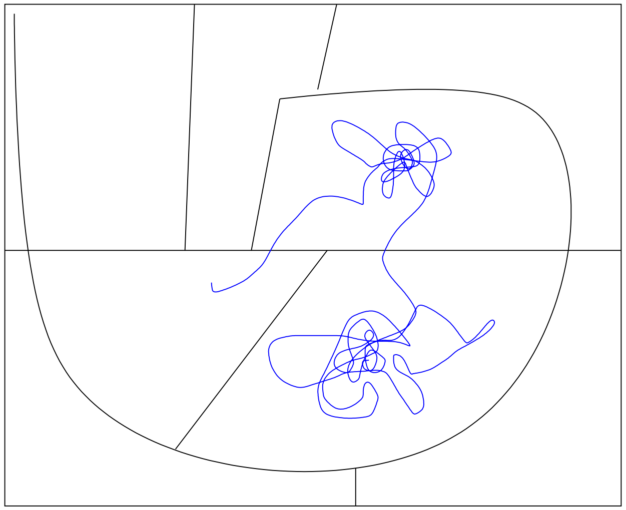
For $C \subset S$, let

$$\tau_C = \inf\{n \in \mathbb{N}\colon\ X_n \in C\}.$$

The fundamental feature we would like to associate with metastability is the existence of two well-separated time scales and the partition of the state space into disjoint sets S_i, $i \in I$, such that, when X starts in S_i:

- On a short time scale X reaches some sort of local equilibrium concentrated on S_i.
- On a long time scale X exits S_i and moves to some S_j with $j \neq i$, where it again reaches local equilibrium.

Etcetera.



Think of X as hopping between quasi-invariant sets. An appealing way to characterise the rapid approach to local equilibrium is by saying that X is locally recurrent: each S_i contains a small set $B_i \subset S_i$ that is revisited by X frequently before it moves out of S_i.

An intuitively appealing definition of metastability could therefore be the following.

DEFINITION 3.1

A family of Markov processes is called metastable if there exists a collection of disjoint sets $B_i \subset S$, $i \in I$, such that

$$\frac{\sup_{x \notin \cup_{i \in I} B_i} \mathbb{E}_x[\tau_{\cup_{i \in I} B_i}]}{\inf_{i \in I} \inf_{x \in B_i} \mathbb{E}_x[\tau_{\cup_{j \in I \setminus i} B_j}]} = o(1).$$

Here, $o(1)$ is a small intrinsic parameter that characterises the degree of metastability.

Since, typically, we deal with a family of Markov processes indexed by a parameter (like temperature, system size, etc.), we can make the quotient as small as we like in an appropriate metastable regime.

DEFINITION 3.1 characterises metastability in terms of average hitting times. Certainly we want such a property to hold in a metastable setting.

However, one of our goals is to compute average hitting times, and so the condition would put us in a circular set-up. It is desirable to have a definition involving more manageable quantities.

The relations in Lecture 2 between average hitting times and capacities suggest that we pursue a characterisation of metastability through capacities.

DEFINITION 3.2

A family of Markov processes is called metastable if there exists a collection of disjoint sets $B_i \subset S$, $i \in I$, such that

$$\frac{\sup_{i\in I} \sup_{x\in B_i} \mathbb{P}_x(\tau_{\cup_{j\in I\setminus i} B_j} < \tau_{B_i})}{\inf_{x\notin \cup_{i\in I} B_i} \mathbb{P}_x(\tau_{\cup_{i\in I} B_i} < \tau^{\circlearrowleft}_{B(x)})} = o(1),$$

where

$$B(x) \text{ is an appropriate neighbourhood of } x$$

and

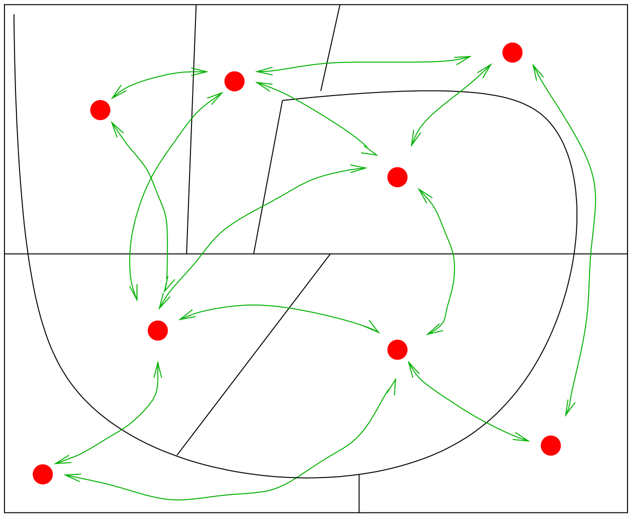
$$\tau^{\circlearrowleft}_{B(x)} \equiv \inf\{t > \tau_{B(x)^c} \colon X_t \in B(x)\}$$

is the first time when X returns to $B(x)$ after having left $B(x)$.

