Metastability in stochastic dynamics: Poincaré and logarithmic Sobolev inequality via two-scale decomposition

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joint work with A. Schlichting

Mathematics of kinetically constrained dynamics and metastability, Warwick

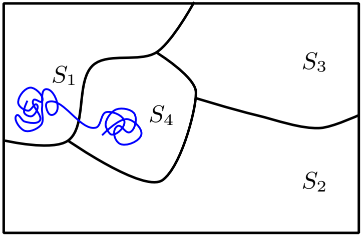
Metastability: A common phenomenon

The paradigm. Related to the dynamics of first order phase transitions

Change parameters quickly across the line of first order phase transition, the system reveals the existence of multiple time scales:

Short time scales.

- Existence of disjoint subsets S_i trapping effectively the system
- Quasi-equilibrium ($\hat{=}$ metastable states) is reached within S_i

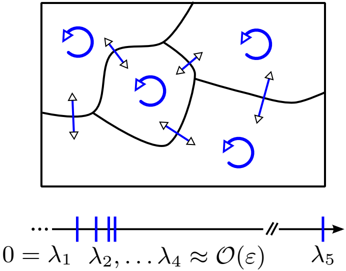


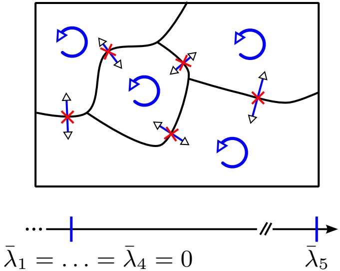
Larger time scales.

- Rapid transitions between S_i and S_j occur induced by random fluctuations

Spectrum and metastability

Heuristic. Reversible Markov process $\{X_t : t \geq 0\}$, generator L, $\lambda_i \in \mathrm{spec}(-L)$





The goal. Understanding of quantitative aspects of dynamical phase transitions:

- expected time of a transition from a metastable to a stable state
- distribution of the exit time from a metastable state
- spectral properties of the generator and mixing times

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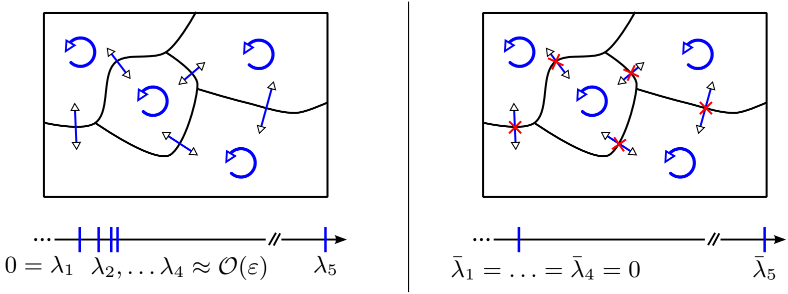

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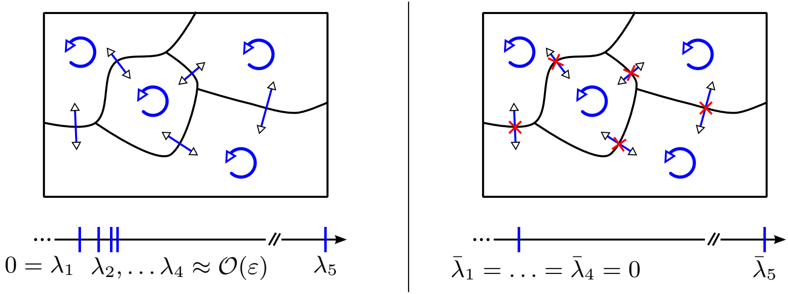

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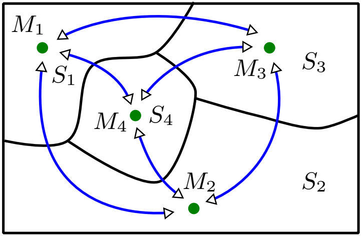
Elements of a definition.

- Represent S_i by small sets $M_i \subset S_i$ (or even single points)
- Consider transitions between M_i's, e.g.

