Optimal Poincaré and logarithmic Sobolev constants by decomposition of the energy landscape

André Schlichting

joint work with Georg Menz (Stanford)

Perspectives in Analysis and Probability
— Opening Conference

April 12, 2013

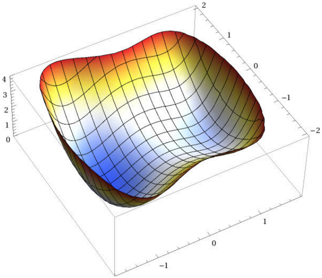
Outline

1. Description and Question
2. Main results
3. Sketch of the Proofs
   - Local PI and LSI
   - Mean-difference estimate
4. Application to entropic switching

Introduction

Overdamped Langevin dynamics

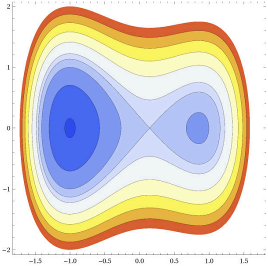
Hamiltonian $H : \mathbb{R}^n \to \mathbb{R}$ *energy landscape*



Dynamic at temperature $\varepsilon \ll 1$
$$\mathrm{d}X_t = -\nabla H(X_t)\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

Fokker-Planck evolution of law $X_t = \varrho_t$
$$\partial_t \varrho_t = \nabla \cdot (\varepsilon \nabla \varrho_t + \varrho_t \nabla H)$$

Gibbs measure $\mu(\mathrm{d}x) = \frac{1}{Z_\mu} \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x,$
where $\quad Z_\mu = \int \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x$



Generator evolution of $f_t = \varrho_t / \mu$
$$\partial_t f_t = L f_t := \varepsilon \Delta f_t - \nabla H \cdot \nabla f_t.$$

Dirichlet form $\mathcal{E}(f) := \int (-Lf) f \,\mathrm{d}\mu$
$$= \varepsilon \int |\nabla f|^2 \,\mathrm{d}\mu.$$

Hamiltonian $H : \mathbb{R}^n \to \mathbb{R}$ *energy landscape*

Dynamic at temperature $\varepsilon \ll 1$

$$\mathrm{d}X_t = -\nabla H(X_t)\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

Fokker-Planck evolution of law $X_t = \varrho_t$

$$\partial_t \varrho_t = \nabla \cdot (\varepsilon \nabla \varrho_t + \varrho_t \nabla H)$$

Gibbs measure $\mu(\mathrm{d}x) = \frac{1}{Z_\mu} \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x$,

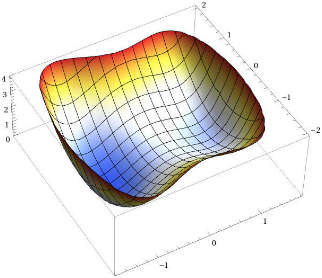
where $Z_\mu = \int \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x$

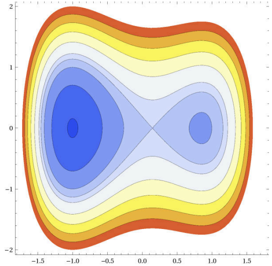
Generator evolution of $f_t = \varrho_t / \mu$

$$\partial_t f_t = L f_t := \varepsilon \Delta f_t - \nabla H \cdot \nabla f_t.$$

Dirichlet form $\mathcal{E}(f) := \int (-Lf) f \,\mathrm{d}\mu$

$$= \varepsilon \int |\nabla f|^2 \,\mathrm{d}\mu.$$

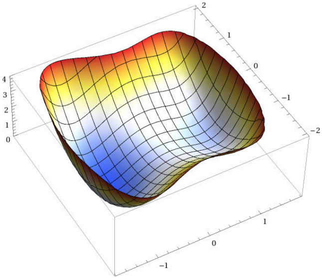




Introduction

Overdamped Langevin dynamics

Hamiltonian $H : \mathbb{R}^n \to \mathbb{R}$ *energy landscape*



Dynamic at temperature $\varepsilon \ll 1$

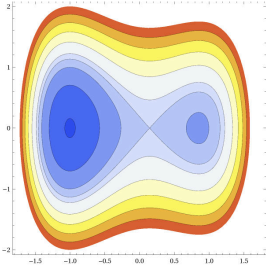
$$\mathrm{d}X_t = -\nabla H(X_t)\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

Fokker-Planck evolution of law $X_t = \varrho_t$

$$\partial_t \varrho_t = \nabla \cdot (\varepsilon \nabla \varrho_t + \varrho_t \nabla H)$$

Gibbs measure $\mu(\mathrm{d}x) = \frac{1}{Z_\mu} \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x,$

where $\quad Z_\mu = \int \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x$



Generator evolution of $f_t = \varrho_t / \mu$

$$\partial_t f_t = L f_t := \varepsilon \Delta f_t - \nabla H \cdot \nabla f_t.$$

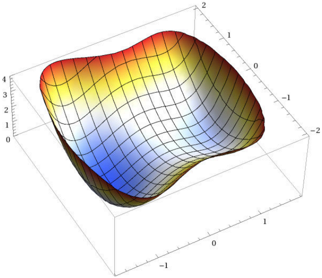
Dirichlet form $\mathcal{E}(f) := \int (-Lf) f \,\mathrm{d}\mu$

$$= \varepsilon \int |\nabla f|^2 \,\mathrm{d}\mu.$$

Introduction

Overdamped Langevin dynamics

Hamiltonian $H : \mathbb{R}^n \to \mathbb{R}$ *energy landscape*



Dynamic at temperature $\varepsilon \ll 1$

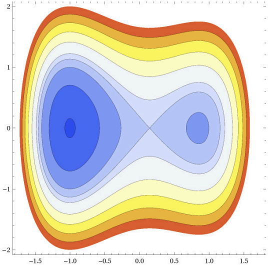
$$\mathrm{d}X_t = -\nabla H(X_t)\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

Fokker-Planck evolution of law $X_t = \varrho_t$

$$\partial_t \varrho_t = \nabla \cdot (\varepsilon \nabla \varrho_t + \varrho_t \nabla H)$$

Gibbs measure $\mu(\mathrm{d}x) = \frac{1}{Z_\mu} \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x$,

where $\quad Z_\mu = \int \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x$



Generator evolution of $f_t = \varrho_t / \mu$

$$\partial_t f_t = L f_t := \varepsilon \Delta f_t - \nabla H \cdot \nabla f_t.$$

Dirichlet form $\mathcal{E}(f) := \int (-Lf) f \,\mathrm{d}\mu$

$$= \varepsilon \int |\nabla f|^2 \,\mathrm{d}\mu.$$

Introduction

Overdamped Langevin dynamics

Hamiltonian $H : \mathbb{R}^n \to \mathbb{R}$ *energy landscape*

Dynamic at temperature $\varepsilon \ll 1$

$$\mathrm{d}X_t = -\nabla H(X_t)\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

Fokker-Planck evolution of law $X_t = \varrho_t$

$$\partial_t \varrho_t = \nabla \cdot (\varepsilon \nabla \varrho_t + \varrho_t \nabla H)$$

Gibbs measure $\mu(\mathrm{d}x) = \frac{1}{Z_\mu} \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x$,

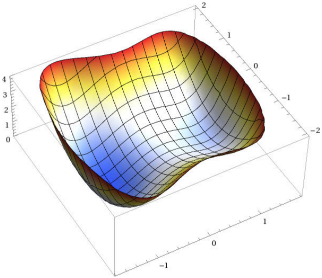
where $Z_\mu = \int \exp\left(-\frac{H}{\varepsilon}\right) \mathrm{d}x$

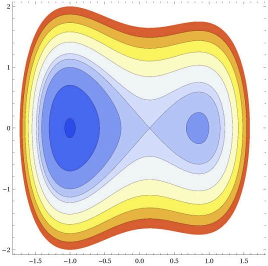
Generator evolution of $f_t = \varrho_t / \mu$

$$\partial_t f_t = L f_t := \varepsilon \Delta f_t - \nabla H \cdot \nabla f_t.$$

Dirichlet form $\mathcal{E}(f) := \int (-Lf) f \,\mathrm{d}\mu$

$$= \varepsilon \int |\nabla f|^2 \,\mathrm{d}\mu.$$

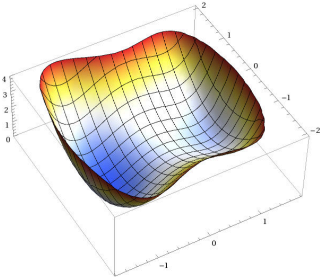




Introduction

Overdamped Langevin dynamics

Hamiltonian $H : \mathbb{R}^n \to \mathbb{R}$ *energy landscape*



Dynamic at temperature $\varepsilon \ll 1$

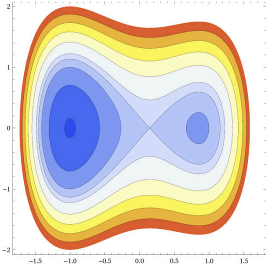
$$dX_t = -\nabla H(X_t)dt + \sqrt{2\varepsilon}\, dW_t$$

Fokker-Planck evolution of law $X_t = \varrho_t$

$$\partial_t \varrho_t = \nabla \cdot (\varepsilon \nabla \varrho_t + \varrho_t \nabla H)$$

Gibbs measure $\mu(dx) = \frac{1}{Z_\mu} \exp\left(-\frac{H}{\varepsilon}\right) dx,$

where $\quad Z_\mu = \int \exp\left(-\frac{H}{\varepsilon}\right) dx$



Generator evolution of $f_t = \varrho_t / \mu$

$$\partial_t f_t = L f_t := \varepsilon \Delta f_t - \nabla H \cdot \nabla f_t.$$

Dirichlet form $\mathcal{E}(f) := \int (-Lf) f \, d\mu$

$$= \varepsilon \int |\nabla f|^2 \, d\mu.$$

Poincaré and logarithmic Sobolev inequality

Definition

μ satisfies the Poincaré inequality PI(ϱ) if $\forall f : \mathbb{R}^n \to \mathbb{R}$

$$\operatorname{var}_\mu(f) := \int f^2 - \left(\int f \,\mathrm{d}\mu\right)^2 \mathrm{d}\mu \le \frac{1}{\varrho}\int |\nabla f|^2 \,\mathrm{d}\mu. \qquad \text{PI}(\varrho)$$

and the logarithmic Sobolev inequality LSI(α) if $\forall f : \mathbb{R}^n \to \mathbb{R}$

$$\operatorname{Ent}_\mu(f) := \int f \log \frac{f}{\int f \,\mathrm{d}\mu} \mathrm{d}\mu \le \frac{1}{\alpha}\int \frac{|\nabla f|^2}{2f} \mathrm{d}\mu. \qquad \text{LSI}(\alpha)$$

PI(ϱ) and LSI(α) imply exponential convergence to μ:

$$\text{PI}(\varrho) \;\Rightarrow\; \operatorname{var}_\mu(f_t) \le \operatorname{var}_\mu(f_0) e^{-2\varrho\varepsilon t}$$

$$\text{LSI}(\alpha) \;\Rightarrow\; \operatorname{Ent}_\mu(f_t) \le \operatorname{Ent}_\mu(f_0) e^{-2\alpha\varepsilon t}.$$

Poincaré and logarithmic Sobolev inequality

Definition

μ satisfies the Poincaré inequality $\mathrm{PI}(\varrho)$ if $\forall f : \mathbb{R}^n \to \mathbb{R}$

$$\mathrm{var}_\mu(f) := \int f^2 - \left(\int f \,\mathrm{d}\mu\right)^2 \mathrm{d}\mu \le \frac{1}{\varrho} \int |\nabla f|^2 \,\mathrm{d}\mu. \qquad \mathrm{PI}(\varrho)$$

and the logarithmic Sobolev inequality $\mathrm{LSI}(\alpha)$ if $\forall f : \mathbb{R}^n \to \mathbb{R}$

$$\mathrm{Ent}_\mu(f) := \int f \log \frac{f}{\int f \,\mathrm{d}\mu} \mathrm{d}\mu \le \frac{1}{\alpha} \int \frac{|\nabla f|^2}{2f} \mathrm{d}\mu. \qquad \mathrm{LSI}(\alpha)$$

$\mathrm{PI}(\varrho)$ and $\mathrm{LSI}(\alpha)$ imply exponential convergence to μ:

$$\mathrm{PI}(\varrho) \;\Rightarrow\; \mathrm{var}_\mu(f_t) \le \mathrm{var}_\mu(f_0) e^{-2\varrho\varepsilon t}$$
$$\mathrm{LSI}(\alpha) \;\Rightarrow\; \mathrm{Ent}_\mu(f_t) \le \mathrm{Ent}_\mu(f_0) e^{-2\alpha\varepsilon t}.$$

