Eyring-Kramers formula for Poincaré and logarithmic Sobolev inequalities

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joint work with Georg Menz (Stanford)

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Introduction

Overdamped Langevin dynamics

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

Dynamic at temperature $\varepsilon \ll 1$

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

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

where $Z_\mu = \int e^{-\frac{H}{\varepsilon}} dx$

Generator law $X_t = f_t \mu$ evolves

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

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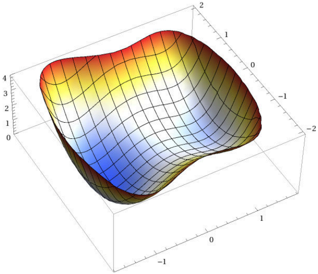

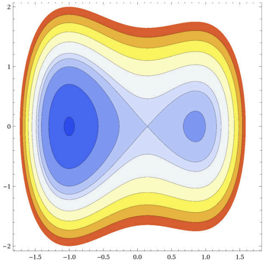

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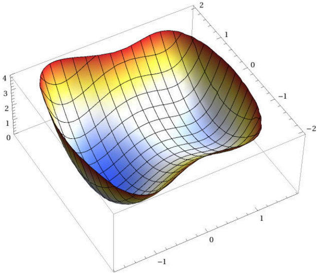

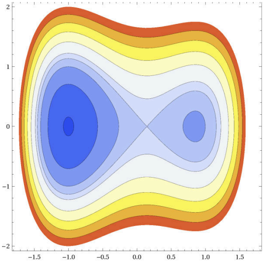

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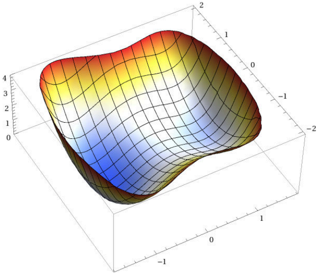

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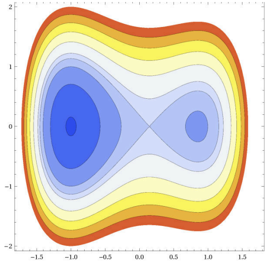

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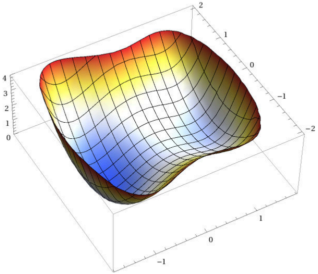

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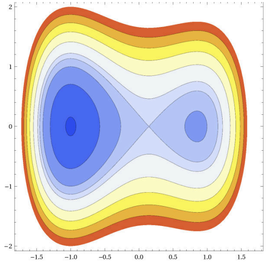

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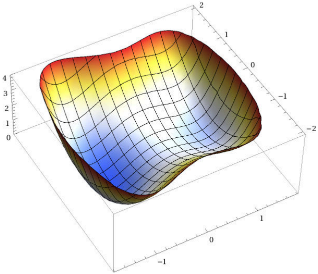

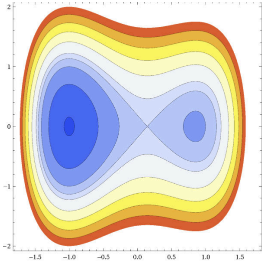

Poincaré and logarithmic Sobolev inequality

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 $\forall f : \mathbb{R}^n \to \mathbb{R}$

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

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

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

Basins of attraction $\Omega_0 \uplus \Omega_1 = \mathbb{R}^n$ of local minima m_0, m_1:

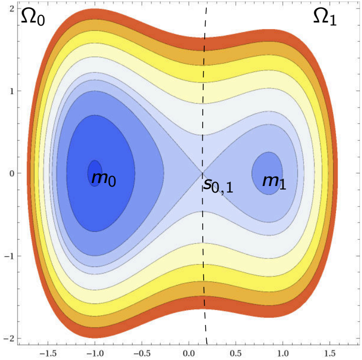
$$\Omega_i := \left\{ y_0 \in \mathbb{R}^n : \dot{y}_t = -\nabla H(y_t), y_t \to m_i \right\}.$$

