Peer Seminar
'23.11.9.
Younghun Jo.

Capacity of Markov Processes and Variational Principles.

Table of Contents.

References

- R. Durrett, Probability : Theory and Examples.
- T. M. Liggett, Continuous Time Markov Processes : An Introduction.
- A. Bovier, F. den Hollander, Metastability : A Potential-Theoretic Approach.
- I. Seo, Generalized Dirichlet and Thomson Principles and Their Applications.

§ 0. Preliminary

Recall R. Durnett, T. M. Liggett, ...

- S : (finite) state space.
- A stochastic process $(X_t)_{t\in I}$ is a Markov process if
  - (i) it is casual, i.e., the law of X_t can be described in $\mathcal{F}_{t-} = \sigma(X_s,\ 0\le s<t)$;
  - (ii) it is forgetful of the past, i.e., the law of X_t is independent of the values of $X_u,\ 0\le u<s$ for all $0\le s<t$.

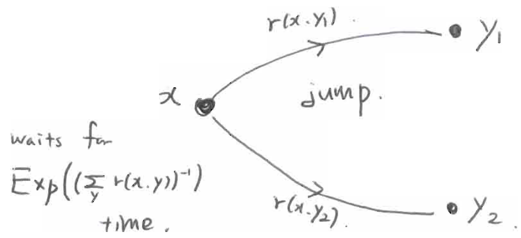
  If $I=\mathbb{Z}_{\ge 0}$, then (X_t) can be described w/ its transition probability $p: S\times S\to[0,1]$ given by $\mathbb{P}_x[X_1=y]=p(x,y)$.

- One can also define a continuous-time Markov process (i.e., $I=\mathbb{R}_{\ge 0}$) in the same manner.

  There are several equivalent formulations :
  - Transition rate (or, jump rate) $r: S\times S\longrightarrow[0,\infty)$. $\quad (r(x,x)=0)$
  - Jump chain & holding time $(\hat{X}_n)_{n\in\mathbb{Z}_{\ge0}}$: position of X_t after nth jump.

    $\rightsquigarrow$ transition probability $p(x,y)=\dfrac{r(x,y)}{\sum_z r(x,z)}$

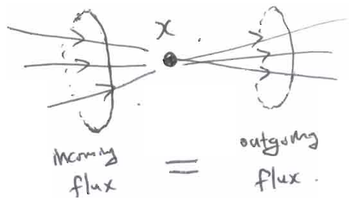
    holding time $S_n \sim \mathrm{Exp}\left(\left(\sum_y r(X_n,y)\right)^{-1}\right)$.
  - Markov semigroup $(P_t)_{t\ge0}$: $\mathcal{P}(S)\longrightarrow\mathcal{P}(S)$.



- If (X_t) is irreducible, i.e., "$\forall x,y\in S$, X can go from x to y w/ nonzero probability,"

  then $\exists!$ invariant probability measure μ on S.

  that is, $\displaystyle\sum_y \mu(x)\,r(x,y)=\sum_y \mu(y)\,r(y,x)\quad \forall x\in S.$



- Note that every real ftn on S is in $L^2(\mu)$ since S is finite.

The <u>probability generator</u> $\mathcal{L} : L^2(\mu) \longrightarrow L^2(\mu)$ is defined by

$$\mathcal{L} f(x) = \sum_y r(x,y)\big(f(y) - f(x)\big).$$

then it satisfies $\displaystyle \mathcal{L} f = \lim_{t \searrow 0} \frac{P_t f - f}{t}$.

- let $\langle \cdot , \cdot \rangle_\mu$ be the inner product on $L^2(\mu)$.

The <u>Dirichlet form</u> associated to $(X_t)_{t \geq 0}$ is

$$\begin{aligned} \mathcal{D}(f) &:= \langle f, -\mathcal{L} f \rangle_\mu \\ &= \frac{1}{2} \sum_x \sum_y \mu(x)\, r(x,y)\, [f(y) - f(x)]^2 \geq 0. \end{aligned}$$

- We assume that $(X_t)_{t \geq 0}$ is <u>reversible</u>,

that is, $\mu(x)\, r(x,y) = \mu(y)\, r(y,x) \quad \forall x, y \in S$.

