Eyring-Kramers formula
for
Poincaré
and
logarithmic Sobolev inequalities

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joint work with Georg Menz (Stanford)

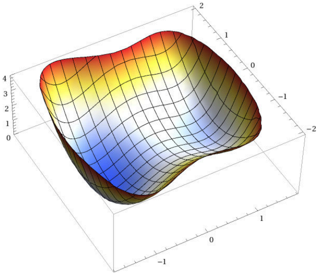
Bielefeld Stochastics Afternoon

November 14, 2012

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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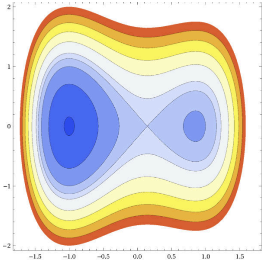

Generator evolution of $f_t = \varrho_t / \mu$

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

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

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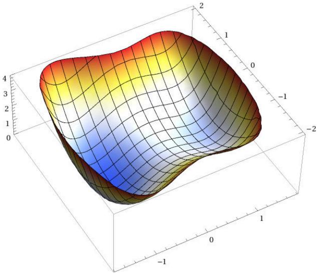

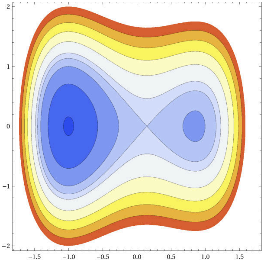

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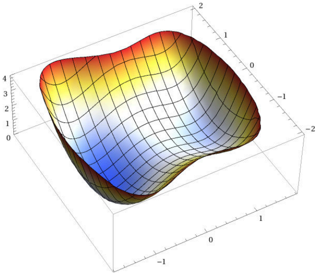

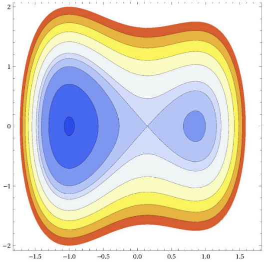

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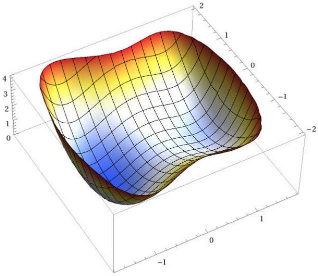

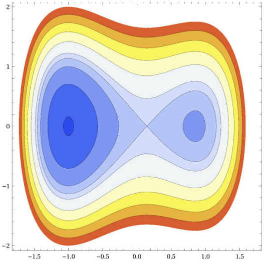

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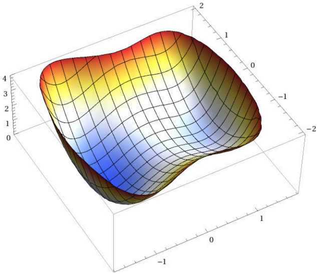

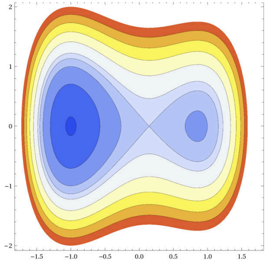

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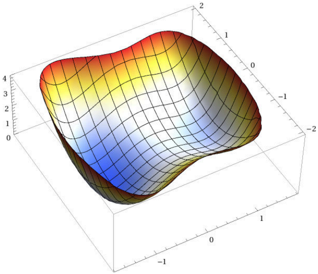

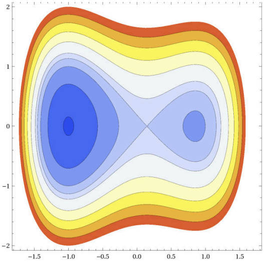

Distance and convergence to equilibrium

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 $\partial f_t = Lf_t$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Xi(f_t) = \int \xi' \circ f \underbrace{\partial_t f_t}_{=Lf_t} \mathrm{d}\mu = -\varepsilon \int \underbrace{\xi'' \circ f}_{>0} |\nabla f_t|^2 \,\mathrm{d}\mu.$$

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Convergence to equilibrium is established by FI(β)

Poincaré and logarithmic Sobolev inequality

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

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

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Goal: Eyring-Kramers formula

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

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

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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