Restricted measures μ_0, μ_1:

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

Mixture representation

$$\mu = Z_0 \mu_0 + Z_1 \mu_1, \quad Z_i := \mu(\Omega_i).$$



Splitting

Lemma

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

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

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
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Main results

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Theorem (Local PI and LSI)

The measures μ_0 *and* μ_1 *satisfy* $\mathrm{PI}(\varrho_{loc})$ *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 convex potential
- Non-convexity of potential worsens LSI
- Both results scale optimal in one dimension

Theorem (Mean-difference estimate)

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

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Eyring-Kramers formula

Corollary

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

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

Asymptotic evaluation of the factor $\frac{Z_0 Z_1 Z_\mu}{(2\pi\varepsilon)^{\frac{n}{2}}}$ for two special cases:

$$H(m_0) < H(m_1): \quad 1 \leq \frac{\varrho}{\alpha} \lesssim O(\varepsilon^{-1})$$

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Proof: Mean-difference estimate

Goal: Find a good estimate for C in

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

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Approximation step

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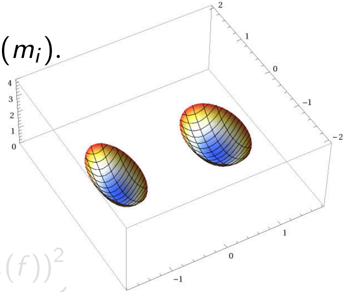

Introduce ν_0 and ν_1 as coupling:

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

Approximation bound follows from local PI and local LSI.

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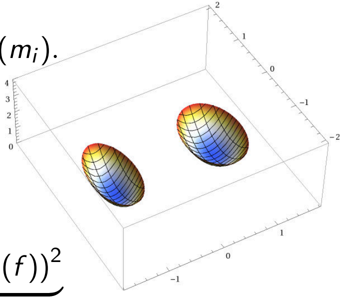

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Transport interpolation

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

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

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

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

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

Proof: Mean-difference estimate

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

Proof: Mean-difference estimate

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Proof: Mean-difference estimate

Transport interpolation

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&\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

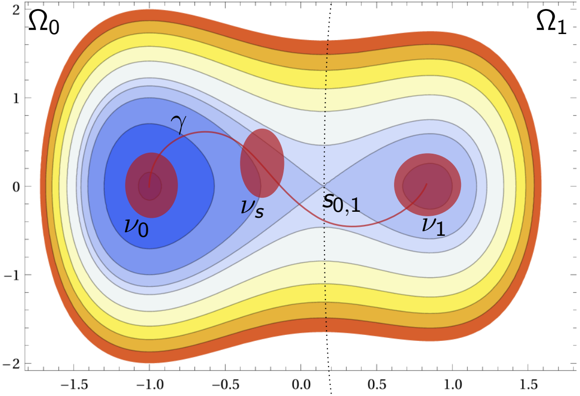
Construction of transport interpolation

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 $s_{0,1}$



Proof: Mean-difference estimate

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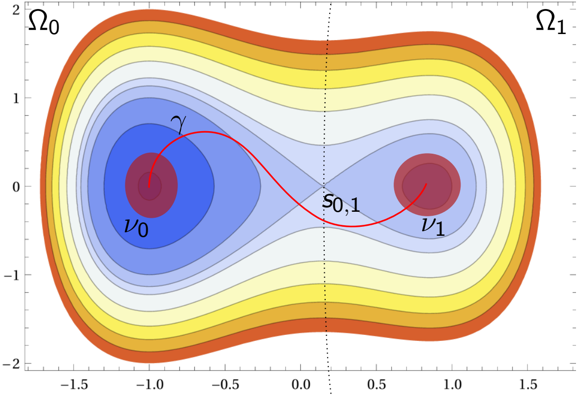