Poincaré and logarithmic Sobolev inequality

Definition

μ satisfies the Poincaré inequality PI(ϱ) if $\forall f : \mathbb{R}^n \to \mathbb{R}$

$$\operatorname{var}_\mu(f) := \int f^2 - \left(\int f \,\mathrm{d}\mu\right)^2 \mathrm{d}\mu \le \frac{1}{\varrho} \int |\nabla f|^2 \,\mathrm{d}\mu. \qquad \mathrm{PI}(\varrho)$$

and the logarithmic Sobolev inequality LSI(α) if $\forall f : \mathbb{R}^n \to \mathbb{R}$

$$\operatorname{Ent}_\mu(f^2) := \int f^2 \log \frac{f^2}{\int f^2 \mathrm{d}\mu} \mathrm{d}\mu \le \frac{2}{\alpha} \int |\nabla f|^2 \,\mathrm{d}\mu. \qquad \mathrm{LSI}(\alpha)$$

PI(ϱ) and LSI(α) imply exponential convergence to μ:

$$\mathrm{PI}(\varrho) \Rightarrow \operatorname{var}_\mu(f_t) \le \operatorname{var}_\mu(f_0) e^{-2\varrho\varepsilon t}$$

$$\mathrm{LSI}(\alpha) \Rightarrow \operatorname{Ent}_\mu(f_t) \le \operatorname{Ent}_\mu(f_0) e^{-2\alpha\varepsilon t}.$$

Poincaré and logarithmic Sobolev inequality

universitätbonn iam

Definition

μ satisfies the Poincaré inequality PI(ϱ) if $\forall f : \mathbb{R}^n \to \mathbb{R}$

$$\operatorname{var}_\mu(f) := \int f^2 - \left(\int f \,\mathrm{d}\mu\right)^2 \mathrm{d}\mu \le \frac{1}{\varrho} \int |\nabla f|^2 \,\mathrm{d}\mu. \qquad \text{PI}(\varrho)$$

and the logarithmic Sobolev inequality LSI(α) if $\forall f : \mathbb{R}^n \to \mathbb{R}$

$$\operatorname{Ent}_\mu(f^2) := \int f^2 \log \frac{f^2}{\int f^2 \mathrm{d}\mu} \mathrm{d}\mu \le \frac{2}{\alpha} \int |\nabla f|^2 \,\mathrm{d}\mu. \qquad \text{LSI}(\alpha)$$

PI(ϱ) and LSI(α) imply exponential convergence to μ:

$$\text{PI}(\varrho) \;\Rightarrow\; \operatorname{var}_\mu(f_t) \le \operatorname{var}_\mu(f_0) e^{-2\varrho\varepsilon t}$$

$$\text{LSI}(\alpha) \;\Rightarrow\; \operatorname{Ent}_\mu(f_t) \le \operatorname{Ent}_\mu(f_0) e^{-2\alpha\varepsilon t}.$$

Goal: Optimal constants in PI and LSI

Accurate estimates of ϱ and α in the regime $\varepsilon \ll 1$:

$$\varrho = C_\varrho(\varepsilon) e^{-\frac{\Delta H}{\varepsilon}}(1 + o(1)) \qquad \text{and} \qquad \alpha = C_\alpha(\varepsilon) e^{-\frac{\Delta H}{\varepsilon}}(1 + o(1)).$$

Goal: Optimal constants in PI and LSI

Accurate estimates of ϱ and α in the regime $\varepsilon \ll 1$:

$$\varrho = C_\varrho(\varepsilon) e^{-\frac{\Delta H}{\varepsilon}}(1 + o(1)) \qquad \text{and} \qquad \alpha = C_\alpha(\varepsilon) e^{-\frac{\Delta H}{\varepsilon}}(1 + o(1)).$$

Heuristics

$$dX_t = -\nabla H(X_t)\,dt + \sqrt{2\varepsilon}\,dW_t$$

- particle follows $-\nabla H$ as long as $|\nabla H| \sim 1$
- noise is dominant, if $|\nabla H| \lesssim \sqrt{\varepsilon}$

Heuristics

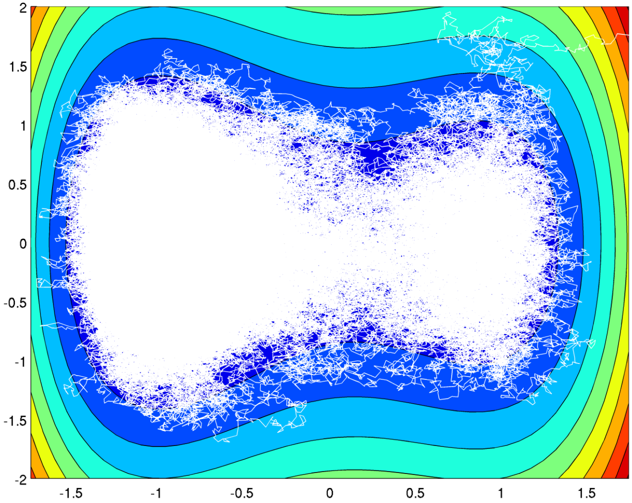


Figure : Trajectory for $\varepsilon = 0.4$

Heuristics

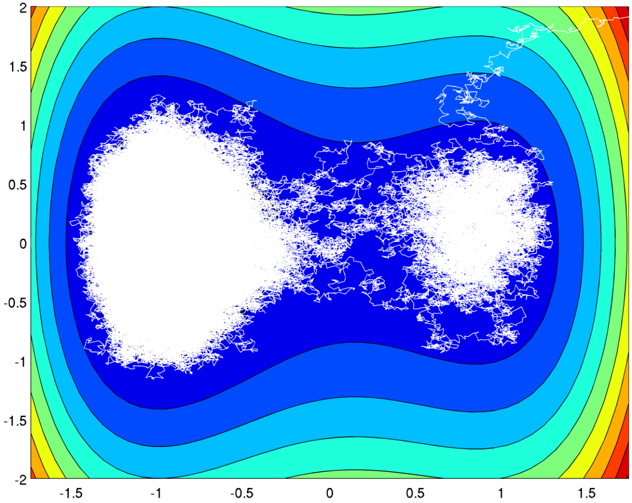


Figure : Trajectory for $\varepsilon = 0.2$

Heuristics

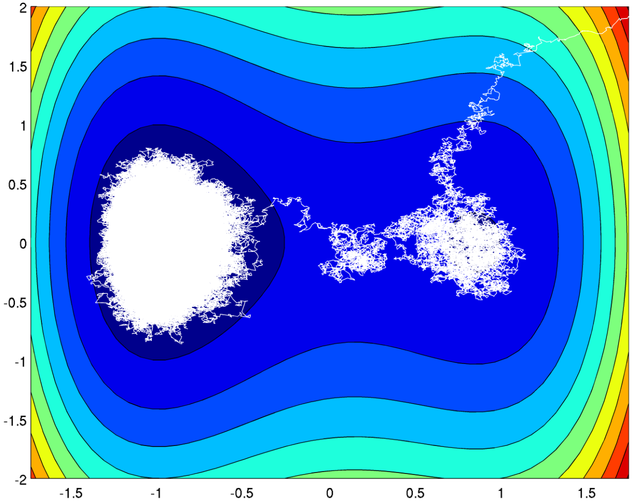


Figure : Trajectory for $\varepsilon = 0.1$

Heuristics

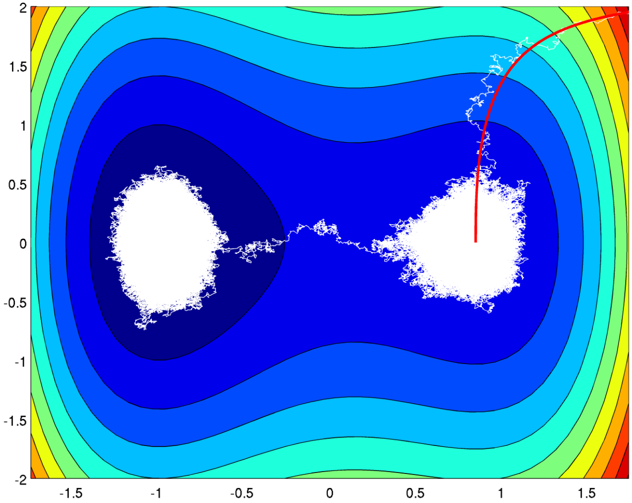


Figure : Trajectory for $\varepsilon = 0.05$ (red $\varepsilon = 0$)

Two scales by decomposition à la [GOVW09][1]

The partition $\biguplus_i \Omega_i = \mathbb{R}^n$ is called admissible for μ if:

(i) For each local minimum $m_i \in \mathcal{M}$ exists $\Omega_i \in \mathcal{P}_{\mathcal{M}}$ with $m_i \in \Omega_i$

(ii) The partition sum of each Ω_i is approximately Gaussian

$$\mu(\Omega_i) Z_\mu = \frac{(2\pi\varepsilon)^{\frac{n}{2}}}{\sqrt{\det \nabla^2 H(m_i)}} \exp\left(-\frac{H(m_i)}{\varepsilon}\right)(1+o(1)) .$$

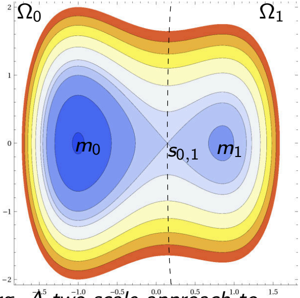
Restricted measures: $\mu_i := \mu \llcorner \Omega_i, \quad i = 0, 1.$

Macroscopic measures $\bar{\mu}$ on $\{0,1\}$:

$$\bar{\mu} := Z_0 \delta_0 + Z_1 \delta_1 .$$

Mixture representation:

$$\mu = Z_0 \mu_0 + Z_1 \mu_1 \text{ with } Z_i := \mu(\Omega_i).$$



[1] N. Grunewald, F. Otto, C. Villani, and M. G. Westdickenberg, *A two-scale approach to logarithmic Sobolev inequalities and the hydrodynamic limit*, Annales de l'Institut Henri Poincaré, Probabilités et Statistiques, 45:**2**, 2009.

Splitting

Ideas motivated from [CM10][2]

$$\mathrm{var}_\mu(f) = \underbrace{Z_0\,\mathrm{var}_{\mu_0}(f) + Z_1\,\mathrm{var}_{\mu_1}(f)}_{\text{local variances}} + Z_0 Z_1 \underbrace{\left(\mathbb{E}_{\mu_0}(f) - \mathbb{E}_{\mu_1}(f)\right)^2}_{\text{mean-difference}}$$

$$\mathrm{Ent}_\mu(f^2) = \overbrace{Z_0\,\mathrm{Ent}_{\mu_0}(f^2) + Z_1\,\mathrm{Ent}_{\mu_1}(f^2)}^{\text{local entropies}} + \overbrace{\mathrm{Ent}_{\bar\mu}\left(\mathbb{E}_{\mu_\bullet}(f^2)\right)}^{\text{macroscopic entropy}}$$

where $\Lambda(Z_0, Z_1) = \frac{Z_0 - Z_1}{\log Z_0 - \log Z_1}$ is the logarithmic mean.

Expect from heuristics:

- *good* estimate for local variances/entropies
- *exponential* estimate for mean-difference

[2] D. Chafaï and F. Malrieu, *On fine properties of mixtures with respect to concentration of measure and Sobolev type inequalities*, Annales de l'Institut Henri Poincaré, Probabilités et Statistiques, 46:**1**, 2010.

Splitting

Ideas motivated from [CM10][2]

$$\operatorname{var}_\mu(f) = \underbrace{Z_0 \operatorname{var}_{\mu_0}(f) + Z_1 \operatorname{var}_{\mu_1}(f)}_{\text{local variances}} + Z_0 Z_1 \underbrace{\left(\mathbb{E}_{\mu_0}(f) - \mathbb{E}_{\mu_1}(f)\right)^2}_{\text{mean-difference}}$$

$$\operatorname{Ent}_\mu(f^2) \le \overbrace{Z_0 \operatorname{Ent}_{\mu_0}(f^2) + Z_1 \operatorname{Ent}_{\mu_1}(f^2)}^{\text{local entropies}} + \\ + \frac{Z_0 Z_1}{\Lambda(Z_0, Z_1)} \left(\operatorname{var}_{\mu_0}(f) + \operatorname{var}_{\mu_1}(f) + \left(\mathbb{E}_{\mu_0}(f) - \mathbb{E}_{\mu_1}(f)\right)^2 \right),$$

where $\Lambda(Z_0, Z_1) = \frac{Z_0 - Z_1}{\log Z_0 - \log Z_1}$ is the logarithmic mean.

Expect from heuristics:

- *good* estimate for local variances/entropies
- *exponential* estimate for mean-difference

[2] D. Chafaï and F. Malrieu, *On fine properties of mixtures with respect to concentration of measure and Sobolev type inequalities*, Annales de l'Institut Henri Poincaré, Probabilités et Statistiques, 46:**1**, 2010.