It is equivalent to saying that $\mathcal{L}$ is self-adjoint w.r.t. $\langle \cdot , \cdot \rangle_\mu$:

$$\langle f, \mathcal{L} g \rangle_\mu = \langle \mathcal{L} f, g \rangle_\mu \qquad \text{i.e.,} \quad \mathcal{L}^{+} = \mathcal{L}.$$

[<u>Note</u> The generator for time-reversed process of $(X_t)_{t \geq 0}$ is given by $\mathcal{L}^{+}$.].

- $h \in L^2(\mu)$ is said to be <u>harmonic</u> if $\mathcal{L} h \equiv 0$.

Note that in this case, $\big(h(X_t)\big)_{t \geq 0}$ is a martingale.

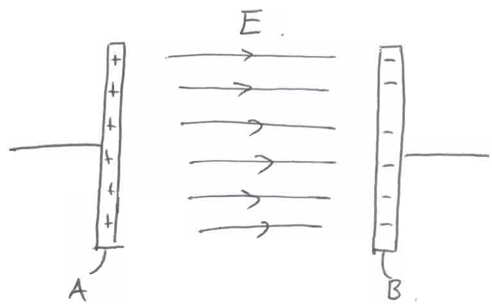
§1. Electrostatic Analogue

- $\Omega = \mathbb{R}^2$ or cpt $K \subseteq \mathbb{R}^2$.
- Consider the diffusion $(X_t)_{t\geq 0}$ on Ω, then $\mathcal{L} = \Delta$.
- Electrostatic potential V : $E = -\nabla V$.

  $\Rightarrow \Delta V = -\dfrac{\rho}{\varepsilon_0}$. ρ: charge density
- Dirichlet form : "Electrostatic energy"

$$\mathcal{D}(V) = \int V \, (-\Delta V) \, d^3r = \int |\nabla V|^2 \, d^3r = \int |E|^2 \, d^3r = \frac{2}{\varepsilon_0} \mathcal{U}.$$

- Capacitor :



  - V satisfies $V|_A \equiv V_0$. $V|_B \equiv 0$. $\Delta V \equiv 0$ on $(A \cup B)^c$.

    ↳ minimizes energy!

    : "Dirichlet problem".
  - Capacity : $C = \dfrac{2\mathcal{U}}{V_0^2} = \mathcal{D}(h_{A,B})$

    where $h_{A,B}|_A \equiv 1$. $h_{A,B}|_0 \equiv 0$. $\Delta h_{A,B} \equiv 0$ on $(A \cup B)^c$.

§2 Dirichlet Problem and Capacity

def For disjoint $A, B \subseteq S$,

the *equilibrium potential* $h_{A,B}$ between A and B w.r.t. $(X_t)_{t\geq 0}$ is

the unique solution of the Dirichlet problem :

$$h|_A \equiv 1, \quad h|_B \equiv 0, \quad \mathcal{L}h \equiv 0 \quad \text{on} \quad (A \cup B)^c.$$

The *capacity* between A and B is $\quad \mathrm{cap}(A, B) := \mathcal{D}(h_{A,B})$.

$\boxed{\text{lemma}}$ $\quad h_{A,B}(x) = \mathbb{P}_x[\tau_A < \tau_B], \quad \forall x \in S.$

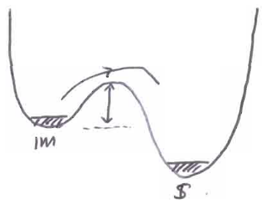
where $\tau_A = \inf\{t \geq 0 : X_t \in A\}$ is the *hitting time* of A.

$$\left[\begin{array}{l} \text{pf} \quad \mathbb{P}_x[\tau_A < \tau_B] \underset{\text{Markov}}{=} \sum_y \dfrac{r(x,y)}{\sum_z r(x,z)} \mathbb{P}_y[\tau_A < \tau_B], \\ \quad \Rightarrow \sum_y r(x,y) \left(\mathbb{P}_y[\tau_A < \tau_B] - \mathbb{P}_x[\tau_A < \tau_B]\right) = 0. \quad \blacksquare \end{array}\right].$$

Note
- $h_{B,A} = 1 - h_{A,B}$.
- $\langle 1, \mathcal{L}g \rangle_\mu = 0 \quad \forall g$.
- $\mathrm{cap}(A, B) = \mathcal{D}(h_{A,B}) = \mathcal{D}(h_{B,A}) = \mathrm{cap}(B, A)$.