A Markov process is called metastable if there exists a collection $\mathcal{M}$ of disjoint sets M_i such that

$$\frac{\sup_{x \notin \mathcal{M}} \mathbb{E}_x \left[\tau_{\mathcal{M}}\right]}{\inf_i \ \inf_{m \in M_i} \mathbb{E}_m \left[\tau_{\mathcal{M} \setminus M_i}\right]} \ll 1$$



- Involves only well-computable quantities

Reversible Markov chains

Setting.

- state space $\mathcal{S}$ (finite or countable infinite)
- μ measure on $\mathcal{S}$
- $\big(p(x,y) : x, y \in \mathcal{S}\big)$ stochastic matrix, irreducible (positive recurrent)

Dynamics. Discrete-time Markov chain $X = \{X_t : t \geq 0\}$ on $\mathcal{S}$ with generator

$$(Lf)(x) \;=\; \sum_{y} p(x,y)\,\big(f(y) - f(x)\big)$$

The Markov process X is reversible with respect to μ.

First return time. For any $A \subset \mathcal{S}$, let

$$\tau_A \;=\; \inf\{t > 0 \,:\, X_t \in A\}$$

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Poincaré and logarithmic Sobolev inequality

$$\mathcal{E}(f,f) \;=\; \frac{1}{2}\sum_{x,y\in\mathcal{S}} \mu(x)\, p(x,y)\, \big(f(x) - f(y)\big)^2$$

Poincaré inequality.

$$\operatorname{var}_\mu[f] \;\leq\; \frac{1}{\lambda}\,\mathcal{E}(f,f), \qquad \forall\, f : \mathcal{S} \to \mathbb{R} \qquad \text{(PI}(\lambda))$$

Logarithmic Sobolev inequality.

$$\operatorname{Ent}_\mu[f^2] \;=\; \mathrm{E}_\mu\Big[f^2\,\ln\frac{f^2}{\mathrm{E}_\mu[f^2]}\Big] \;\leq\; \frac{\mathcal{E}(f,f)}{\alpha}, \qquad \forall\, f : \mathcal{S} \to \mathbb{R} \qquad \text{(LSI}(\alpha))$$

The goal: Compute for metastable Markov chains

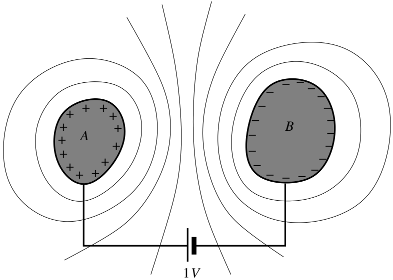
- the optimal constant λ_{PI} in the Poincaré inequality (spetral gap)
- the optimal constant α_{LSI} in the logarithmic Sobolev inequlity

Equilibrium potential. Given $A, B \subset \mathcal{S}$ disjoint

$$\begin{cases} Lh_{A,B} = 0, & \text{on } (A \cup B)^c \\ h_{A,B} = \mathbb{1}_A, & \text{on } A \cup B \end{cases} \qquad h_{A,B}(x) = \mathbb{P}_x\big[\tau_A < \tau_B\big]$$

Capacity.

$$\begin{aligned} \operatorname{cap}(A,B) &= \sum_{x \in A} \mu(x)\,(-Lh_{A,B})(x) \\ &= \langle h_{A,B}, -Lh_{A,B} \rangle_\mu \\ &= \sum_{x \in A} \mu(x)\, \mathbb{P}_x\big[\tau_B < \tau_A\big] \end{aligned}$$



Fact.

$$\operatorname{cap}(A,B) = \operatorname{cap}(B,A) \quad \text{and} \quad \operatorname{cap}(A',B) \le \operatorname{cap}(A,B), \quad \forall\, A' \subset A$$

Computation of capacities

Variational principles. Allows to bound capacities from above and from below

Dirichlet principle.

$$\mathrm{cap}(A,B) = \inf_{h \in \mathcal{H}_{A,B}} \frac{1}{2} \sum_{x,y} \mu(x)\, p(x,y)\, \big(h(x) - h(y)\big)^2$$

$\mathcal{H}_{A,B}$: space of functions with boundary constraints; minimizer harmonic function

Thomson principle.

$$\frac{1}{\mathrm{cap}(A,B)} = \inf_{f \in \mathcal{U}_{A,B}} \frac{1}{2} \sum_{x,y} \frac{f(x,y)^2}{\mu(x)\, p(x,y)}$$

$\mathcal{U}_{A,B}$: space of unit AB-flows; maximizer harmonic flow.