Splitting

Ideas motivated from [CM10][2]

$$\operatorname{var}_\mu(f) = \underbrace{Z_0 \operatorname{var}_{\mu_0}(f) + Z_1 \operatorname{var}_{\mu_1}(f)}_{\text{local variances}} + Z_0 Z_1 \underbrace{\left(\mathbb{E}_{\mu_0}(f) - \mathbb{E}_{\mu_1}(f)\right)^2}_{\text{mean-difference}}$$

$$\begin{aligned}\operatorname{Ent}_\mu(f^2) \le{}& \overbrace{Z_0 \operatorname{Ent}_{\mu_0}(f^2) + Z_1 \operatorname{Ent}_{\mu_1}(f^2)}^{\text{local entropies}} + \\ &+ \frac{Z_0 Z_1}{\Lambda(Z_0, Z_1)} \left(\operatorname{var}_{\mu_0}(f) + \operatorname{var}_{\mu_1}(f) + \left(\mathbb{E}_{\mu_0}(f) - \mathbb{E}_{\mu_1}(f)\right)^2\right),\end{aligned}$$

where $\Lambda(Z_0, Z_1) = \frac{Z_0 - Z_1}{\log Z_0 - \log Z_1}$ is the logarithmic mean.

Expect from heuristics:

- *good* estimate for local variances/entropies
- *exponential* estimate for mean-difference

[2] D. Chafaï and F. Malrieu, *On fine properties of mixtures with respect to concentration of measure and Sobolev type inequalities*, Annales de l'Institut Henri Poincaré, Probabilités et Statistiques, 46:**1**, 2010.

Outline

Main results

Theorem (Local PI and LSI)

There exists an admissible partition $\biguplus_i \Omega_i = \mathbb{R}^n$ *such that each local measure* $\mu_i = \mu \llcorner \Omega_i$ *satisfies* $\mathrm{PI}(\varrho_{loc})$ *and* $\mathrm{LSI}(\alpha_{loc})$ *with*

$$\varrho_{loc}^{-1} = O(\varepsilon) \quad \textit{and} \quad \alpha_{loc}^{-1} = O(1).$$

- PI is as good as for convex potential
- Non-convexity of potential worsens LSI
- Both results scale optimal in one dimension

Theorem (Mean-difference estimate)

$$(\mathbb{E}_{\mu_0} f - \mathbb{E}_{\mu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 d\mu.$$

"$\lesssim$": *up to multiplicative error* $1 + o(1)$ *as* $\varepsilon \to 0$.

Main results

Theorem (Local PI and LSI)

There exists an admissible partition $\biguplus_i \Omega_i = \mathbb{R}^n$ *such that each local measure* $\mu_i = \mu \llcorner \Omega_i$ *satisfies* $\mathrm{PI}(\varrho_{loc})$ *and* $\mathrm{LSI}(\alpha_{loc})$ *with*

$$\varrho_{loc}^{-1} = O(\varepsilon) \quad \text{and} \quad \alpha_{loc}^{-1} = O(1).$$

- PI is as good as for convex potential
- Non-convexity of potential worsens LSI
- Both results scale optimal in one dimension

Theorem (Mean-difference estimate)

$$(\mathbb{E}_{\mu_0} f - \mathbb{E}_{\mu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

"$\lesssim$": *up to multiplicative error* $1 + o(1)$ *as* $\varepsilon \to 0$.

Main results

Theorem (Local PI and LSI)

There exists an admissible partition $\biguplus_i \Omega_i = \mathbb{R}^n$ such that each local measure $\mu_i = \mu \llcorner \Omega_i$ satisfies PI(ϱ_{loc}) *and* LSI(α_{loc}) *with*

$$\varrho_{loc}^{-1} = O(\varepsilon) \quad \text{and} \quad \alpha_{loc}^{-1} = O(1).$$

- PI is as good as for convex potential
- Non-convexity of potential worsens LSI
- Both results scale optimal in one dimension

Theorem (Mean-difference estimate)

$$(\mathbb{E}_{\mu_0} f - \mathbb{E}_{\mu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \, \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} \, e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

"$\lesssim$": *up to multiplicative error* $1 + o(1)$ *as* $\varepsilon \to 0$.

Main results

Theorem (Local PI and LSI)

There exists an admissible partition $\biguplus_i \Omega_i = \mathbb{R}^n$ *such that each local measure* $\mu_i = \mu \llcorner \Omega_i$ *satisfies* $\mathrm{PI}(\varrho_{loc})$ *and* $\mathrm{LSI}(\alpha_{loc})$ *with*

$$\varrho_{loc}^{-1} = O(\varepsilon) \quad \text{and} \quad \alpha_{loc}^{-1} = O(1).$$

- PI is as good as for convex potential
- Non-convexity of potential worsens LSI
- Both results scale optimal in one dimension

Theorem (Mean-difference estimate)

$$(\mathbb{E}_{\mu_0} f - \mathbb{E}_{\mu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \,\mathrm{d}\mu.$$

"$\lesssim$": up to multiplicative error $1 + o(1)$ *as* $\varepsilon \to 0$.

Main results

Theorem (Local PI and LSI)

There exists an admissible partition $\biguplus_i \Omega_i = \mathbb{R}^n$ *such that each local measure* $\mu_i = \mu \llcorner \Omega_i$ *satisfies* $\mathrm{PI}(\varrho_{loc})$ *and* $\mathrm{LSI}(\alpha_{loc})$ *with*

$$\varrho_{loc}^{-1} = O(\varepsilon) \quad \text{and} \quad \alpha_{loc}^{-1} = O(1).$$

- PI is as good as for convex potential
- Non-convexity of potential worsens LSI
- Both results scale optimal in one dimension

Theorem (Mean-difference estimate)

$$(\mathbb{E}_{\mu_0} f - \mathbb{E}_{\mu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \, \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} \, e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, \mathrm{d}\mu.$$

"$\lesssim$": *up to multiplicative error* $1 + o(1)$ *as* $\varepsilon \to 0$.

Eyring-Kramers formula

Corollary

The measure μ *satisfies* PI(ϱ) *and* LSI(α) *with*

$$\frac{1}{\varrho} \approx Z_0 Z_1 \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\frac{H(s_{0,1})}{\varepsilon}} \quad \text{and} \quad \frac{2}{\alpha} \approx \frac{1}{\Lambda(Z_0, Z_1)\ \varrho}.$$

Asymptotic evaluation of the factor $\Lambda(Z_0, Z_1)$ for two special cases:

$$H(m_0) < H(m_1): \quad \frac{\varrho}{\alpha} \approx \frac{1}{2}\left(\frac{H(m_1) - H(m_0)}{\varepsilon} + \log\left(\frac{\kappa_0}{\kappa_1}\right)\right) = O(\varepsilon^{-1})$$

$$H(m_0) = H(m_1): \quad \frac{\varrho}{\alpha} \approx \frac{\frac{\kappa_0 + \kappa_1}{2}}{\Lambda(\kappa_0, \kappa_1)} = O(1),$$

where $\kappa_i := \sqrt{\det \nabla^2 H(m_i)}$.

Eyring-Kramers formula

Corollary

The measure μ *satisfies* $\mathrm{PI}(\varrho)$ *and* $\mathrm{LSI}(\alpha)$ *with*

$$\frac{1}{\varrho} \approx Z_0 Z_1 \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\frac{H(s_{0,1})}{\varepsilon}} \quad \text{and} \quad \frac{2}{\alpha} \approx \frac{1}{\Lambda(Z_0, Z_1)\ \varrho}.$$

Asymptotic evaluation of the factor $\Lambda(Z_0, Z_1)$ for two special cases:

$$H(m_0) < H(m_1): \quad \frac{\varrho}{\alpha} \approx \frac{1}{2}\left(\frac{H(m_1) - H(m_0)}{\varepsilon} + \log\left(\frac{\kappa_0}{\kappa_1}\right)\right) = O(\varepsilon^{-1})$$

$$H(m_0) = H(m_1): \quad \frac{\varrho}{\alpha} \approx \frac{\frac{\kappa_0+\kappa_1}{2}}{\Lambda(\kappa_0, \kappa_1)} = O(1),$$

where $\kappa_i := \sqrt{\det \nabla^2 H(m_i)}$.

Outline

Proof: Local PI and LSI

Theorem (Local PI and LSI)

There exists an admissible partition $\biguplus_i \Omega_i = \mathbb{R}^n$ such that each local measure $\mu_i = \mu \llcorner \Omega_i$ satisfies $\mathrm{PI}(\varrho_{loc})$ *and* $\mathrm{LSI}(\alpha_{loc})$ *with*

$$\varrho_{loc}^{-1} = O(\varepsilon) \quad \text{and} \quad \alpha_{loc}^{-1} = O(1).$$

- lack of convexity of H on Ω
  $\Rightarrow$ rules out Bakry-Émery criterion
- non-exponential behavior of constants
  $\Rightarrow$ rules out Holley-Stroock perturbation principle
- optimality available in one dimension
  $\Rightarrow$ Muckenhoupt and Bobkov/Götze functional

Proof: Local PI and LSI

Theorem (Local PI and LSI)

There exists an admissible partition $\biguplus_i \Omega_i = \mathbb{R}^n$ such that each local measure $\mu_i = \mu \llcorner \Omega_i$ satisfies PI(ϱ_{loc}) *and* LSI(α_{loc}) *with*

$$\varrho_{loc}^{-1} = O(\varepsilon) \quad \text{and} \quad \alpha_{loc}^{-1} = O(1).$$

- lack of convexity of H on Ω
  $\Rightarrow$ rules out Bakry-Émery criterion
- non-exponential behavior of constants
  $\Rightarrow$ rules out Holley-Stroock perturbation principle
- optimality available in one dimension
  $\Rightarrow$ Muckenhoupt and Bobkov/Götze functional

Proof: Local PI and LSI

Theorem (Local PI and LSI)

There exists an admissible partition $\biguplus_i \Omega_i = \mathbb{R}^n$ *such that each local measure* $\mu_i = \mu \llcorner \Omega_i$ *satisfies* $\mathrm{PI}(\varrho_{loc})$ *and* $\mathrm{LSI}(\alpha_{loc})$ *with*

$$\varrho_{loc}^{-1} = O(\varepsilon) \quad \text{and} \quad \alpha_{loc}^{-1} = O(1).$$

- lack of convexity of H on Ω
  $\Rightarrow$ rules out Bakry-Émery criterion
- non-exponential behavior of constants
  $\Rightarrow$ rules out Holley-Stroock perturbation principle
- optimality available in one dimension
  $\Rightarrow$ Muckenhoupt and Bobkov/Götze functional

Proof: Local PI and LSI

Theorem (Local PI and LSI)

There exists an admissible partition $\biguplus_i \Omega_i = \mathbb{R}^n$ such that each local measure $\mu_i = \mu \llcorner \Omega_i$ satisfies PI(ϱ_{loc}) *and* LSI(α_{loc}) *with*

$$\varrho_{loc}^{-1} = O(\varepsilon) \quad \text{and} \quad \alpha_{loc}^{-1} = O(1).$$

- lack of convexity of H on Ω
  $\Rightarrow$ rules out Bakry-Émery criterion
- non-exponential behavior of constants
  $\Rightarrow$ rules out Holley-Stroock perturbation principle
- optimality available in one dimension
  $\Rightarrow$ Muckenhoupt and Bobkov/Götze functional

Proof: Local PI and LSI via Lyapunov condition

Technique developed by Bakry, Barthe, Cattiaux, Guillin, Wang and Wu 2008–

Definition (Lyapunov condition on domains)

L satisfies a Lyapunov condition with constants $\lambda, b > 0$ and some $U \subset \Omega$, if there exists a Lyapunov function $W : \Omega \to [1, \infty)$ satisfying

$$\frac{LW}{\varepsilon W} \leq -\lambda + b\,\mathbb{1}_U.$$

and Neumann boundary condition on Ω, such that integration by parts holds

$$\int_\Omega f(-LW)\,\mathrm{d}\mu = \varepsilon \int_\Omega \langle \nabla f, \nabla W \rangle\,\mathrm{d}\mu.$$

Theorem ([BBCG08])

Suppose L satisfies a Lyapunov condition and $\mu \llcorner U$ satisfies $\mathrm{PI}(\varrho_U)$, then μ satisfies $\mathrm{PI}(\varrho)$ with

$$\varrho \geq \frac{\lambda}{b + \varrho_U}\varrho_U$$

Proof: Local PI and LSI via Lyapunov condition

Technique developed by Bakry, Barthe, Cattiaux, Guillin, Wang and Wu 2008–

Definition (Lyapunov condition on domains)

L satisfies a Lyapunov condition with constants $\lambda, b > 0$ and some $U \subset \Omega$, if there exists a Lyapunov function $W : \Omega \to [1, \infty)$ satisfying

$$\frac{LW}{\varepsilon W} \leq -\lambda + b\, \mathbb{1}_U.$$

and Neumann boundary condition on Ω, such that integration by parts holds

$$\int_\Omega f(-LW)\, \mathrm{d}\mu = \varepsilon \int_\Omega \langle \nabla f, \nabla W \rangle\, \mathrm{d}\mu.$$

Theorem ([BBCG08])

Suppose L satisfies a Lyapunov condition and $\mu \llcorner U$ satisfies PI(ϱ_U), *then μ satisfies* PI(ϱ) *with*

$$\varrho \geq \frac{\lambda}{b + \varrho_U} \varrho_U$$

Proof: Local PI and LSI

Proof: Lyapunov $\Rightarrow$ PI(ϱ)