This definition leaves several questions open:
- What should be the choice for $B(x)$?
- How can we relate the probabilities appearing in the definition to capacities, as advertised in Lecture 2?

It will become clear that the usefulness of DEFINITION 3.2 depends crucially on further properties of the sets B_i, $i \in I$, and on local mixing properties of X.

Everything becomes transparent when the state space S is finite, and we replace the sets B_i, $i \in I$, and $B(x)$, $x \in S$, by single points. It is useful to understand this simple setting first and later look for generalisations.



The red configurations form a set $\mathcal{M} \subset \Omega$ of metastable points.

DEFINITION 3.3

Suppose that $|S| < \infty$. A Markov processes X is said to be ρ-metastable with respect to a set of points $\mathcal{M} \subset S$ if

$$|S| \frac{\text{sup}_{x \in \mathcal{M}} [\text{cap}(x, \mathcal{M} \backslash x)/\mu(x)]}{\text{inf}_{y \notin \mathcal{M}} [\text{cap}(y, \mathcal{M})/\mu(y)]} \leq \rho,$$

which can be written alternatively as

$$|S| \frac{\text{sup}_{x \in \mathcal{M}} \mathbb{P}_x(\tau_{\mathcal{M} \backslash x} < \tau_x)}{\text{inf}_{y \notin \mathcal{M}} \mathbb{P}_y(\tau_{\mathcal{M}} < \tau_y)} \leq \rho.$$

Here, ρ is a small intrinsic parameter that characterises the degree of metastability.

We want to show that if a process is metastable in the sense of DEFINITION 3.3, then we can express the average crossover times between points of $\mathcal{M}$ in terms of capacities and the reversible invariant measure alone.

This approach is based on the key formula that we derived in Lecture 2, which here reads

$$\mathbb{E}_m[\tau_{\mathcal{M}'}] = \frac{1}{\mathrm{cap}(m, \mathcal{M}')} \sum_{y \in S} \mu(y) h_{m,\mathcal{M}'}(y),$$

$$\mathcal{M}' \subset \mathcal{M}, \; m \in \mathcal{M} \setminus \mathcal{M}',$$

where typically $\mathcal{M}'$ is a set of points with a free energy lower than that of m.

The denominator can be estimated with the help of the Dirichlet Principle and the Thomson Principle presented in Lecture 2. The numerator can be estimated by controlling the equilibrium potential in terms of capacities.

§ RENEWAL ESTIMATES

Estimation of the equilibrium potential through capacities is based on a renewal argumentthat is simple in the case of a discrete state space.

LEMMA 3.4

Let $A, B \subset S$ *be non-empty disjoint sets, and let* $x \notin A \cup B$*. Then*

$$\max\left(1 - \frac{\text{cap}(x, B)}{\text{cap}(x, A)}, 0\right) \leq h_{A,B}(x) \leq \min\left(\frac{\text{cap}(x, A)}{\text{cap}(x, B)}, 1\right).$$

PROOF:

The upper bound follows from the estimate

$$h_{A,B}(x) = \mathbb{P}_x(\tau_A < \tau_B) = \frac{\mathbb{P}_x(\tau_A < \tau_{B\cup x})}{1 - \mathbb{P}_x(\tau_x < \tau_{A\cup B})}$$

$$= \frac{\mathbb{P}_x(\tau_A < \tau_{B\cup x})}{\mathbb{P}_x(\tau_{A\cup B} < \tau_x)} \leq \frac{\mathbb{P}_x(\tau_A < \tau_x)}{\mathbb{P}_x(\tau_B < \tau_x)} = \frac{\mathrm{cap}(x,A)}{\mathrm{cap}(x,B)},$$

where the second equality comes from counting the returns to x without a hit of A or B. The lower bound follows from the upper bound via the symmetry relation $h_{A,B}(x) = 1 - h_{B,A}(x)$. $\square$

§ TOWARDS INTERACTING PARTICLE SYSTEMS

We think of an interacting particle system whose state space consists of a finite set of configurations Ω and whose evolution is given by a Markov generator L acting on a class of test functions $\phi\colon\ \Omega \to \mathbb{R}$ as

$$(L\phi)(\eta) = \sum_{\eta' \in \Omega} c(\eta, \eta')[\phi(\eta') - \phi(\eta)], \qquad \eta \in \Omega,$$

with $c(\eta, \eta')$ the rate at which the Markov dynamics moves from η to η'.