Q. Why is capacity important?

- Metastability : "Spontaneous transition from a 'fake' stable state to the stable state"
- Common indicators of metastability :
  - exponential hitting time : $\tau_S^{(n)} = \inf\{t : X_t^{(n)} \in S\}$.
    $$\Rightarrow \frac{\log \mathbb{E}_{M}\, \tau_S^{(n)}}{n} \xrightarrow{n\to\infty} \exists\, c > 0 .$$
  - "independent" attempts : $\dfrac{\tau_S^{(n)}}{\mathbb{E}\,\tau_S^{(n)}} \xrightarrow{n\to\infty} \mathrm{Exp}(1)$ in distribution.



$\rightsquigarrow$ Essentially, we only need to know the mean hitting time $\mathbb{E}\tau$.

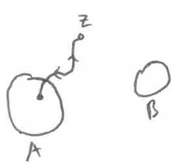
def The equilibrium measure $\nu_{A,B}$ between A and B on A is

$$\nu_{A,B}(x) := \frac{\mu(x) \sum_y r(x,y) \cdot \mathbb{P}_x[\tau_B < \tau_A^+]}{\mathrm{cap}(A,B)}$$

where $\tau_A^+ = \inf\{t>0 : X_t \in A \text{ and } \exists s\in[0,t] \text{ s.t. } X_s \neq X_0\}$ is the return time to A.

$\boxed{\text{Thm}}$ $$\mathbb{E}_{\nu_{A,B}} \tau_B = \frac{\sum_x h_{A,B}(x)\cdot \mu(x)}{\mathrm{cap}(A,B)} .$$

pf Write $\hat{\mathbb{P}}$ for the associated jump chain $(\hat{X}_n)$.
Note that the stationary measure for $\hat{X}$ is given by $M(x) = \mu(x)\cdot \sum_y r(x,y)$.
Fix $z \in S$.
Then,
$$h_{A,B}(z) = \mathbb{P}_z[\tau_A < \tau_B] = \hat{\mathbb{P}}_z[\hat\tau_A < \hat\tau_B]$$
$$\underset{\text{Markov}}{=} \sum_{n\geq 0}\sum_{y\in A} \hat{\mathbb{P}}_z[\hat{X}_n = y,\ n<\hat\tau_B]\cdot \hat{\mathbb{P}}_y[\hat\tau_B < \hat\tau_A^+]$$
$$= \sum_{y\in A}\Big(\hat{\mathbb{P}}_y[\hat\tau_B<\hat\tau_A^+]\cdot \sum_{n\geq0}\hat{\mathbb{P}}_z[\hat{X}_n=y,\ n<\hat\tau_B]\Big)$$
$$= \sum_{y\in A}\Big(\frac{M(y)}{M(z)}\hat{\mathbb{P}}_y[\hat\tau_B<\hat\tau_A^+]\cdot\sum_{n\geq0}\hat{\mathbb{P}}_y[\hat{X}_n=z,\ n<\hat\tau_B]\Big)$$
$$= \frac{\mathrm{cap}(A,B)}{M(z)}\sum_{y\in A}\Big(\nu_{A,B}(y)\cdot\sum_{n=0}^{\hat\tau_B-1}\hat{\mathbb{P}}_y[\hat{X}_n=z]\Big)$$
$$= \frac{\mathrm{cap}(A,B)}{M(z)}\,\mathbb{E}_{\nu_{A,B}}\Big[\int_0^{\tau_B}\mathbb{1}_z(X_t)\,dt\Big]$$
Sum over z. ∎



§3 Flow and Capacity

def
- Write $x \sim y$ if $r(x,y) > 0$. ($\Leftrightarrow r(y,x) > 0$).
  let $\mathcal{E} = \{(x,y) \in S \times S : x \sim y\}$ be the set of directed edges.
- $\phi : \mathcal{E} \longrightarrow \mathbb{R}$ is a flow if it is anti-symmetric. i.e., $\phi(x,y) = -\phi(y,x)$.
- The divergence of ϕ at x is $\nabla\phi(x) := \sum_{y \sim x} \phi(x,y)$.
  ϕ is said to be divergence-free at x if $\nabla\phi(x) = 0$.