Integration by parts of W wrt. to L yields

$$\int_\Omega f^2 \frac{(-LW)}{\varepsilon W} \mathrm{d}\mu = \int_\Omega \left\langle \nabla \frac{f^2}{W}, \nabla W \right\rangle \mathrm{d}\mu$$

$$= 2 \int_\Omega \frac{f}{W} \langle \nabla f, \nabla W \rangle \mathrm{d}\mu - \int_\Omega \frac{f^2 |\nabla W|^2}{W^2} \mathrm{d}\mu$$

$$= \int_\Omega |\nabla f|^2 \mathrm{d}\mu - \int_\Omega \left| \nabla f - \frac{f}{W} \nabla W \right|^2 \mathrm{d}\mu.$$

The Lyapunov conditions ensures $1 \le \frac{-LW}{\lambda \varepsilon W} + \frac{b}{\lambda} \mathbb{1}_U$:

$$\operatorname{var}_\mu(f) = \int_\Omega (f - \bar{f})^2 \mathrm{d}\mu$$

universitätbonn iam

Proof: Lyapunov ⇒ PI(ϱ)

Integration by parts of W wrt. to L yields

$$\begin{aligned}\int_\Omega f^2 \frac{(-LW)}{\varepsilon W} \mathrm{d}\mu &= \int_\Omega \left\langle \nabla \frac{f^2}{W}, \nabla W \right\rangle \mathrm{d}\mu \\ &= 2 \int_\Omega \frac{f}{W} \left\langle \nabla f, \nabla W \right\rangle \mathrm{d}\mu - \int_\Omega \frac{f^2 \left|\nabla W\right|^2}{W^2} \mathrm{d}\mu \\ &\leq \int_\Omega \left|\nabla f\right|^2 \mathrm{d}\mu\end{aligned}$$

The Lyapunov conditions ensures $1 \leq \frac{-LW}{\lambda \varepsilon W} + \frac{b}{\lambda} \mathbb{1}_U$:

$$\mathrm{var}_\mu(f) = \int_\Omega (f - \bar{f})^2 \mathrm{d}\mu$$

Proof: Local PI and LSI

Proof: Lyapunov $\Rightarrow$ PI(ϱ)

Integration by parts of W wrt. to L yields

$$\int_\Omega f^2 \frac{(-LW)}{\varepsilon W} \mathrm{d}\mu = \int_\Omega \left\langle \nabla \frac{f^2}{W}, \nabla W \right\rangle \mathrm{d}\mu$$

$$= 2 \int_\Omega \frac{f}{W} \langle \nabla f, \nabla W \rangle \, \mathrm{d}\mu - \int_\Omega \frac{f^2 \left|\nabla W\right|^2}{W^2} \mathrm{d}\mu$$

$$\leq \int_\Omega \left|\nabla f\right|^2 \mathrm{d}\mu$$

The Lyapunov conditions ensures $1 \leq \frac{-LW}{\lambda \varepsilon W} + \frac{b}{\lambda} \mathbb{1}_U$:

$$\operatorname{var}_\mu(f) = \int_\Omega (f - \bar{f})^2 \mathrm{d}\mu$$

Proof: Local PI and LSI

Proof: Lyapunov $\Rightarrow$ PI(ϱ)

Integration by parts of W wrt. to L yields

$$\int_\Omega f^2 \frac{(-LW)}{\varepsilon W} \mathrm{d}\mu = \int_\Omega \left\langle \nabla \frac{f^2}{W}, \nabla W \right\rangle \mathrm{d}\mu$$

$$= 2 \int_\Omega \frac{f}{W} \langle \nabla f, \nabla W \rangle \,\mathrm{d}\mu - \int_\Omega \frac{f^2 \left|\nabla W\right|^2}{W^2} \mathrm{d}\mu$$

$$\leq \int_\Omega \left|\nabla f\right|^2 \mathrm{d}\mu$$

The Lyapunov conditions ensures $1 \leq \frac{-LW}{\lambda \varepsilon W} + \frac{b}{\lambda} \mathbb{1}_U$:

$$\mathrm{var}_\mu(f) \leq \int_\Omega (f - \bar{f}_U)^2 \mathrm{d}\mu$$

Proof: Local PI and LSI

Proof: Lyapunov $\Rightarrow$ PI(ϱ)

Integration by parts of W wrt. to L yields

$$\int_\Omega f^2 \frac{(-LW)}{\varepsilon W} \mathrm{d}\mu = \int_\Omega \left\langle \nabla \frac{f^2}{W}, \nabla W \right\rangle \mathrm{d}\mu$$
$$= 2 \int_\Omega \frac{f}{W} \langle \nabla f, \nabla W \rangle \,\mathrm{d}\mu - \int_\Omega \frac{f^2 \left|\nabla W\right|^2}{W^2} \mathrm{d}\mu$$
$$\leq \int_\Omega \left|\nabla f\right|^2 \mathrm{d}\mu$$

The Lyapunov conditions ensures $1 \leq \frac{-LW}{\lambda \varepsilon W} + \frac{b}{\lambda} \mathbb{1}_U$:

$$\operatorname{var}_\mu(f) \leq \int_\Omega (f - \bar{f}_U)^2 \mathrm{d}\mu \leq \int_\Omega (f - \bar{f}_U)^2 \frac{-LW}{\lambda \varepsilon W} \mathrm{d}\mu + \frac{b}{\lambda} \int_U (f - \bar{f}_U)^2 \mathrm{d}\mu$$

Proof: Local PI and LSI

Proof: Lyapunov $\Rightarrow$ PI(ϱ)

Integration by parts of W wrt. to L yields

$$\int_\Omega f^2 \frac{(-LW)}{\varepsilon W} \mathrm{d}\mu = \int_\Omega \left\langle \nabla \frac{f^2}{W}, \nabla W \right\rangle \mathrm{d}\mu$$

$$= 2 \int_\Omega \frac{f}{W} \langle \nabla f, \nabla W \rangle \,\mathrm{d}\mu - \int_\Omega \frac{f^2 \left|\nabla W\right|^2}{W^2} \mathrm{d}\mu$$

$$\leq \int_\Omega \left|\nabla f\right|^2 \mathrm{d}\mu$$

The Lyapunov conditions ensures $1 \leq \frac{-LW}{\lambda \varepsilon W} + \frac{b}{\lambda} \mathbb{1}_U$:

$$\operatorname{var}_\mu(f) \leq \int_\Omega (f - \bar{f}_U)^2 \mathrm{d}\mu \leq \int_\Omega (f - \bar{f}_U)^2 \frac{-LW}{\lambda \varepsilon W} \mathrm{d}\mu + \frac{b}{\lambda} \int_U (f - \bar{f}_U)^2 \mathrm{d}\mu$$

$$\leq \frac{1}{\lambda} \int_\Omega \left|\nabla f\right|^2 \mathrm{d}\mu + \frac{b}{\lambda \varrho_U} \int_U \left|\nabla f\right|^2 \mathrm{d}\mu.$$

Proof: Local PI and LSI

Lyapunov function

- Task: Find a function $W : \Omega \to [1, \infty)$ such that

$$\frac{LW}{W} \le -\lambda + b\, \mathbb{1}_{B_{a\sqrt{\varepsilon}}(m)}.$$

- Ansatz $W = \exp\left(\frac{\tilde{H}}{2\varepsilon}\right)$, where $\tilde{H}$ is an ε-perturbation of H

$$\frac{\tilde{L}W}{W} = \frac{1}{2}\Delta\tilde{H} - \frac{1}{4\varepsilon}|\nabla\tilde{H}|^2 \overset{!}{\le} -\lambda.$$

  - if x is $\sqrt{\varepsilon}$-away from critical points: $\varepsilon^{-1}|\nabla\tilde{H}(x)|^2 \ge 4\lambda$
  - if x is $\sqrt{\varepsilon}$-nearby a critical point of index $k \ge 1$

$$\Delta\tilde{H}(x) = \underbrace{\tilde{\lambda}_1^- + \cdots + \tilde{\lambda}_k^-}_{<0} + \underbrace{\tilde{\lambda}_{k+1}^+ + \cdots + \tilde{\lambda}_n^+}_{>0} + O(\sqrt{\varepsilon})$$

Can negative eigenvalues be enforced such that $\Delta\tilde{H}(x) \le -2\lambda$?

Proof: Local PI and LSI

Lyapunov function

- Task: Find a function $W : \Omega \to [1, \infty)$ such that

$$\frac{LW}{W} \leq -\lambda + b\, \mathbb{1}_{B_{a\sqrt{\varepsilon}}(m)}.$$

- Ansatz $W = \exp\left(\frac{\tilde{H}}{2\varepsilon}\right)$, where $\tilde{H}$ is an ε-perturbation of H

$$\frac{\tilde{L}W}{W} = \frac{1}{2}\Delta\tilde{H} - \frac{1}{4\varepsilon}|\nabla\tilde{H}|^2 \overset{!}{\leq} -\lambda.$$

  - if x is $\sqrt{\varepsilon}$-away from critical points: $\varepsilon^{-1}|\nabla\tilde{H}(x)|^2 \geq 4\lambda$
  - if x is $\sqrt{\varepsilon}$-nearby a critical point of index $k \geq 1$

$$\Delta\tilde{H}(x) = \underbrace{\tilde{\lambda}_1^- + \cdots + \tilde{\lambda}_k^-}_{<0} + \underbrace{\tilde{\lambda}_{k+1}^+ + \cdots + \tilde{\lambda}_n^+}_{>0} + O(\sqrt{\varepsilon})$$

Can negative eigenvalues be enforced such that $\Delta\tilde{H}(x) \leq -2\lambda$?

Proof: Local PI and LSI

Lyapunov function

- Task: Find a function $W : \Omega \to [1, \infty)$ such that

$$\frac{LW}{W} \leq -\lambda + b\,\mathbb{1}_{B_{a\sqrt{\varepsilon}}(m)}.$$

- Ansatz $W = \exp\left(\frac{\tilde{H}}{2\varepsilon}\right)$, where $\tilde{H}$ is an ε-perturbation of H

$$\frac{\tilde{L}W}{W} = \frac{1}{2}\Delta\tilde{H} - \frac{1}{4\varepsilon}|\nabla\tilde{H}|^2 \overset{!}{\leq} -\lambda.$$

  - if x is $\sqrt{\varepsilon}$-away from critical points: $\varepsilon^{-1}|\nabla\tilde{H}(x)|^2 \geq 4\lambda$
  - if x is $\sqrt{\varepsilon}$-nearby a critical point of index $k \geq 1$

$$\Delta\tilde{H}(x) = \underbrace{\tilde{\lambda}_1^- + \cdots + \tilde{\lambda}_k^-}_{<0} + \underbrace{\tilde{\lambda}_{k+1}^+ + \cdots + \tilde{\lambda}_n^+}_{>0} + O(\sqrt{\varepsilon})$$

Can negative eigenvalues be enforced such that $\Delta\tilde{H}(x) \leq -2\lambda$?

Proof: Local PI and LSI

Lyapunov function

- Task: Find a function $W : \Omega \to [1,\infty)$ such that

$$\frac{LW}{W} \le -\lambda + b\,\mathbb{1}_{B_{a\sqrt{\varepsilon}}(m)}.$$

- Ansatz $W = \exp\left(\frac{\tilde{H}}{2\varepsilon}\right)$, where $\tilde{H}$ is an ε-perturbation of H

$$\frac{\tilde{L}W}{W} = \frac{1}{2}\Delta\tilde{H} - \frac{1}{4\varepsilon}|\nabla\tilde{H}|^2 \overset{!}{\le} -\lambda.$$

  - if x is $\sqrt{\varepsilon}$-away from critical points: $\varepsilon^{-1}|\nabla\tilde{H}(x)|^2 \ge 4\lambda$
  - if x is $\sqrt{\varepsilon}$-nearby a critical point of index $k \ge 1$

$$\Delta\tilde{H}(x) = \underbrace{\tilde{\lambda}_1^- + \cdots + \tilde{\lambda}_k^-}_{<0} + \underbrace{\tilde{\lambda}_{k+1}^+ + \cdots + \tilde{\lambda}_n^+}_{>0} + O(\sqrt{\varepsilon})$$

Can negative eigenvalues be enforced such that $\Delta\tilde{H}(x) \le -2\lambda$?