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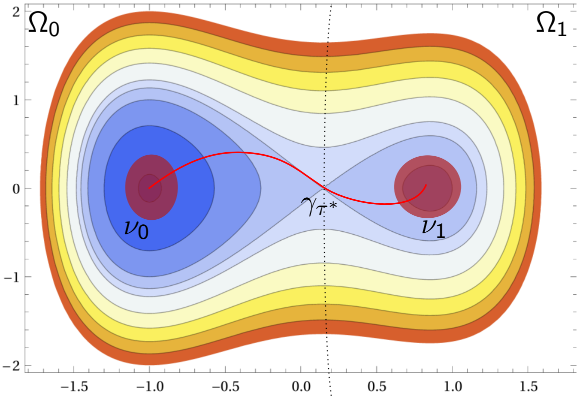

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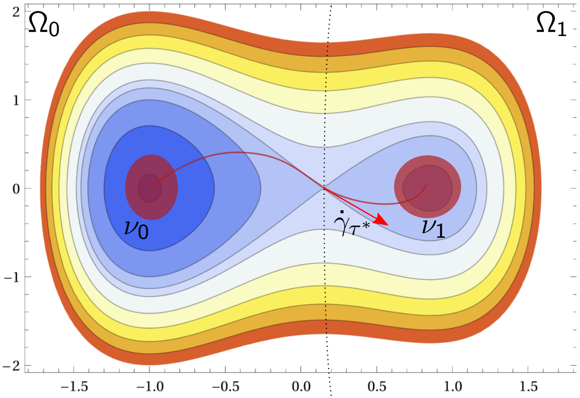

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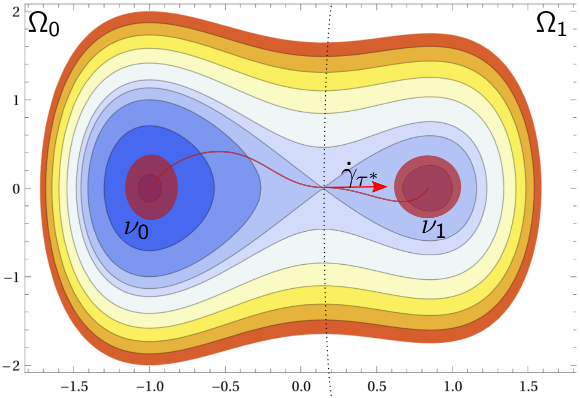

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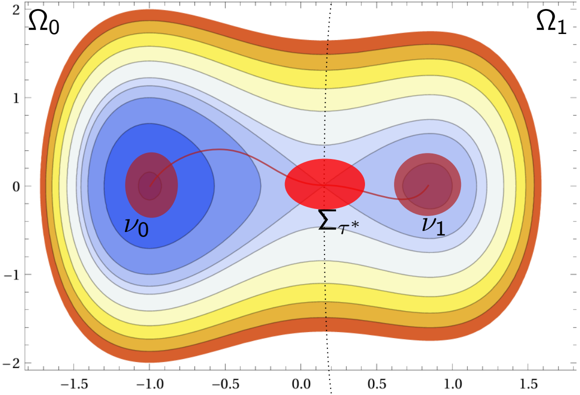

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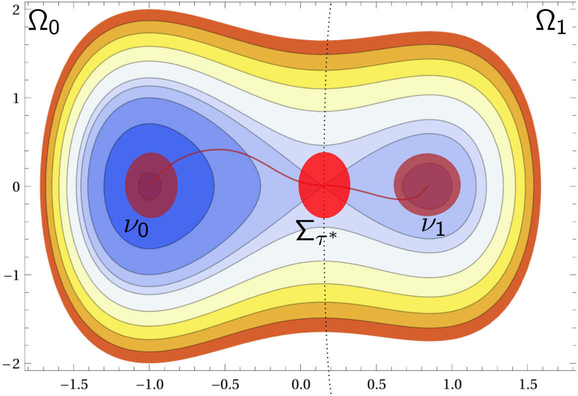

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