Eyring-Kramers formula
for
Poincaré
and
logarithmic Sobolev inequalities

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joint work with Georg Menz (Stanford)

Oberseminar Analysis

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Introduction

Overdamped Langevin dynamics

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

Dynamic at temperature $\varepsilon \ll 1$
$$dX_t = -\nabla H(X_t)dt + \sqrt{2\varepsilon}\, dW_t$$

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

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

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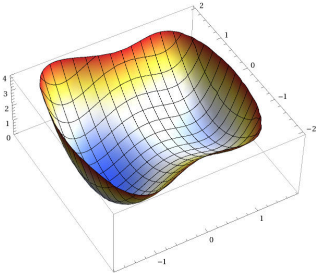

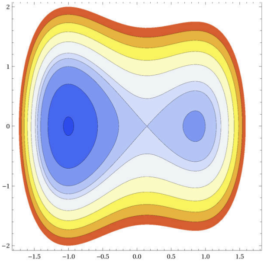

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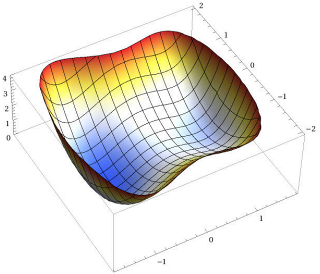

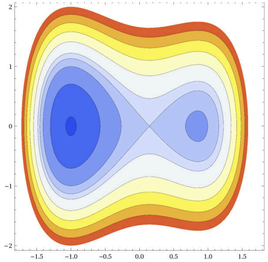

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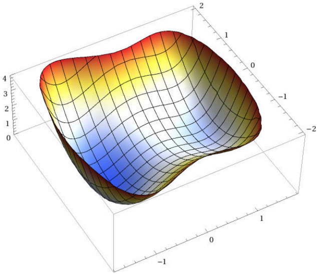

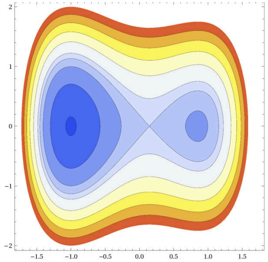

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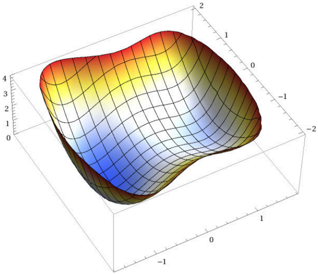

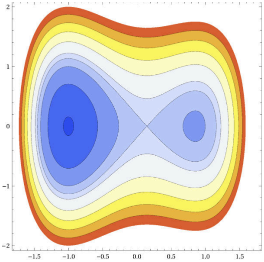

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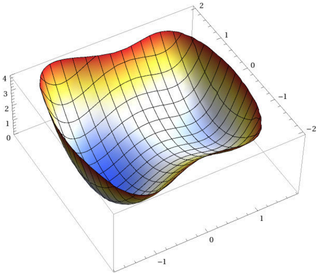

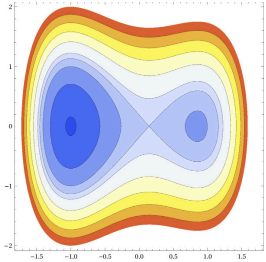

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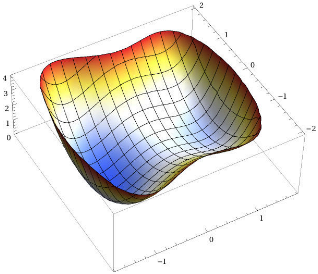

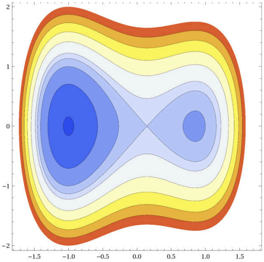

Distance and convergence to equilibrium

Quantification via functional inequalities

- $f \equiv$ const. is equilibrium state
- for a strictly convex function $\xi : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ define

$$\Xi(f) := \int \xi \circ f \, \mathrm{d}\mu - \xi\left(\int f \, \mathrm{d}\mu\right).$$