Proof: Local PI and LSI

Lyapunov function

- Task: Find a function $W : \Omega \to [1, \infty)$ such that

$$\frac{LW}{W} \le -\lambda + b\, \mathbb{1}_{B_{a\sqrt{\varepsilon}}(m)}.$$

- Ansatz $W = \exp\left(\frac{\tilde{H}}{2\varepsilon}\right)$, where $\tilde{H}$ is an ε-perturbation of H

$$\frac{\tilde{L}W}{W} = \frac{1}{2}\Delta\tilde{H} - \frac{1}{4\varepsilon}|\nabla\tilde{H}|^2 \overset{!}{\le} -\lambda.$$

  - if x is $\sqrt{\varepsilon}$-away from critical points: $\varepsilon^{-1}|\nabla\tilde{H}(x)|^2 \ge 4\lambda$
  - if x is $\sqrt{\varepsilon}$-nearby a critical point of index $k \ge 1$

$$\Delta\tilde{H}(x) = \underbrace{\tilde{\lambda}_1^- + \cdots + \tilde{\lambda}_k^-}_{<0} + \underbrace{\tilde{\lambda}_{k+1}^+ + \cdots + \tilde{\lambda}_n^+}_{>0} + O(\sqrt{\varepsilon})$$

Can negative eigenvalues be enforced such that $\Delta\tilde{H}(x) \le -2\lambda$?

Proof: Local PI and LSI

Lyapunov function

- Task: Find a function $W : \Omega \to [1, \infty)$ such that

$$\frac{LW}{W} \leq -\lambda + b\, \mathbb{1}_{B_{a\sqrt{\varepsilon}}(m)}.$$

- Ansatz $W = \exp\left(\frac{\tilde{H}}{2\varepsilon}\right)$, where $\tilde{H}$ is an ε-perturbation of H

$$\frac{\tilde{L}W}{W} = \frac{1}{2}\Delta\tilde{H} - \frac{1}{4\varepsilon}|\nabla\tilde{H}|^2 \overset{!}{\leq} -\lambda.$$

  - if x is $\sqrt{\varepsilon}$-away from critical points: $\varepsilon^{-1}|\nabla\tilde{H}(x)|^2 \geq 4\lambda$
  - if x is $\sqrt{\varepsilon}$-nearby a critical point of index $k \geq 1$

$$\Delta\tilde{H}(x) = \underbrace{\tilde{\lambda}_1^- + \cdots + \tilde{\lambda}_k^-}_{<0} + \underbrace{\tilde{\lambda}_{k+1}^+ + \cdots + \tilde{\lambda}_n^+}_{>0} + O(\sqrt{\varepsilon})$$

Can negative eigenvalues be enforced such that $\Delta\tilde{H}(x) \leq -2\lambda$?

Proof: Local PI and LSI

universitätbonn iam

Lyapunov function

- Task: Find a function $W : \Omega \to [1, \infty)$ such that

$$\frac{LW}{W} \leq -\lambda + b\, \mathbb{1}_{B_{a\sqrt{\varepsilon}}(m)}.$$

- Ansatz $W = \exp\left(\frac{\tilde{H}}{2\varepsilon}\right)$, where $\tilde{H}$ is an ε-perturbation of H

$$\frac{\tilde{L}W}{W} = \frac{1}{2}\Delta\tilde{H} - \frac{1}{4\varepsilon}|\nabla\tilde{H}|^2 \overset{!}{\leq} -\lambda.$$

  - if x is $\sqrt{\varepsilon}$-away from critical points: $\varepsilon^{-1}|\nabla\tilde{H}(x)|^2 \geq 4\lambda$
  - if x is $\sqrt{\varepsilon}$-nearby a critical point of index $k \geq 1$

$$\Delta\tilde{H}(x) = \underbrace{\tilde{\lambda}_1^- + \cdots + \tilde{\lambda}_k^-}_{<0} + \underbrace{\tilde{\lambda}_{k+1}^+ + \cdots + \tilde{\lambda}_n^+}_{>0} + O(\sqrt{\varepsilon})$$

Can negative eigenvalues be enforced such that $\Delta\tilde{H}(x) \leq -2\lambda$? YES!

Proof: Local PI and LSI

Construction of Lyapunov function

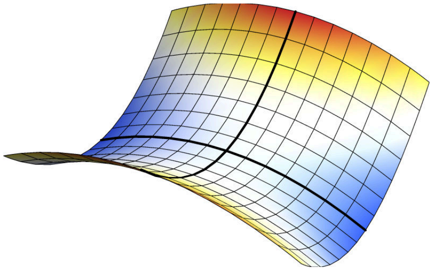


Figure : H around a saddle point

$\tilde{H}$ is quadratic perturbation of H in $\sqrt{\varepsilon}$-neighborhoods of critical points:

$$\sup_x \left| H(x) - \tilde{H}(x) \right| = O(\varepsilon).$$

Proof: Local PI and LSI

Construction of Lyapunov function

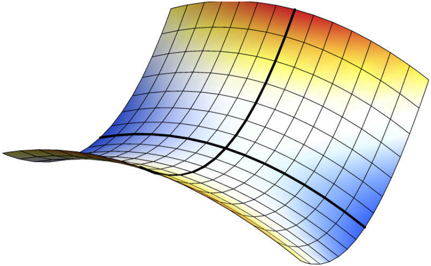


Figure : H around a saddle point

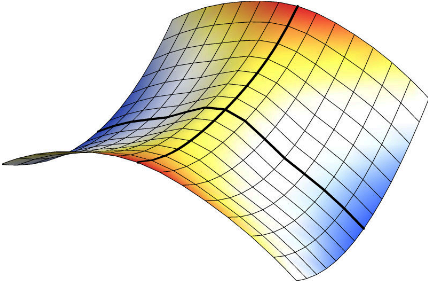


Figure : $\tilde{H}$ around a saddle point

$\tilde{H}$ is quadratic perturbation of H in $\sqrt{\varepsilon}$-neighborhoods of critical points:

$$\sup_x \left| H(x) - \tilde{H}(x) \right| = O(\varepsilon).$$

Proof: Mean-difference estimate

Goal: Find a good estimate for C in

$$(\mathbb{E}_{\mu_0}(f) - \mathbb{E}_{\mu_1}(f))^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Proof: Mean-difference estimate

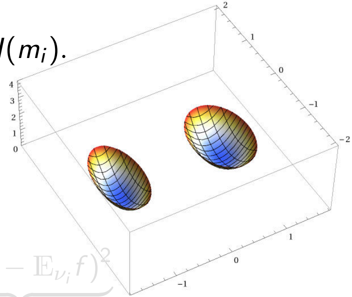
Approximation step

Goal: Find a good estimate for C in

$$(\mathbb{E}_{\mu_0}(f) - \mathbb{E}_{\mu_1}(f))^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Step 1: Approximate μ_0 and μ_1 by truncated Gaussians ν_0 and ν_1:

$$\nu_i \sim \mathcal{N}(m_i, \varepsilon\Sigma_i) \llcorner B_{\sqrt{\varepsilon}}(m_i) \text{ with } \Sigma_i^{-1} := \nabla^2 H(m_i).$$



Introduce ν_0 and ν_1 as coupling:

$$(\mathbb{E}_{\mu_0} f - \mathbb{E}_{\mu_1} f)^2 \leq (1+\tau) \underbrace{(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f)^2}_{\text{transport argument}} + 2(1+\tau^{-1}) \sum_{i=\{0,1\}} \underbrace{(\mathbb{E}_{\mu_i} f - \mathbb{E}_{\nu_i} f)^2}_{\text{approximation bound}}$$

Approximation bound follows from local PI and local LSI.

Proof: Mean-difference estimate

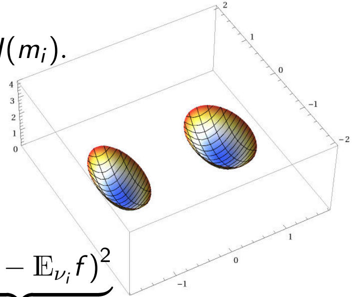
Approximation step

Goal: Find a good estimate for C in

$$\left(\mathbb{E}_{\mu_0}(f) - \mathbb{E}_{\mu_1}(f)\right)^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Step 1: Approximate μ_0 and μ_1 by truncated Gaussians ν_0 and ν_1:

$$\nu_i \sim \mathcal{N}(m_i, \varepsilon\Sigma_i) \llcorner B_{\sqrt{\varepsilon}}(m_i) \quad \text{with} \quad \Sigma_i^{-1} := \nabla^2 H(m_i).$$



Introduce ν_0 and ν_1 as coupling:

$$\left(\mathbb{E}_{\mu_0} f - \mathbb{E}_{\mu_1} f\right)^2 \leq (1+\tau) \underbrace{\left(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f\right)^2}_{\text{transport argument}} + 2(1+\tau^{-1}) \sum_{i=\{0,1\}} \underbrace{\left(\mathbb{E}_{\mu_i} f - \mathbb{E}_{\nu_i} f\right)^2}_{\text{approximation bound}}$$

Approximation
bound follows from local PI and local LSI.

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in

$$\left(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f)\right)^2 \leq C \int |\nabla f|^2 \, d\mu.$$

Step 2: Transport $(\Phi_s \in \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n))_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in

$$\left(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f)\right)^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Step 2: Transport $(\Phi_s \in \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n))_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

$$\left(\int f \, \mathrm{d}\nu_0 - \int f \, \mathrm{d}\nu_1\right)^2 = \left(\int \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}(f \circ \Phi_s) \, \mathrm{d}s \, \mathrm{d}\nu_0\right)^2$$

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in

$$(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f))^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Step 2: Transport $(\Phi_s \in \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n))_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

$$\left(\int f \, \mathrm{d}\nu_0 - \int f \, \mathrm{d}\nu_1\right)^2 = \left(\int \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}(f \circ \Phi_s) \, \mathrm{d}s \, \mathrm{d}\nu_0\right)^2$$

$$= \left(\int \int_0^1 \left\langle \dot{\Phi}_s, \nabla f \circ \Phi_s \right\rangle \mathrm{d}s \, \mathrm{d}\nu_0 \right)^2$$

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in

$$\left(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f)\right)^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Step 2: Transport $(\Phi_s \in \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n))_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

$$\left(\int f \, \mathrm{d}\nu_0 - \int f \, \mathrm{d}\nu_1\right)^2 = \left(\int \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}(f \circ \Phi_s) \, \mathrm{d}s \, \mathrm{d}\nu_0\right)^2$$

$$= \left(\int_0^1 \int \left\langle \dot{\Phi}_s, \nabla f \circ \Phi_s \right\rangle \mathrm{d}\nu_0 \, \mathrm{d}s\right)^2$$

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in

$$\left(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f)\right)^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Step 2: Transport $(\Phi_s \in \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n))_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

$$\begin{aligned}
\left(\int f \, \mathrm{d}\nu_0 - \int f \, \mathrm{d}\nu_1\right)^2 &= \left(\int \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}(f \circ \Phi_s) \, \mathrm{d}s \, \mathrm{d}\nu_0\right)^2 \\
&= \left(\int_0^1 \int \left\langle \dot{\Phi}_s, \nabla f \circ \Phi_s \right\rangle \mathrm{d}\nu_0 \, \mathrm{d}s\right)^2 \\
&= \left(\int_0^1 \int \left\langle \dot{\Phi}_s \circ \Phi_s^{-1}, \nabla f \right\rangle \mathrm{d}\nu_s \, \mathrm{d}s\right)^2
\end{aligned}$$

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in

$$\left(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f)\right)^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Step 2: Transport $(\Phi_s \in \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n))_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

$$\begin{aligned}
\left(\int f \, \mathrm{d}\nu_0 - \int f \, \mathrm{d}\nu_1\right)^2 &= \left(\int \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}(f \circ \Phi_s) \, \mathrm{d}s \, \mathrm{d}\nu_0\right)^2 \\
&= \left(\int_0^1 \int \left\langle \dot{\Phi}_s, \nabla f \circ \Phi_s \right\rangle \mathrm{d}\nu_0 \, \mathrm{d}s\right)^2 \\
&= \left(\int_0^1 \int \left\langle \dot{\Phi}_s \circ \Phi_s^{-1}, \nabla f \right\rangle \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \, \mathrm{d}\mu \, \mathrm{d}s\right)^2
\end{aligned}$$

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in

$$(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f))^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Step 2: Transport $(\Phi_s \in \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n))_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

$$\begin{aligned}
\left(\int f \, \mathrm{d}\nu_0 - \int f \, \mathrm{d}\nu_1 \right)^2 &= \left(\int \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s} (f \circ \Phi_s) \, \mathrm{d}s \, \mathrm{d}\nu_0 \right)^2 \\
&= \left(\int_0^1 \int \left\langle \dot{\Phi}_s, \nabla f \circ \Phi_s \right\rangle \mathrm{d}\nu_0 \, \mathrm{d}s \right)^2 \\
&= \left(\int \int_0^1 \left\langle \dot{\Phi}_s \circ \Phi_s^{-1}, \nabla f \right\rangle \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \, \mathrm{d}s \, \mathrm{d}\mu \right)^2
\end{aligned}$$

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in

$$\left(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f)\right)^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Step 2: Transport $(\Phi_s \in \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n))_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

$$\begin{aligned}
\left(\int f \, \mathrm{d}\nu_0 - \int f \, \mathrm{d}\nu_1\right)^2 &= \left(\int \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}(f \circ \Phi_s) \, \mathrm{d}s \, \mathrm{d}\nu_0\right)^2 \\
&= \left(\int_0^1 \int \left\langle \dot{\Phi}_s, \nabla f \circ \Phi_s \right\rangle \mathrm{d}\nu_0 \, \mathrm{d}s\right)^2 \\
&= \left(\int \left\langle \int_0^1 \dot{\Phi}_s \circ \Phi_s^{-1} \, \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \, \mathrm{d}s, \nabla f \right\rangle \mathrm{d}\mu\right)^2
\end{aligned}$$