Note the change of notation

$$S \to \Omega, \qquad x, y \to \eta, \eta',$$

to mark that henceforth we focus on interacting particle systems. Further note that we consider continuous time instead of discrete time.

A natural choice for the transition rates is

$$c(\eta,\eta') = \mathrm{exp}\Big(-\beta[H(\eta')-H(\eta)]_+\Big), \qquad \eta,\eta' \in \Omega,$$

which has reversible equilibrium

$$\mu(\eta) = \frac{1}{\Xi}\,\mathrm{e}^{-\beta H(\eta)}, \qquad \eta \in \Omega,$$

where H, β and Ξ have the following interpretation:

- $H\colon\ \Omega \to \mathbb{R}$ is the Hamiltonian that associates with each configuration η an energy $H(\eta)$.
- $\beta \in (0,\infty)$ is the inverse temperature (= interaction strength).
- Ξ is the normalising partition function.

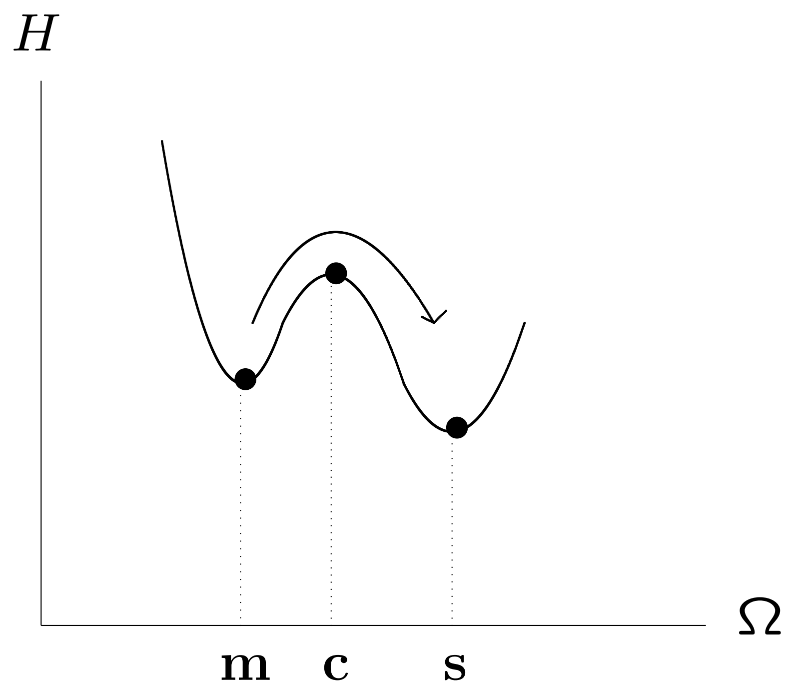
Typically transitions are restricted to a subset of admissible transitions.

The above dynamics is called the Metropolis dynamics associated with (H, β), and its equilibrium is called the Gibbs measure.

The proper choice of Ω, H and β depends on the model at hand. For $\beta \to \infty$ or $|\Omega| \to \infty$ we may expect to see metastability under certain conditions.

Typically, the Hamiltonian H has three important sets of configurations:

- Global minimum $\mathbf{s}$: stable state.
- Local minimum $\mathbf{m}$: metastable state.
  (= bottom of the deepest valley not containing $\mathbf{s}$).
- Saddle point $\mathbf{c}$: critical droplet.
  (= ridge between the valleys containing $\mathbf{m}$ and $\mathbf{s}$).



Caricature of the (free) energy lanscape.

Examples of dynamics:

spin-flip systems	Lecture 7
particle-hop systems	Lecture 8
systems of interacting disks	Lectures 9–11

If $\mathbf{m}$ is a single configuration, then the average metastable crossover time from $\mathbf{m}$ to $\mathbf{s}$ is given by

$$\boxed{\mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) = \frac{\sum_{\eta\in\Omega}\mu(\eta)\,h_{\mathbf{m},\mathbf{s}}(\eta)}{\text{cap}(\mathbf{m},\mathbf{s})}}$$

EXERCISE!