- evaluate $\Xi(f_t)$ along solution $\partial f_t = L f_t$

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Convergence to equilibrium is established by $\mathrm{FI}(\beta)$

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

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

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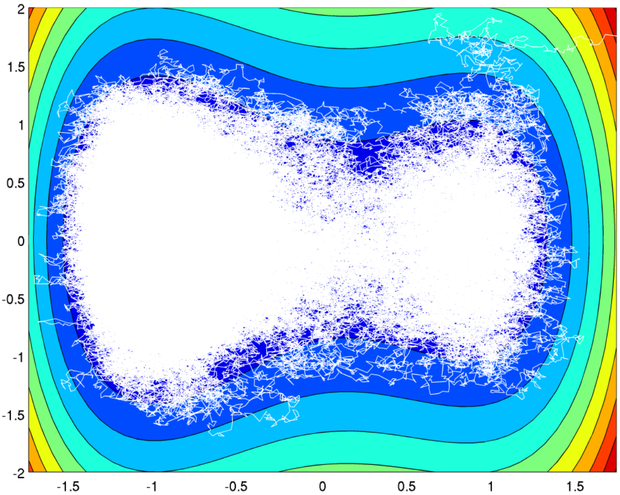


Figure : Trajectory for $\varepsilon = 0.4$

Heuristics

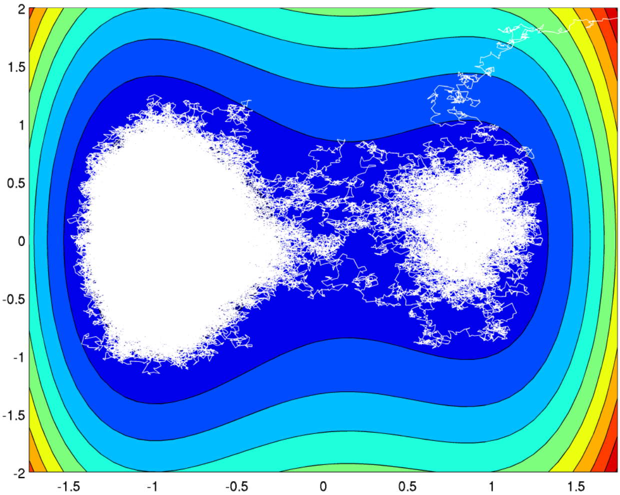


Figure : Trajectory for $\varepsilon = 0.2$

Heuristics

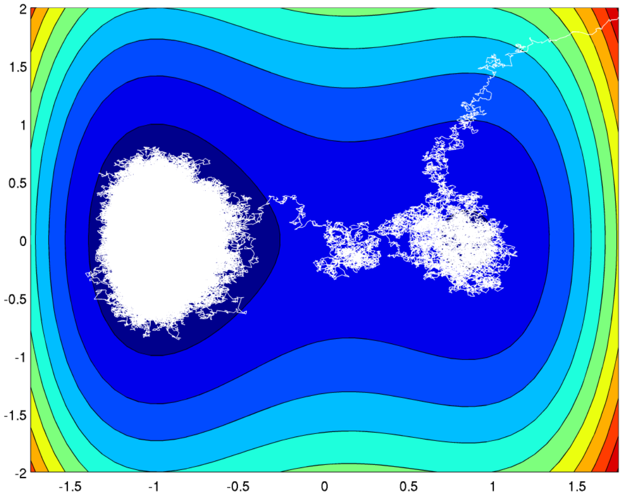


Figure : Trajectory for $\varepsilon = 0.1$

Heuristics

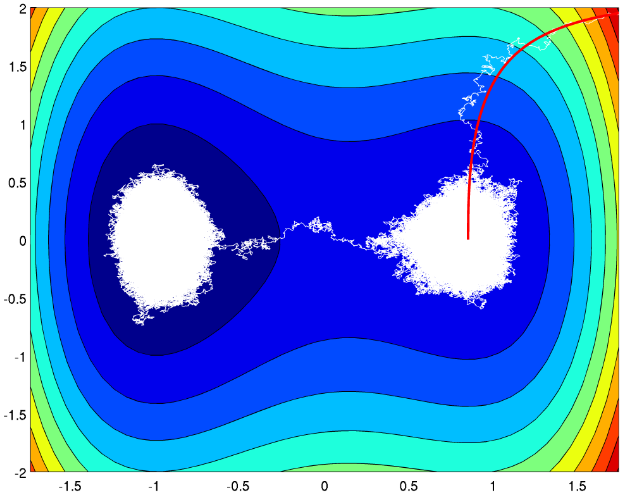


Figure : Trajectory for $\varepsilon = 0.05$ (red $\varepsilon = 0$)

Partitions

Make use of the two scale in dynamics by decomposition [GOVW09]

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

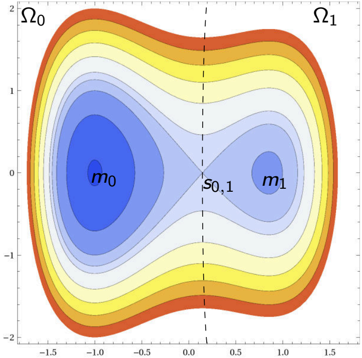
$$\Omega_i := \{y_0 \in \mathbb{R}^n : \dot{y}_t = -\nabla H(y_t), y_t \to m_i\}.$$

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

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

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

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

Splitting

Lemma

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

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

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

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Main results

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

Theorem (Mean-difference estimate)

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