Berman-Konsowa principle.

$$\mathrm{cap}(A,B) = \sup_{f \in \mathcal{U}^{+}_{A,B}} \mathbb{E}^f \left[\left(\sum_{(x,y) \in \mathcal{X}} \frac{f(x,y)}{\mu(x)\, p(x,y)} \right)^{-1} \right]$$

$\mathcal{U}^{+}_{A,B}$: space of cycle-free, non-negative unit AB-flows; maximizer harmonic flow.
$\mathbb{E}^f$ is the law of a directed Markov chain with transition probabilities proportional to f.

Connection between capacities and mean hitting times

Mean hitting times.

$$\begin{cases} Lw_B = -1, & \text{on } B^c \\ w_B = 0, & \text{on } B \end{cases} \qquad w_B(x) = \mathbb{E}_x[\tau_B]$$

Last exit biased distribution. Let $A, B \subset \mathcal{S}$ be disjoint. $\nu_{A,B}$ measure on A

$$\nu_{A,B}(x) = \frac{\mu(x)\ \mathbb{P}_x\left[\tau_B < \tau_A\right]}{\sum_{x \in A} \mu(\sigma)\ \mathbb{P}_x\left[\tau_B < \tau_A\right]}, \qquad x \in A$$

Representation.

$$\mathbb{E}_{\nu_{A,B}}\left[\tau_B\right] = \frac{1}{\operatorname{cap}(A,B)} \sum_{x \notin B} \mu(x)\ h_{A,B}(x)$$

$$\text{Proof: } \operatorname{cap}(A,B)\,\mathbb{E}_{\nu_{A,B}}[\tau_B] = \langle -Lh_{A,B}, w_B\rangle_\mu = \langle h_{A,B}, -Lw_B\rangle_\mu = \langle h_{A,B}, 1\rangle_\mu$$

Capacitary inequalities

$$\langle h, -Lg \rangle_\mu \;=\; \frac{1}{2} \sum_{x,y \in \mathcal{S}} \mu(x)\, p(x,y)\, \big(h(x) - h(y)\big)\big(g(x) - g(y)\big)$$

Proposition

Let $B \subset \mathcal{S}$ be non-empty. For any $f : \mathcal{S} \to \mathbb{R}$ with $f \equiv 0$ on B set

$$A_t \;:=\; \{x \in \mathcal{S} \,:\, |f(x)| > t\}.$$

Then,

$$\int_0^\infty 2t\, \mathrm{cap}(A_t, B)\, \mathrm{d}t \;\le\; 4\,\mathcal{E}(f,f).$$

Previous and related work

- Maz'ya (1972), operators in divergence form on $\mathbb{R}^d$

`Idea of the proof on the blackboard.`

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Consequences

Proposition

Let $B \subset \mathcal{S}$ be non-empty and $\nu \in \mathcal{P}_1(\mathcal{S})$. Then, there exist $C_1, C_2 \in (0, \infty)$ satisfying $C_1 \;\leq\; C_2 \;\leq\; 4C_1$ such that the following statements are equivalent:

(i) *For all $A \subset \mathcal{S} \setminus B$ it holds*

$$\nu[A] \;\leq\; C_1 \operatorname{cap}(A, B).$$

(ii) *For all $f : \mathcal{S} \to \mathbb{R}$ with $f|_B \equiv 0$ holds*

$$\|f^2\|_{\ell^1(\nu)} \;\leq\; C_2 \, \mathcal{E}(f, f).$$

Consequences

$$\|f\|_{\Phi,\nu} \;:=\; \sup\Big\{\, \mathrm{E}_\nu[|f|g] \;:\; g \geq 0,\; \mathrm{E}_\nu[\Psi(g)] \leq 1 \Big\}$$