Example Write $c(x,y) = \mu(x)\, r(x,y)$ $(= c(y,x))$.
For $f : S \longrightarrow \mathbb{R}$, the flow Ψ_f associated to f is given by

$$\Psi_f(x,y) := c(x,y)\big(f(y) - f(x)\big).$$

Prop $\nabla \Psi_f(x) = \mu(x) \cdot \mathcal{L} f(x)$.
In particular, $\Psi_{h_{A,B}}$ is divergence-free on $(A \cup B)^c$.

def let $\mathcal{F}$ be the space of flows.
Define the inner product of two flows ϕ, ψ by

$$\langle \phi, \psi \rangle_{\mathcal{F}} := \frac{1}{2} \sum_{x \sim y} \frac{\phi(x,y)\, \psi(x,y)}{c(x,y)}.$$

Write $\|\phi\|_{\mathcal{F}} = \langle \phi, \phi \rangle_{\mathcal{F}}^{1/2}$.

Prop
- $\langle \Psi_f, \phi \rangle_{\mathcal{F}} = -\sum_{x} f(x) \cdot \nabla\phi(x)$.
- $\|\Psi_f\|_{\mathcal{F}}^2 = \mathcal{D}(f)$.
  In particular, $\|\Psi_{h_{A,B}}\|_{\mathcal{F}}^2 = \mathrm{cap}(A,B)$.

§4 Variational Principles

In most cases, it is hard to find the explicit equilibrium potential.

$\boxed{\text{Thm}}$ (Dirichlet principle)

$$\mathrm{Cap}(A,B) = \inf\left\{ \mathcal{D}(f) : f : S \to \mathbb{R},\ f|_A \equiv 1,\ f|_B \equiv 0 \right\}$$

and the unique minimizer of RHS is $f = h_{A,B}$.

[pf $\mathcal{D}(f) = \mathcal{D}(h) + \mathcal{D}(f-h) - 2\cancel{\langle g, \mathcal{L}h \rangle}^{=0} \geq \mathcal{D}(h)$. ▨].

$\boxed{\text{Thm}}$ (Thomson principle)

$$\mathrm{Cap}(A,B) = \sup\left\{ \frac{1}{\|\phi\|^2} : \phi \in \mathcal{F},\ \nabla\phi(A) = -\nabla\phi(B) = 1,\ \nabla\phi \equiv 0 \text{ on } (A \cup B)^c \right\}.$$

and the unique maximizer of RHS is $\phi = \Psi_{h_{A,B}}$.

[pf Given such ϕ,

$$\langle \Psi_{h_{A,B}}, \phi \rangle = -\sum_x h(x) \cdot \nabla\phi(x) = -1.$$

$$\Rightarrow 1 = \langle \Psi_{h_{A,B}}, \phi \rangle^2 \underset{C-S}{\leq} \|\Psi_{h_{A,B}}\|^2 \cdot \|\phi\|^2 = \mathrm{Cap}(A,B) \cdot \|\phi\|^2. \quad ▨$$].

Indeed, we do not need to find divergence-free flows if we know $h_{A,B}$:

$\boxed{\text{Thm}}$ (Generalized Thomson principle).

$$\mathrm{Cap}(A,B) = \sup\left\{ \frac{1}{\|\phi\|^2} \cdot \left(\sum_x h_{A,B}(x) \cdot \nabla\phi(x)\right)^2 : \phi \in \mathcal{F} \setminus \{0\} \right\}.$$

and the only maximizers of RHS are $\phi = c \cdot \Psi_{h_{A,B}}$, $c \neq 0$.

[pf $\left(\sum_x h(x) \cdot \nabla\phi(x)\right)^2 = \langle \Psi_h, \phi \rangle^2 \underset{C-S}{\leq} \|\Psi_h\|^2 \cdot \|\phi\|^2 = \mathrm{Cap}(A,B) \cdot \|\phi\|^2$. ▨]