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New proof to [BEGK04/05] for PI and extension to LSI:

Corollary

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

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

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Proof: Local PI and LSI

Lyapunov condition

Technique by Bakry, Barthe, Cattiaux, Guillin, Wang and Wu 2008–
Principal eigenvalue characterization for L by Donsker-Varadhan 1975

Definition

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

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

W is called Lyapunov function for L.

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Proof: Lyapunov $\Rightarrow$ PI(ϱ)

With the symmetry of $\varepsilon^{-1}(-L)$ in $L^2(\mu)$ follows

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

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

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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: $\varepsilon^{-1}|\nabla\tilde{H}(x)|^2 \geq 4\lambda$
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$$\Delta\tilde{H}(x) = \underbrace{\tilde{\lambda}_1^- + \cdots + \tilde{\lambda}_k^-}_{<0} + \underbrace{\tilde{\lambda}_{k+1}^+ + \cdots + \tilde{\lambda}_n^+}_{>0} + O(\sqrt{\varepsilon})$$

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

Proof: Local PI and LSI

Construction of Lyapunov function

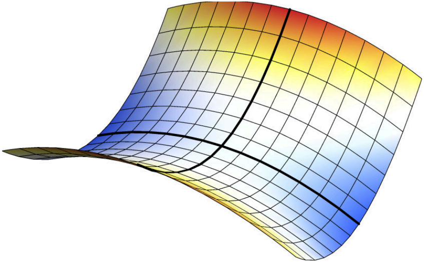

Figure : H around a saddle point

$\tilde{H}$ 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

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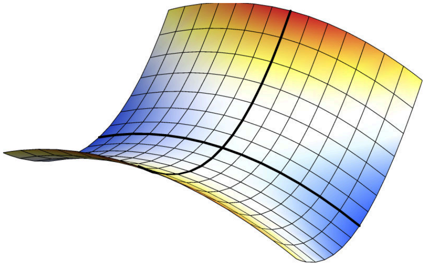