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$$\nu[A]\, \Psi^{-1}\big(1/\nu[A]\big) \;\leq\; C_1 \,\mathrm{cap}(A, B).$$

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Examples.

$$\big(\Phi_p(r), \Psi_p(r)\big) \;:=\; \big(\tfrac{1}{p} r^p, \tfrac{1}{p_*} r^{p_*}\big), \qquad \big(\Phi_{\mathrm{Ent}}(r), \Psi_{\mathrm{Ent}}(r)\big) \;:=\; \big(r \ln r - r + 1, \mathrm{e}^r - 1\big)$$

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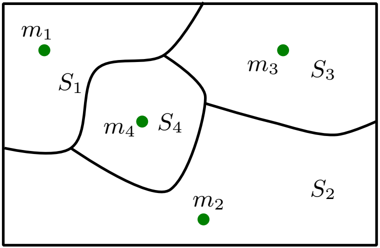
Definition of metastability

Definition

Let $\rho > 0$ and $\mathcal{M} \subset \mathcal{S}$ be finite. $\{X_t : t \geq 0\}$ is ρ-metastable with respect to $\mathcal{M}$ (set of metastable points), if

$$\frac{\max_{m\in\mathcal{M}} \mathbb{P}_m\left[\tau_{\mathcal{M}\backslash m} < \tau_m\right]}{\min_{A\subset\mathcal{S}\backslash\mathcal{M}} \mathbb{P}_{\mu_A}\left[\tau_{\mathcal{M}} < \tau_A\right]} \leq \rho \ll 1.$$



Previous and related definition

- Bovier (2006), reversible Markov chains with finite state space; reversible diffusions

Metastable partition. $\mathcal{S} = \bigcup_{m\in\mathcal{M}} S_m$, the sets S_m, $m \in \mathcal{M}$ are mutually disjoint

$$S_m \subset \left\{x \in \mathcal{S} : \mathbb{P}_x\left[\tau_m < \tau_{\mathcal{M}\backslash m}\right] \geq \max_{m'\in\mathcal{M}\backslash m} \mathbb{P}_x\left[\tau_{m'} < \tau_{\mathcal{M}\backslash m'}\right]\right\}$$

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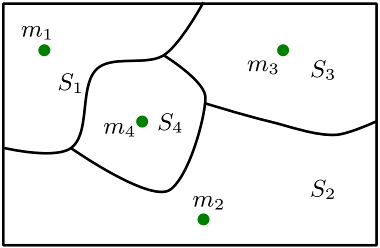

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Main result

Theorem

Suppose $\{X_t : t \geq 0\}$ *is a* ρ*-metastable Markov chain with* $\mathcal{M} = \{m_1, m_2\}$*. Then,*

$$\lambda_{\mathrm{PI}} \;=\; \frac{\operatorname{cap}(m_1, m_2)}{\mu[S_1]\,\mu[S_2]}\,\big(1 + O(\sqrt{\rho})\big).$$

Moreover, under further conditions on $\mu[\cdot|S_i]$*, it holds*

$$\alpha_{\mathrm{LSI}} \;=\; \Lambda(\mu[S_1], \mu[S_2])\,\frac{\operatorname{cap}(m_1, m_2)}{\mu[S_1]\,\mu[S_2]}\,\big(1 + O(\sqrt{\rho})\big),$$

where $\Lambda(s,t) = (s-t)/(\ln s - \ln t)$ *denotes the logarithmic mean.*

Previous and related results

- Bovier, Eckhoff, Gayrard, Klein (2002), low lying spectrum, reversible Markov chains
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Two-scale decomposition

$$\mu_i[\,\cdot\,] \;:=\; \mu[\,\cdot\,|S_i] \qquad \text{and} \qquad \bar{\mu} \;:=\; \mu[S_1]\,\delta_{m_1} \;+\; \mu[S_2]\,\delta_{m_2}$$