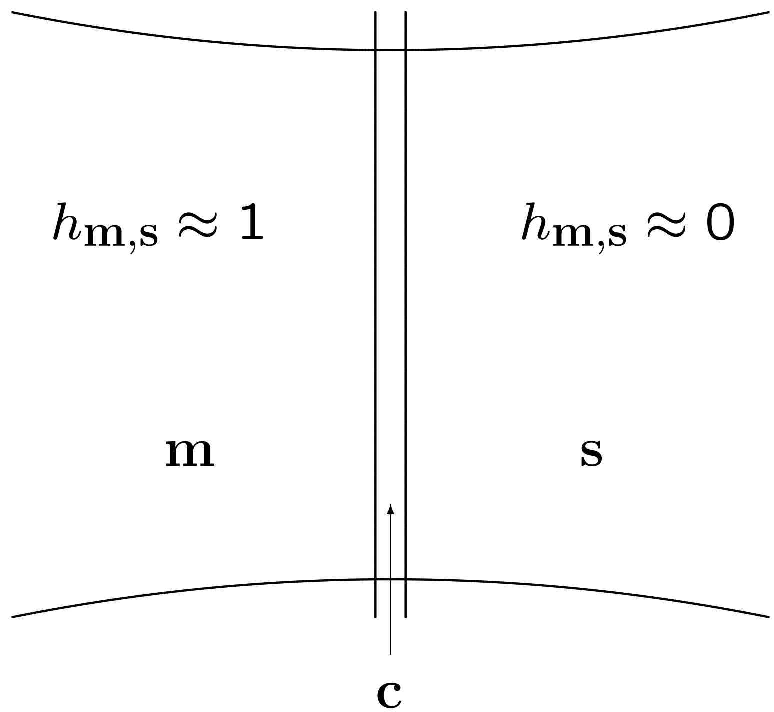
where $\tau_{\mathbf{s}}$ is the first hitting time of $\mathbf{s}$,

$$h_{\mathbf{m},\mathbf{s}}(\eta) = \mathbb{P}_\eta(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}), \qquad \eta \in \Omega,$$

is the harmonic function and

$$\text{cap}(\mathbf{m},\mathbf{s}) = \tfrac{1}{2}\sum_{\eta,\eta'\in\Omega}\mu(\eta)c(\eta,\eta')\,[h_{\mathbf{m},\mathbf{s}}(\eta') - h_{\mathbf{m},\mathbf{s}}(\eta)]^2$$

is the capacity.



Schematic picture of the harmonic function $h_{\mathbf{m},\mathbf{s}}$:

trivial inside the valleys around $\mathbf{m}$ and $\mathbf{s}$, nontrivial around $\mathbf{c}$.

In metastable regimes it often turns out that

$$\sum_{\eta \in \Omega} \mu(\eta)\, h_{\mathbf{m},\mathbf{s}}(\eta) = [1 + o(1)]\, \mu(\mathbf{m})$$

in which case

$$\mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) = [1 + o(1)]\, \frac{\mathrm{e}^{-\beta H(\mathbf{m})}}{\Xi\, \mathrm{cap}(\mathbf{m}, \mathbf{s})}.$$

This formula shows that the average metastable crossover time is essentially controlled by the capacity, which in turn is essentially controlled by the harmonic function near the critical set.

Note that for the Metropolis dynamics

$$\Xi\, \mathrm{cap}(\mathbf{m}, \mathbf{s}) = \tfrac{1}{2} \sum_{\eta, \eta' \in \Omega} \mathrm{e}^{-\beta [H(\eta) \vee H(\eta')]} [h_{\mathbf{m},\mathbf{s}}(\eta') - h_{\mathbf{m},\mathbf{s}}(\eta)]^2.$$

§ SUPPORTING TECHNIQUES

Various methods are available to tackle specific hurdles that arise when we want to apply the potential-theoretic tools described in Lecture 2 to describe the metastable behaviour of interacting particle systems. These include:

- approximation via test functions and test flows
- coarse-graining
- lumping
- coupling
- isoperimetric inequalities

We will see plenty of examples in Lectures 4–16.

LITERATURE:

Chapters 8–9 of Bovier and den Hollander 2015, and references therein.