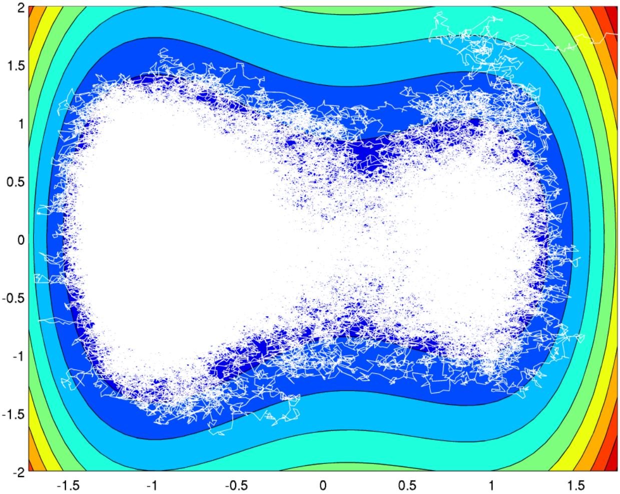


Figure : Trajectory for $\varepsilon = 0.4$

Heuristics

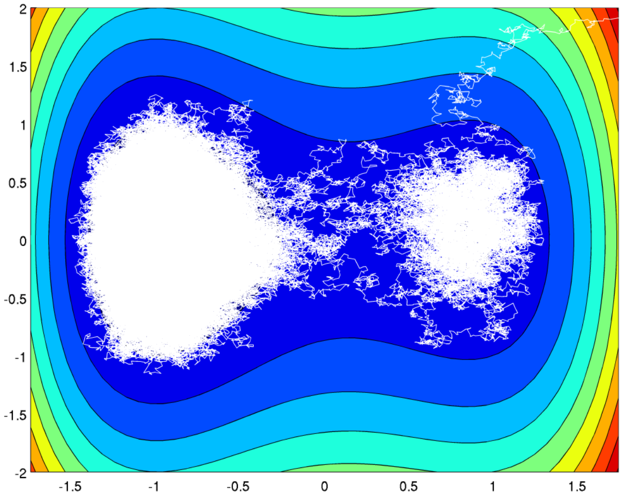


Figure : Trajectory for $\varepsilon = 0.2$

Heuristics

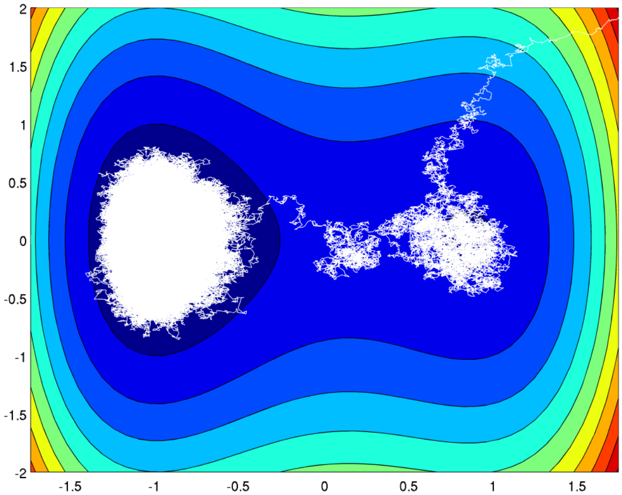


Figure : Trajectory for $\varepsilon = 0.1$

Heuristics

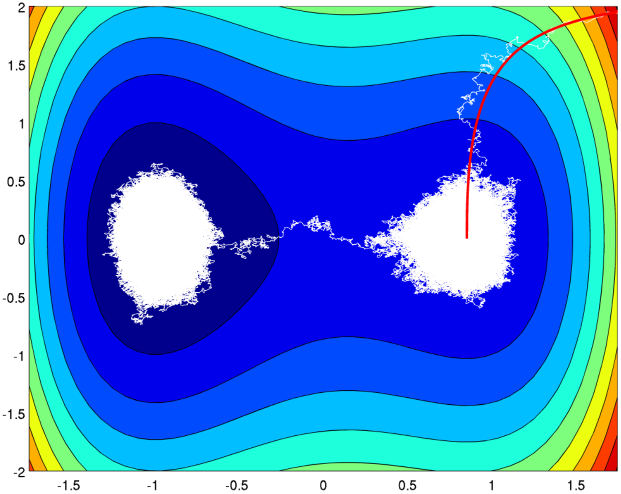


Figure : Trajectory for $\varepsilon = 0.05$ (red $\varepsilon = 0$)

Partitions

Make use of the two scales by decomposition [GOVW09][1]

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:

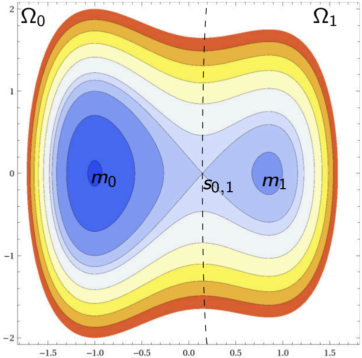
$$\mu_i := \mu \llcorner \Omega_i, \quad i = 0, 1.$$

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

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

Mixture representation

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



[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

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

Similar ideas used in [CM10]: 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

Lemma

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

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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*

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

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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* $\mathrm{PI}(\varrho)$ *and* $\mathrm{LSI}(\alpha)$ *with*

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Proof: Local PI and LSI

Lyapunov condition

Technique developed 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

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W is called Lyapunov function for L.