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in

$$\left(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f)\right)^2 \leq C \int |\nabla f|^2 \,\mathrm{d}\mu.$$

Step 2: Transport $(\Phi_s \in \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n))_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

$$\begin{aligned}
\left(\int f \,\mathrm{d}\nu_0 - \int f \,\mathrm{d}\nu_1\right)^2 &= \left(\int \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}(f \circ \Phi_s) \,\mathrm{d}s \,\mathrm{d}\nu_0\right)^2 \\
&= \left(\int_0^1 \int \left\langle \dot{\Phi}_s, \nabla f \circ \Phi_s \right\rangle \mathrm{d}\nu_0 \,\mathrm{d}s\right)^2 \\
&= \left(\int \left\langle \int_0^1 \dot{\Phi}_s \circ \Phi_s^{-1} \, \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \,\mathrm{d}s, \nabla f \right\rangle \mathrm{d}\mu\right)^2 \\
&\leq \int \left| \int_0^1 \dot{\Phi}_s \circ \Phi_s^{-1} \, \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \,\mathrm{d}s \right|^2 \mathrm{d}\mu \quad \int |\nabla f|^2 \,\mathrm{d}\mu
\end{aligned}$$

Proof: Mean-difference estimate

Sideremark: Weighted transport distance

Definition

For $\nu_0, \nu_1 \ll \mu$ define the weighted transport distance by

$$\mathcal{T}_\mu^2(\nu_0, \nu_1) = \inf_{\{\Phi_s\}} \int \left| \int_0^1 \dot{\Phi}_s \circ \Phi_s^{-1} \, \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \, \mathrm{d}s \right|^2 \mathrm{d}\mu.$$

$(\Phi_s)_{s\in[0,1]}$ is absolutely continuous in s: $(\Phi_s)_\sharp \nu_0 = \nu_s$.

Mean-difference revisited: Identify $\int |\nabla f|^2 \, \mathrm{d}\mu = \|f\|_{\dot{H}^1(\mu)}^2$, then

$$\left(\int f \, \mathrm{d}\nu_0 - \int f \, \mathrm{d}\nu_1\right)^2 = \left({}_{\dot{H}^{-1}(\mu)}\langle \nu_0 - \nu_1, f\rangle_{\dot{H}^1(\mu)}\right)^2 \le \mathcal{T}_\mu^2(\nu_0, \nu_1) \, \|f\|_{\dot{H}^1(\mu)}^2.$$

Indeed, it holds: $\mathcal{T}_\mu^2(\nu_0, \nu_1) = \|\nu_0 - \nu_1\|_{\dot{H}^{-1}(\mu)}^2$.

Proof: Mean-difference estimate

Sideremark: Weighted transport distance

Definition

For $\nu_0, \nu_1 \ll \mu$ define the weighted transport distance by

$$\mathcal{T}_\mu^2(\nu_0,\nu_1) = \inf_{\{\Phi_s\}} \int \left| \int_0^1 \dot{\Phi}_s \circ \Phi_s^{-1} \, \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \, \mathrm{d}s \right|^2 \mathrm{d}\mu.$$

$(\Phi_s)_{s\in[0,1]}$ is absolutely continuous in s: $(\Phi_s)_\sharp \nu_0 = \nu_s$.

Mean-difference revisited: Identify $\int |\nabla f|^2 \, \mathrm{d}\mu = \|f\|^2_{\dot{H}^1(\mu)}$, then

$$\begin{aligned}\left(\int f \, \mathrm{d}\nu_0 - \int f \, \mathrm{d}\nu_1\right)^2 &= \left({}_{\dot{H}^{-1}(\mu)}\langle \nu_0 - \nu_1, f\rangle_{\dot{H}^1(\mu)}\right)^2 \\ &\le \mathcal{T}_\mu^2(\nu_0,\nu_1)\, \|f\|^2_{\dot{H}^1(\mu)} .\end{aligned}$$

Indeed, it holds: $\mathcal{T}_\mu^2(\nu_0,\nu_1) = \|\nu_0 - \nu_1\|^2_{\dot{H}^{-1}(\mu)}$.

Proof: Mean-difference estimate

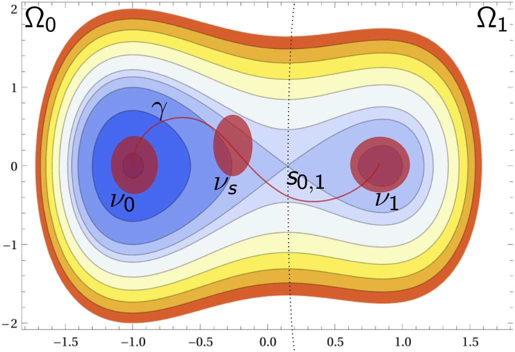
Construction of transport interpolation

Step 3: Ansatz Φ_s such that $\nu_s = (\Phi_s)_\sharp \nu_0 = \mathcal{N}(\gamma_s, \Sigma_s) \llcorner B_{\sqrt{\varepsilon}}(\gamma_s)$

(1) optimize $\gamma \Rightarrow$ passage of saddle $\gamma_{\tau^*} = s_{0,1}$

(2) optimize $\dot{\gamma}_{\tau^*} \Rightarrow$ direction of eigenvector to $\lambda^-(\nabla^2 H(s_{0,1}))$

(3) optimize $\Sigma_{\tau^*} \Rightarrow \Sigma_{\tau^*}^{-1} = \nabla^2 H(s_{0,1})$ on stable manifold of $s_{0,1}$



$$(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

Proof: Mean-difference estimate

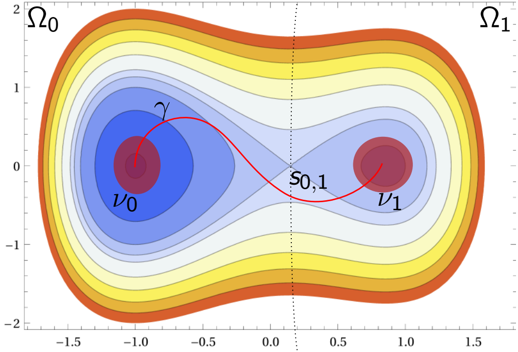
Construction of transport interpolation

Step 3: Ansatz Φ_s such that $\nu_s = (\Phi_s)_\sharp \nu_0 = \mathcal{N}(\gamma_s, \Sigma_s) \llcorner B_{\sqrt{\varepsilon}}(\gamma_s)$

(1) optimize $\gamma \Rightarrow$ passage of saddle $\gamma_{\tau^*} = s_{0,1}$

(2) optimize $\dot\gamma_{\tau^*} \Rightarrow$ direction of eigenvector to $\lambda^-(\nabla^2 H(s_{0,1}))$

(3) optimize $\Sigma_{\tau^*} \Rightarrow \Sigma_{\tau^*}^{-1} = \nabla^2 H(s_{0,1})$ on stable manifold of $s_{0,1}$



$$(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

Proof: Mean-difference estimate

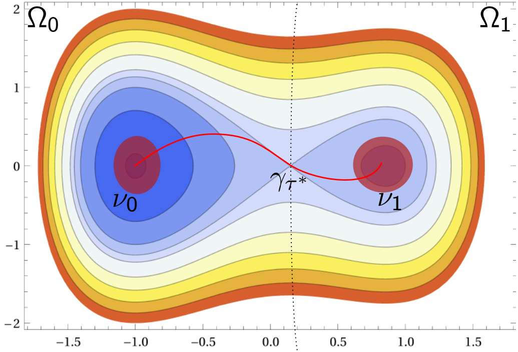
Construction of transport interpolation

Step 3: Ansatz Φ_s such that $\nu_s = (\Phi_s)_\sharp \nu_0 = \mathcal{N}(\gamma_s, \Sigma_s) \llcorner B_{\sqrt{\varepsilon}}(\gamma_s)$

(1) optimize $\gamma \Rightarrow$ passage of saddle $\gamma_{\tau^*} = s_{0,1}$

(2) optimize $\dot{\gamma}_{\tau^*} \Rightarrow$ direction of eigenvector to $\lambda^-(\nabla^2 H(s_{0,1}))$

(3) optimize $\Sigma_{\tau^*} \Rightarrow \Sigma_{\tau^*}^{-1} = \nabla^2 H(s_{0,1})$ on stable manifold of $s_{0,1}$



$$(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

Proof: Mean-difference estimate

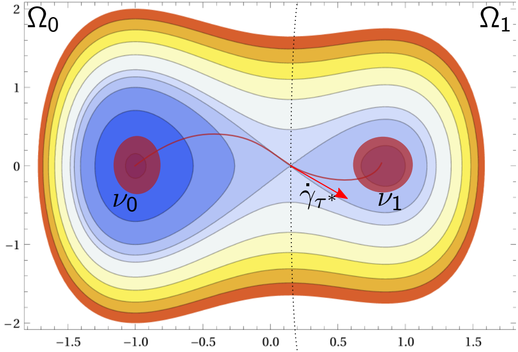
Construction of transport interpolation

Step 3: Ansatz Φ_s such that $\nu_s = (\Phi_s)_\sharp \nu_0 = \mathcal{N}(\gamma_s, \Sigma_s) \llcorner B_{\sqrt{\varepsilon}}(\gamma_s)$

(1) optimize $\gamma \Rightarrow$ passage of saddle $\gamma_{\tau^*} = s_{0,1}$

(2) optimize $\dot{\gamma}_{\tau^*} \Rightarrow$ direction of eigenvector to $\lambda^-(\nabla^2 H(s_{0,1}))$

(3) optimize $\Sigma_{\tau^*} \Rightarrow \Sigma_{\tau^*}^{-1} = \nabla^2 H(s_{0,1})$ on stable manifold of $s_{0,1}$



$$\left(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f\right)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

Proof: Mean-difference estimate

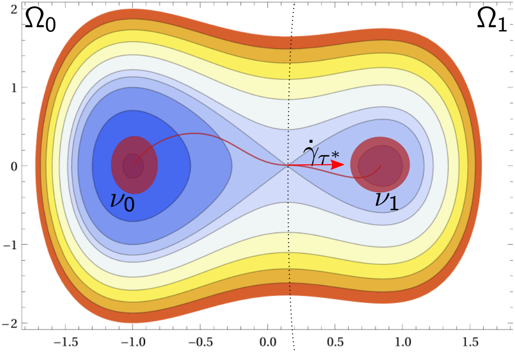
Construction of transport interpolation

Step 3: Ansatz Φ_s such that $\nu_s = (\Phi_s)_\sharp \nu_0 = \mathcal{N}(\gamma_s, \Sigma_s) \llcorner B_{\sqrt{\varepsilon}}(\gamma_s)$

(1) optimize $\gamma \Rightarrow$ passage of saddle $\gamma_{\tau^*} = s_{0,1}$

(2) optimize $\dot{\gamma}_{\tau^*} \Rightarrow$ direction of eigenvector to $\lambda^-(\nabla^2 H(s_{0,1}))$

(3) optimize $\Sigma_{\tau^*} \Rightarrow \Sigma_{\tau^*}^{-1} = \nabla^2 H(s_{0,1})$ on stable manifold of $s_{0,1}$



$$\left(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f\right)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

Proof: Mean-difference estimate

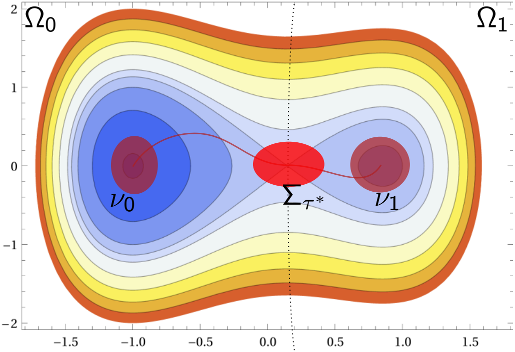
Construction of transport interpolation

Step 3: Ansatz Φ_s such that $\nu_s = (\Phi_s)_\sharp \nu_0 = \mathcal{N}(\gamma_s, \Sigma_s) \llcorner B_{\sqrt{\varepsilon}}(\gamma_s)$

(1) optimize $\gamma \Rightarrow$ passage of saddle $\gamma_{\tau^*} = s_{0,1}$

(2) optimize $\dot{\gamma}_{\tau^*} \Rightarrow$ direction of eigenvector to $\lambda^-(\nabla^2 H(s_{0,1}))$