Figure : H around a saddle point

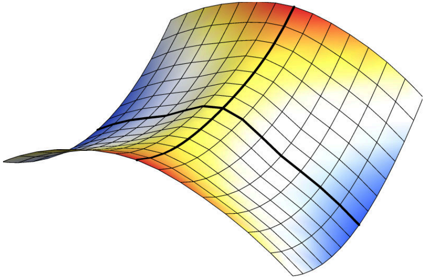

Figure : $\tilde{H}$ around a saddle point

$\tilde{H}$ 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

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

Proof: Mean-difference estimate

Approximation step

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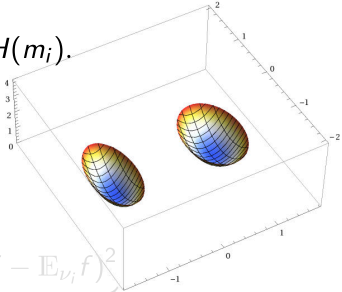
$$(\mathbb{E}_{\mu_0}(f) - \mathbb{E}_{\mu_1}(f))^2 \leq C \int |\nabla f|^2 \, \mathrm{d}\mu.$$

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

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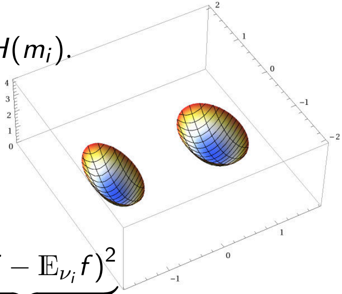

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Step 2: Transport $(\Phi_s : \mathbb{R}^n \to \mathbb{R}^n)_{s\in[0,1]}$ interpolating $(\Phi_s)_\sharp \nu_0 = \nu_s$

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Definition

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

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

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

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

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

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

Proof: Mean-difference estimate

Sideremark: Weighted transport distance

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Proof: Mean-difference estimate

Construction of transport interpolation

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

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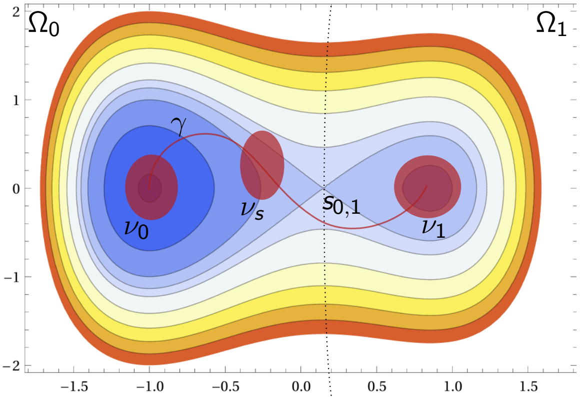

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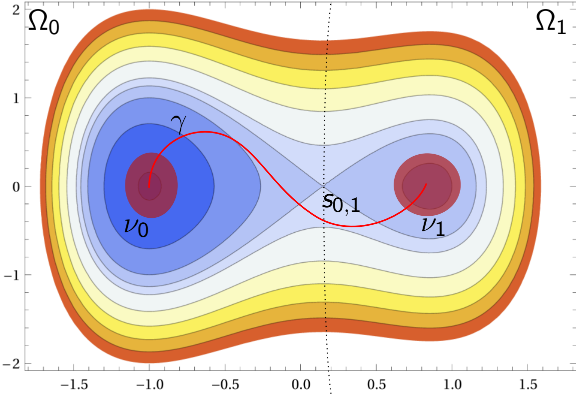

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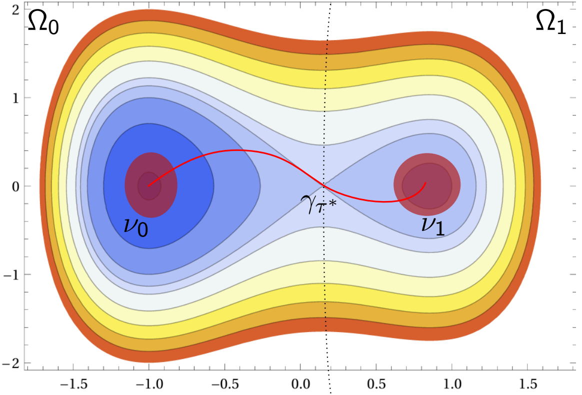