Splitting the variance.

$$\operatorname{var}_\mu[f] \;=\; \mu[S_1]\,\underbrace{\operatorname{var}_{\mu_1}[f]}_{\text{local variance}} + \mu[S_2]\,\underbrace{\operatorname{var}_{\mu_2}[f]}_{\text{local variance}} + \mu[S_1]\,\mu[S_2]\,\big(\underbrace{\mathrm{E}_{\mu_1}[f] - \mathrm{E}_{\mu_2}[f]}_{\text{mean difference}}\big)^2$$

Splitting the entropy.

$$\operatorname{Ent}_\mu[f^2] \;=\; \mu[S_1]\,\underbrace{\operatorname{Ent}_{\mu_1}[f^2]}_{\text{local entropy}} + \mu[S_2]\,\underbrace{\operatorname{Ent}_{\mu_2}[f^2]}_{\text{local entropy}} + \underbrace{\operatorname{Ent}_{\bar{\mu}}\big[\,\mathrm{E}_{\mu_\cdot}[f^2]\big]}_{\text{macroscopic entropy}}$$

$$\operatorname{Ent}_{\bar{\mu}}\big[\,\mathrm{E}_{\mu_\cdot}[f^2]\big] \;\leq\; \frac{\mu[S_1]\,\mu[S_2]}{\Lambda(\mu[S_1],\mu[S_2])}\Big(\operatorname{var}_{\mu_1}[f] + \operatorname{var}_{\mu_2}[f] + \big(\mathrm{E}_{\mu_1}[f] - \mathrm{E}_{\mu_2}[f]\big)^2\Big)$$

The strategy.

- rough bounds for local quantities,
- sharp bounds for the mean difference

Local variances and mean difference estimate

Fact.

$$\mathbb{P}_{\mu_A}\left[\tau_{m_i} < \tau_A\right] \;\geq\; \frac{1}{|\mathcal{M}|}\,\mathbb{P}_{\mu_A}\left[\tau_{\mathcal{M}} < \tau_A\right] \qquad \forall\, A \subset S_i \setminus \{m_i\}$$

Key estimate. For all $A \subset S_i \setminus \{m_i\}$

$$\mu_1[A] \;\leq\; \frac{\rho|\mathcal{M}|}{\mu[S_i]} \left(\max_{m \in \mathcal{M}\setminus\{m_i\}} \mathbb{P}_m\left[\tau_{\mathcal{M}\setminus\{m\}} < \tau_m\right]\right) \operatorname{cap}(A, m_i)$$

Local variances. $\mathcal{M} = \{m_1, m_2\}$

$$\mu[S_i]\; \operatorname{var}_{\mu_i}[f] \;\leq\; 2\,\rho\,|\mathcal{M}|\, \frac{\mu[S_1]\,\mu[S_2]}{\operatorname{cap}(m_1, m_2)}\,\mathcal{E}(f,f)$$

Mean difference estimate.

$$\mu[S_1]\,\mu[S_2]\,\big(\mathrm{E}_{\mu_1}[f] - \mathrm{E}_{\mu_2}[f]\big)^2 \;\leq\; \frac{\mu[S_1]\,\mu[S_2]}{\operatorname{cap}(m_1, m_2)}\,\mathcal{E}(f,f)\,\big(1 + O(\sqrt{\rho|\mathcal{M}|})\big)$$

Summary and open Problems

What have been done so far.

- Capacitary inequality that allows to establish a local PI and LSI inequality
- Method can be applied beyond the situtation of metastable points (e.g. RFCW)

Next task and major challenges.

- Establish a $\ell^2(\mu_i)$-bound on the density of the last exit biased distribution wrt. μ_i

Previous and related results

- Dahlberg (1977), Jerrison, Kenig (1982), Brownian motion on Lipschitz domains, $L^{2+\varepsilon}$ bound on the density of the harmonic measure