(3) optimize $\Sigma_{\tau^*} \Rightarrow \Sigma_{\tau^*}^{-1} = \nabla^2 H(s_{0,1})$ on stable manifold of $s_{0,1}$



$$(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

Proof: Mean-difference estimate

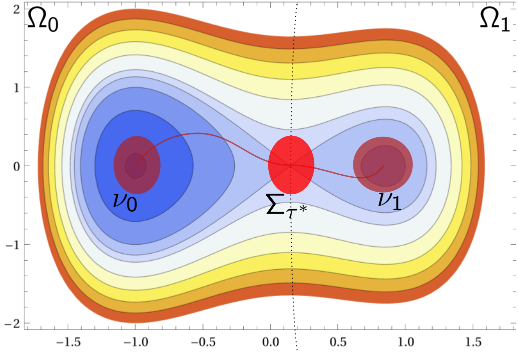
Construction of transport interpolation

Step 3: Ansatz Φ_s such that $\nu_s = (\Phi_s)_\sharp \nu_0 = \mathcal{N}(\gamma_s, \Sigma_s) \llcorner B_{\sqrt{\varepsilon}}(\gamma_s)$

(1) optimize $\gamma \Rightarrow$ passage of saddle $\gamma_{\tau^*} = s_{0,1}$

(2) optimize $\dot{\gamma}_{\tau^*} \Rightarrow$ direction of eigenvector to $\lambda^-(\nabla^2 H(s_{0,1}))$

(3) optimize $\Sigma_{\tau^*} \Rightarrow \Sigma_{\tau^*}^{-1} = \nabla^2 H(s_{0,1})$ on stable manifold of $s_{0,1}$



$$(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

Proof: Mean-difference estimate

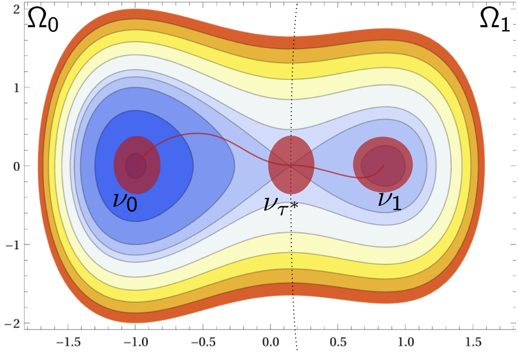
Construction of transport interpolation

Step 3: Ansatz Φ_s such that $\nu_s = (\Phi_s)_\sharp \nu_0 = \mathcal{N}(\gamma_s, \Sigma_s) \llcorner B_{\sqrt{\varepsilon}}(\gamma_s)$

(1) optimize $\gamma \Rightarrow$ passage of saddle $\gamma_{\tau^*} = s_{0,1}$

(2) optimize $\dot{\gamma}_{\tau^*} \Rightarrow$ direction of eigenvector to $\lambda^-(\nabla^2 H(s_{0,1}))$

(3) optimize $\Sigma_{\tau^*} \Rightarrow \Sigma_{\tau^*}^{-1} = \nabla^2 H(s_{0,1})$ on stable manifold of $s_{0,1}$

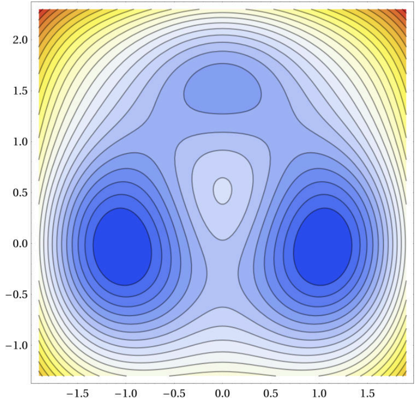


$$(\mathbb{E}_{\nu_0} f - \mathbb{E}_{\nu_1} f)^2 \lesssim \frac{Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}} \frac{2\pi\varepsilon\sqrt{|\det \nabla^2 H(s_{0,1})|}}{|\lambda^-(\nabla^2 H(s_{0,1}))|} e^{\varepsilon^{-1} H(s_{0,1})} \int |\nabla f|^2 \, d\mu.$$

Outline

1. Description and Question
2. Main results
3. Sketch of the Proofs
    - Local PI and LSI
    - Mean-difference estimate
4. Application to entropic switching

Investigation of specific energy landscape:



Features:

- two global minima a, b
- additional local minimum c
- saddle points $s_{a,b}, s_{a,c}, s_{c,b}$

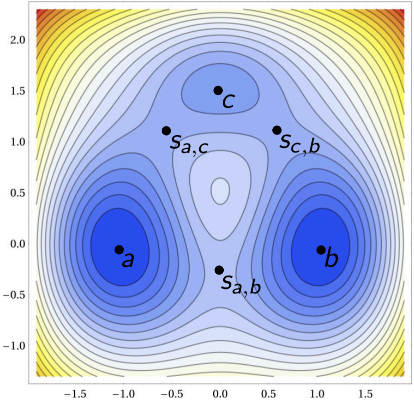
degenerated:

$$|H(s_{a,b}) - H(s_{a,c})| = \delta \text{ small}$$

two small parameters: ε and δ

Application to entropic switching

Investigation of specific energy landscape:



Features:

- two global minima a, b
- additional local minimum c
- saddle points $s_{a,b}$, $s_{a,c}$, $s_{c,b}$

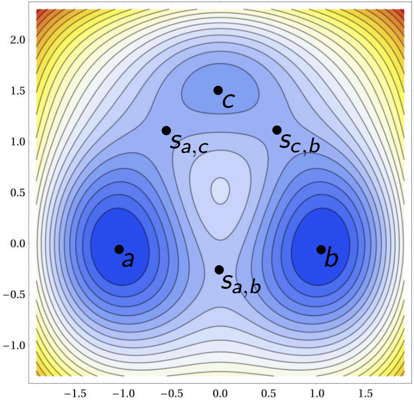
degenerated:

$$|H(s_{a,b}) - H(s_{a,c})| = \delta \text{ small}$$

two small parameters: ε and δ

Application to entropic switching

Investigation of specific energy landscape:



Features:

- two global minima a, b
- additional local minimum c
- saddle points $s_{a,b}$, $s_{a,c}$, $s_{c,b}$

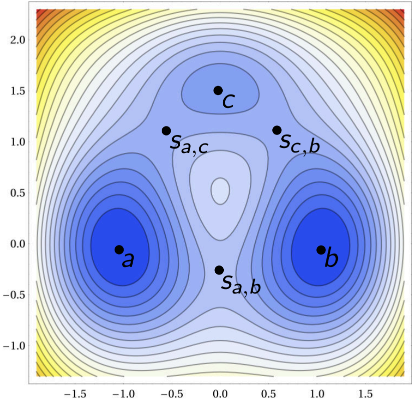
degenerated:

$$|H(s_{a,b}) - H(s_{a,c})| = \delta \text{ small}$$

two small parameters: ε and δ

Application to entropic switching

Investigation of specific energy landscape:



Features:

- two global minima a, b
- additional local minimum c
- saddle points $s_{a,b}$, $s_{a,c}$, $s_{c,b}$

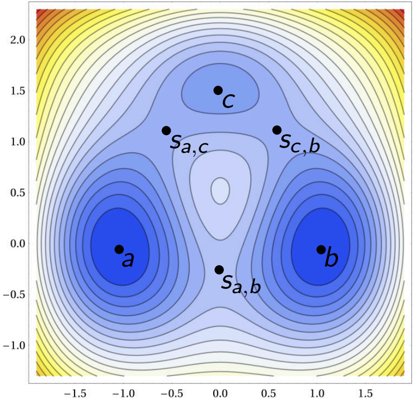
degenerated:

$$|H(s_{a,b}) - H(s_{a,c})| = \delta \text{ small}$$

two small parameters: ε and δ

Application to entropic switching

Investigation of specific energy landscape:



Features:

- two global minima a, b
- additional local minimum c
- saddle points $s_{a,b}$, $s_{a,c}$, $s_{c,b}$

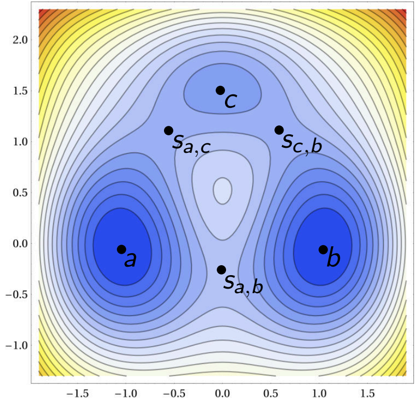
degenerated:

$$|H(s_{a,b}) - H(s_{a,c})| = \delta \text{ small}$$

two small parameters: ε and δ

Application to entropic switching

Investigation of specific energy landscape:



Features:

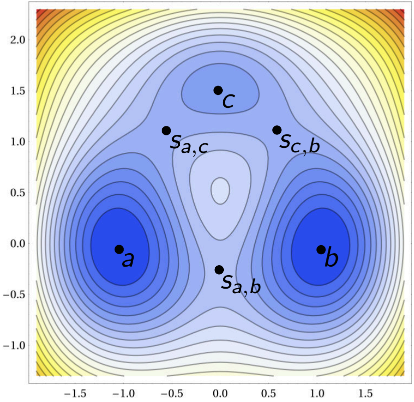
- two global minima a, b
- additional local minimum c
- saddle points $s_{a,b}$, $s_{a,c}$, $s_{c,b}$

degenerated:

$$|H(s_{a,b}) - H(s_{a,c})| = \delta \text{ small}$$

two small parameters: ε and δ

Investigation of specific energy landscape:



Features:

- two global minima a, b
- additional local minimum c
- saddle points $s_{a,b}$, $s_{a,c}$, $s_{c,b}$

degenerated:

$$|H(s_{a,b}) - H(s_{a,c})| = \delta \text{ small}$$

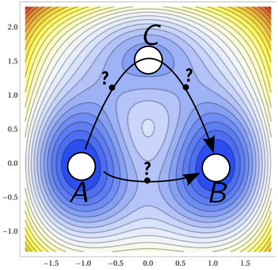
two small parameters: ε and δ

Fluxes and reaction rates

Interpretation as chemical reactions

- $A = \{|x-a| \le r\}$ reactant
- $B = \{|x-a| \le r\}$ product
- $C = \{|x-a| \le r\}$ intermediate product

What are typical reaction rates and paths?



How to define the reaction rate?

Steady state with inflow of reactants and outflow of products:

$$Lh_{A,B} = 0 \quad \text{in } (A \cup B)^c \quad \text{and} \quad h_{A,B} = \mathbb{1}_A \quad \text{in } A \cup B.$$

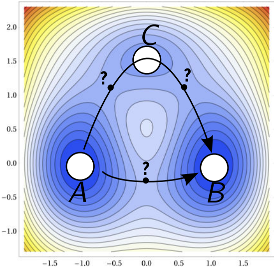
Definition (Reaction rate)

$$k_{A,B} := \varepsilon \int |J_{A,B}|^2 \, d\mu = \varepsilon \int |\nabla h_{A,B}|^2 \, d\mu.$$

Fluxes and reaction rates

Interpretation as chemical reactions

- $A = \{|x - a| \leq r\}$ reactant
- $B = \{|x - a| \leq r\}$ product
- $C = \{|x - a| \leq r\}$ intermediate product



What are typical reaction rates and paths?

How to define the reaction rate?

Steady state with inflow of reactants and outflow of products:

$$Lh_{A,B} = 0 \quad \text{in } (A \cup B)^c \quad \text{and} \quad h_{A,B} = \mathbb{1}_A \quad \text{in } A \cup B.$$

Definition (Reaction rate)

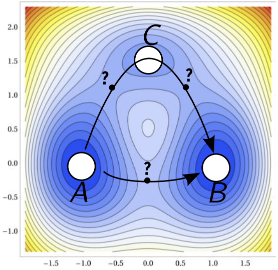
$$k_{A,B} := \varepsilon \int |J_{A,B}|^2 \, d\mu = \varepsilon \int |\nabla h_{A,B}|^2 \, d\mu.$$

Fluxes and reaction rates

Interpretation as chemical reactions

- $A = \{|x - a| \leq r\}$ reactant
- $B = \{|x - a| \leq r\}$ product
- $C = \{|x - a| \leq r\}$ intermediate product

What are typical reaction rates and paths?



How to define the reaction rate?