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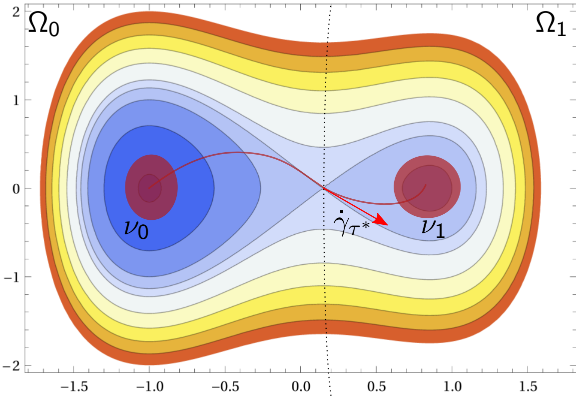

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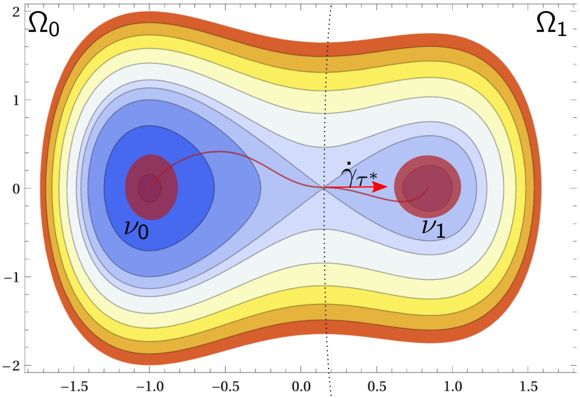

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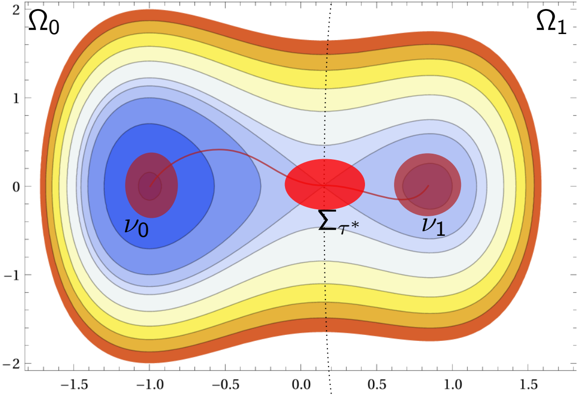

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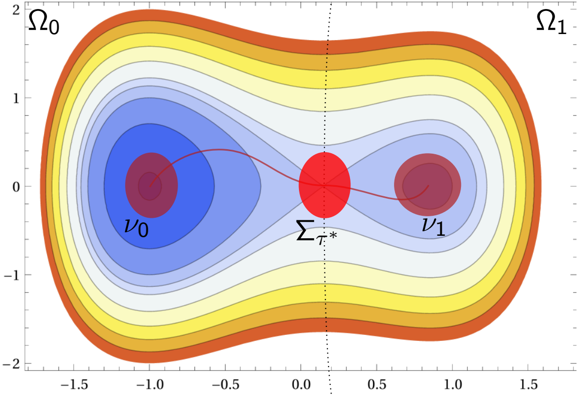

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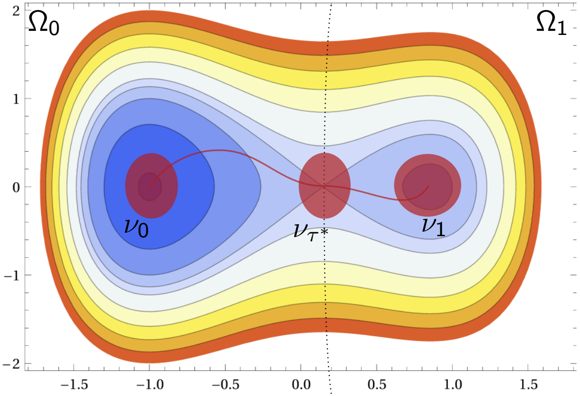

Summary

- Functional inequalities quantify convergence to equilibrium
- Partitions and splitting induced from dynamic (two scales)
- Eyring-Kramers formula follows 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

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