Steady state with inflow of reactants and outflow of products:

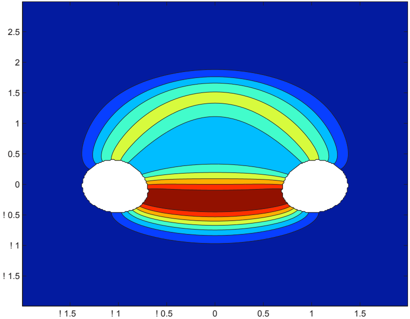
$$Lh_{A,B} = 0 \quad \text{in } (A \cup B)^c \quad \text{and} \quad h_{A,B} = \mathbb{1}_A \quad \text{in } A \cup B.$$

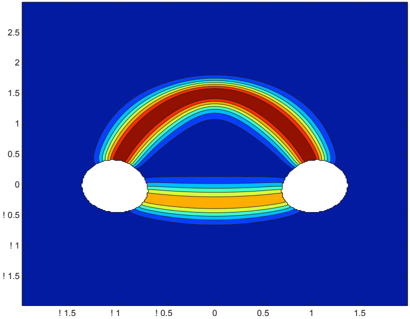
Definition (Reaction rate)

$$k_{A,B} := \varepsilon \int |J_{A,B}|^2 \, \mathrm{d}\mu = \varepsilon \int |\nabla h_{A,B}|^2 \, \mathrm{d}\mu.$$

Entropic switching

Numerics: P. Metzner, C. Schütte and E. Vanden-Eijnden 2006 [MSVE06]



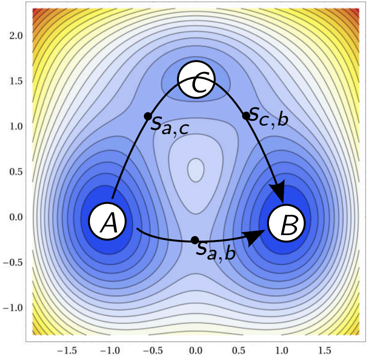


very low temperature $\varepsilon \ll \delta$ vs. low temperature $\varepsilon \approx \delta$

[MSVE06] P. Metzner, C. Schütte, and E. Vanden-Eijnden, *Illustration of transition path theory on a collection of simple examples*. The Journal of chemical physics, 125:**8**, 2006.

Connection to electrical networks

series and parallel law



$\Longrightarrow$

- minima become nodes
- saddles become resistors
- boundary condition becomes voltage source

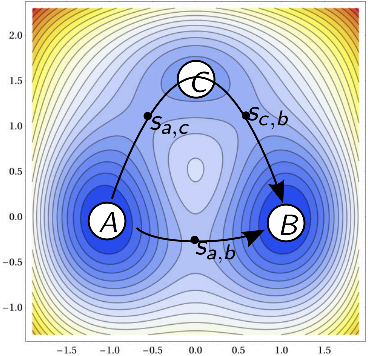
series and parallel law

The total resistance R between A and B of the network satisfies

$$\frac{1}{R} = \frac{1}{R_{AB}} + \frac{1}{R_{AC} + R_{CB}} \qquad .$$

Connection to electrical networks

series and parallel law



$\Longrightarrow$

- minima become nodes
- saddles become resistors
- boundary condition becomes voltage source

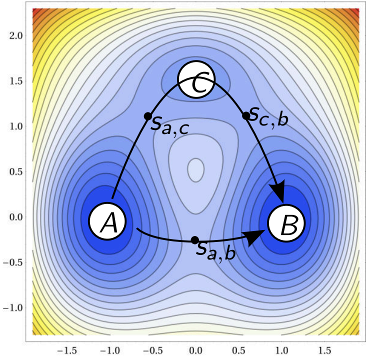
series and parallel law

The total resistance R between A and B of the network satisfies

$$\frac{1}{R} = \frac{1}{R_{AB}} + \frac{1}{R_{AC} + R_{CB}} \quad .$$

Connection to electrical networks

series and parallel law



$\Longrightarrow$

- minima become nodes
- saddles become resistors
- boundary condition becomes voltage source

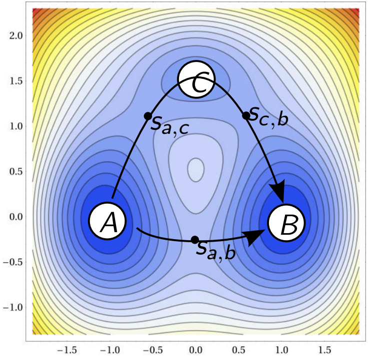
series and parallel law

The total resistance R between A and B of the network satisfies

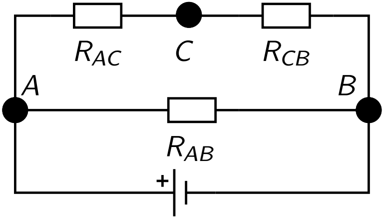
$$\frac{1}{R} = \frac{1}{R_{AB}} + \frac{1}{R_{AC} + R_{CB}} \qquad .$$

Connection to electrical networks

series and parallel law



$\Rightarrow$



Ohm's law: total current $= \frac{\text{voltage}}{\text{total resistance}}$

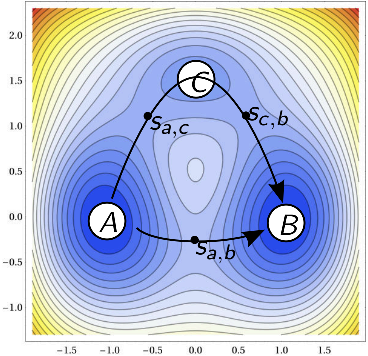
series and parallel law

The total resistance R between A and B of the network satisfies

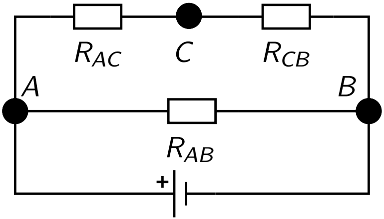
$$\frac{1}{R} = \frac{1}{R_{AB}} + \frac{1}{R_{AC} + R_{CB}} .$$

Connection to electrical networks

series and parallel law



$\Rightarrow$



Ohm's law: total current $= \dfrac{\text{voltage}}{\text{total resistance}}$

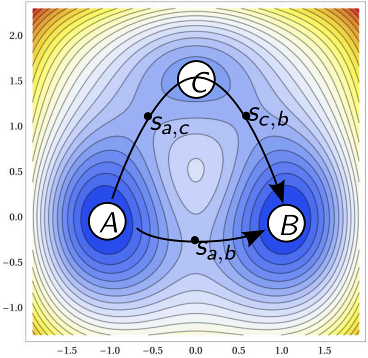
series and parallel law

The total resistance R between A and B of the network satisfies

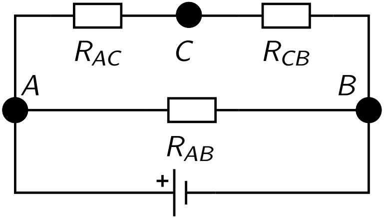
$$\frac{1}{R} = \frac{1}{R_{AB}} + \frac{1}{R_{AC} + R_{CB}} \qquad .$$

Connection to electrical networks

series and parallel law



$\Rightarrow$



Ohm's law: $\text{total current} = \frac{\text{voltage}}{\text{total resistance}}$

series and parallel law

The total resistance R between A and B of the network satisfies

$$\frac{1}{R} = \frac{1}{R_{AB}} + \frac{1}{R_{AC} + R_{CB}} \overset{\text{Ohm}}{=} k_{A,B}.$$

Result and comparison with numerical data

Identification can be justified using the weighted transport distance

Series and parallel law for transport cost

$$k_{A,B} \approx \frac{1}{\mathcal{T}_\mu^2(\mu \llcorner A, \mu \llcorner B)} \approx \frac{1}{T_{AB}} + \frac{1}{T_{AC} + T_{CB}},$$

where

$$T_{AB} = \inf_{\Phi \in \Pi(s_{AB})} \int \left| \int_0^1 \dot{\Phi}_s \circ \Phi_s^{-1} \frac{d\nu_s}{d\mu} \, ds \right|^2 d\mu.$$

$\Pi(s_{AB})$: transport interpolations between $\mu \llcorner A$ and $\mu \llcorner B$ across s_{AB}.

	$\varepsilon = 0.15$	$\varepsilon = 0.6$
[MSVE06] TPT, flux	9.47×10^{-8}	1.912×10^{-2}
[MSVE06] TPT, commitor	9.22×10^{-8}	1.924×10^{-2}
transport, numerical Z_μ	9.33×10^{-8}	1.926×10^{-2}

Result and comparison with numerical data

Identification can be justified using the weighted transport distance

Series and parallel law for transport cost

$$k_{A,B} \approx \frac{1}{\mathcal{T}_\mu^2(\mu \llcorner A, \mu \llcorner B)} \approx \frac{1}{T_{AB}} + \frac{1}{T_{AC} + T_{CB}},$$

where

$$T_{AB} = \inf_{\Phi \in \Pi(s_{AB})} \int \left| \int_0^1 \dot{\Phi}_s \circ \Phi_s^{-1} \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \, \mathrm{d}s \right|^2 \mathrm{d}\mu.$$

$\Pi(s_{AB})$: transport interpolations between $\mu \llcorner A$ and $\mu \llcorner B$ across s_{AB}.

	$\varepsilon = 0.15$	$\varepsilon = 0.6$
[MSVE06] TPT, flux	9.47×10^{-8}	1.912×10^{-2}
[MSVE06] TPT, commitor	9.22×10^{-8}	1.924×10^{-2}
transport, numerical Z_μ	9.33×10^{-8}	1.926×10^{-2}

Result and comparison with numerical data

Identification can be justified using the weighted transport distance

Series and parallel law for transport cost

$$k_{A,B} \approx \frac{1}{\mathcal{T}_\mu^2(\mu \llcorner A, \mu \llcorner B)} \approx \frac{1}{T_{AB}} + \frac{1}{T_{AC} + T_{CB}},$$

where

$$T_{AB} = \inf_{\Phi \in \Pi(s_{AB})} \int \left| \int_0^1 \dot{\Phi}_s \circ \Phi_s^{-1} \, \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \, \mathrm{d}s \right|^2 \mathrm{d}\mu.$$

$\Pi(s_{AB})$: transport interpolations between $\mu \llcorner A$ and $\mu \llcorner B$ across s_{AB}.

	$\varepsilon = 0.15$	$\varepsilon = 0.6$
[MSVE06] TPT, flux	9.47×10^{-8}	1.912×10^{-2}
[MSVE06] TPT, commitor	9.22×10^{-8}	1.924×10^{-2}
transport, numerical Z_μ	9.33×10^{-8}	1.926×10^{-2}

Summary

- Overdamped Langevin dynamics at low temperature
- Partitions and splitting induced from dynamic (two scales)
- Optimal constants in PI and LSI follow from two ingredients:
  - *good* local mixing
    $\Rightarrow$ Lyapunov technique handles non-convex scenario
  - *sharp* estimates of mean-difference
    $\Rightarrow$ transport representation of H^{-1}-norm and approximation
- Relation to electrical networks to estimate reaction rates

Summary

- Overdamped Langevin dynamics at low temperature
- Partitions and splitting induced from dynamic (two scales)
- Optimal constants in PI and LSI follow from two ingredients:
  - *good* local mixing
    $\Rightarrow$ Lyapunov technique handles non-convex situations
  - *sharp* estimates of mean-difference
    $\Rightarrow$ transport representation of H^{-1}-norm and optimization
- Relation to electrical networks to estimate reaction rates

Summary

- Overdamped Langevin dynamics at low temperature
- Partitions and splitting induced from dynamic (two scales)
- Optimal constants in PI and LSI follow from two ingredients:
  - *good* local mixing
    $\Rightarrow$ Lyapunov technique handles non-convex situations
  - *sharp* estimates of mean-difference
    $\Rightarrow$ transport representation of H^{-1}-norm and optimization
- Relation to electrical networks to estimate reaction rates

Summary

- Overdamped Langevin dynamics at low temperature
- Partitions and splitting induced from dynamic (two scales)
- Optimal constants in PI and LSI follow from two ingredients:
  - *good* local mixing
    $\Rightarrow$ Lyapunov technique handles non-convex situations
  - *sharp* estimates of mean-difference
    $\Rightarrow$ transport representation of H^{-1}-norm and optimization
- Relation to electrical networks to estimate reaction rates

Summary

- Overdamped Langevin dynamics at low temperature
- Partitions and splitting induced from dynamic (two scales)
- Optimal constants in PI and LSI follow from two ingredients:
  - *good* local mixing
    $\Rightarrow$ Lyapunov technique handles non-convex situations
  - *sharp* estimates of mean-difference
    $\Rightarrow$ transport representation of H^{-1}-norm and optimization
- Relation to electrical networks to estimate reaction rates

Summary

- Overdamped Langevin dynamics at low temperature
- Partitions and splitting induced from dynamic (two scales)
- Optimal constants in PI and LSI follow from two ingredients:
    - *good* local mixing
      $\Rightarrow$ Lyapunov technique handles non-convex situations
    - *sharp* estimates of mean-difference
      $\Rightarrow$ transport representation of H^{-1}-norm and optimization
- Relation to electrical networks to estimate reaction rates

Summary

- Overdamped Langevin dynamics at low temperature
- Partitions and splitting induced from dynamic (two scales)
- Optimal constants in PI and LSI follow from two ingredients:
  - *good* local mixing
    $\Rightarrow$ Lyapunov technique handles non-convex situations
  - *sharp* estimates of mean-difference
    $\Rightarrow$ transport representation of H^{-1}-norm and optimization
- Relation to electrical networks to estimate reaction rates

Summary

- Overdamped Langevin dynamics at low temperature
- Partitions and splitting induced from dynamic (two scales)
- Optimal constants in PI and LSI follow from two ingredients:
  - *good* local mixing
    $\Rightarrow$ Lyapunov technique handles non-convex situations
  - *sharp* estimates of mean-difference
    $\Rightarrow$ transport representation of H^{-1}-norm and optimization
- Relation to electrical networks to estimate reaction rates