Theorem ([BBCG08])

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

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

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

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

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

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

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

  - 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

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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

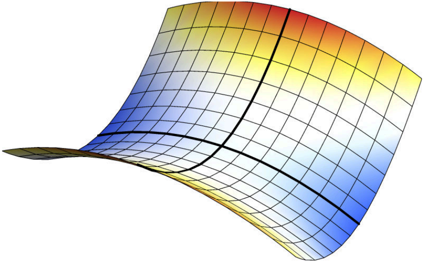

Figure : H around a saddle point

$\tilde{H}$ 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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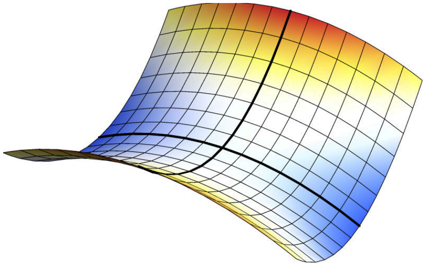

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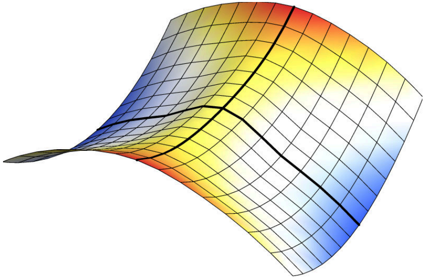

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Proof: Mean-difference estimate

Goal: Find a good estimate for C in

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

Proof: Mean-difference estimate

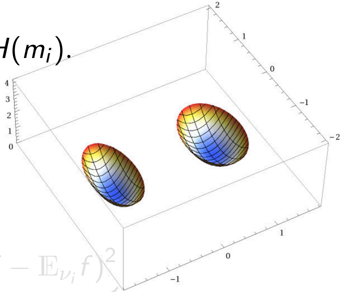
Approximation step

Goal: Find a good estimate for C in

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

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:

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

Approximation bound follows from local PI and local LSI.

Proof: Mean-difference estimate

Approximation step

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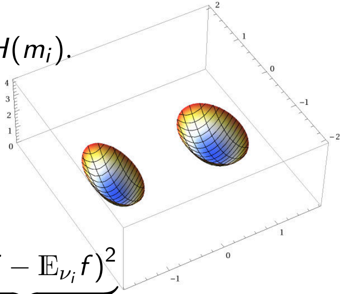

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Approximation
bound follows from local PI and local LSI.

Proof: Mean-difference estimate

Transport interpolation

Goal: Find a good estimate for C in
$$\left(\mathbb{E}_{\nu_0}(f) - \mathbb{E}_{\nu_1}(f)\right)^2 \leq C \int |\nabla f|^2 \,\mathrm{d}\mu.$$

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

Proof: Mean-difference estimate

Transport interpolation

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Proof: Mean-difference estimate

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&= \left(\int_0^1 \int \left\langle \dot\Phi_s \circ \Phi_s^{-1}, \nabla f \right\rangle d\nu_s \, ds\right)^2
\end{aligned}$$

Proof: Mean-difference estimate

Transport interpolation

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\end{aligned}$$

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\end{aligned}$$

Proof: Mean-difference estimate

Sideremark: Weighted transport distance

Definition

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

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

$(\Phi_s)_{s\in[0,1]}$ 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: $\mathcal{T}_\mu^2(\nu_0, \nu_1) = \|\nu_0 - \nu_1\|^2_{\dot{H}^{-1}(\mu)}$.

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

Proof: Mean-difference estimate

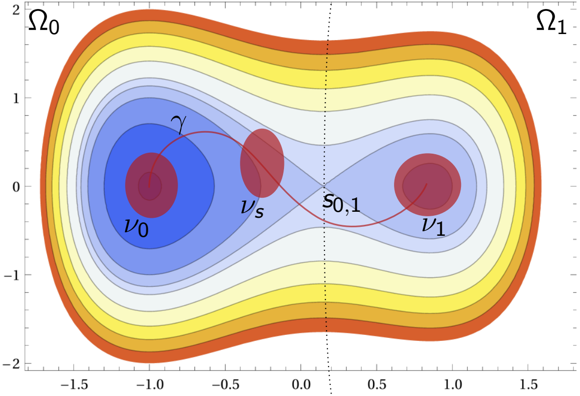
Construction of transport interpolation

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 $s_{0,1}$



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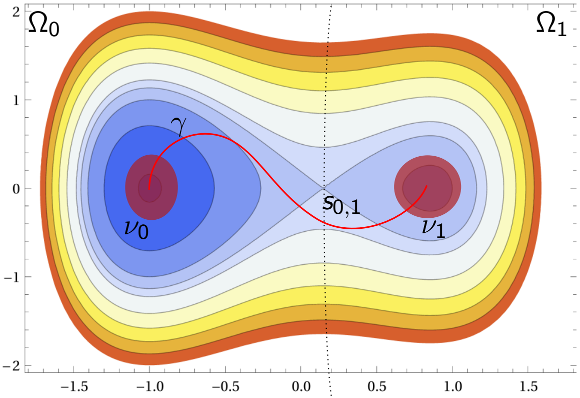

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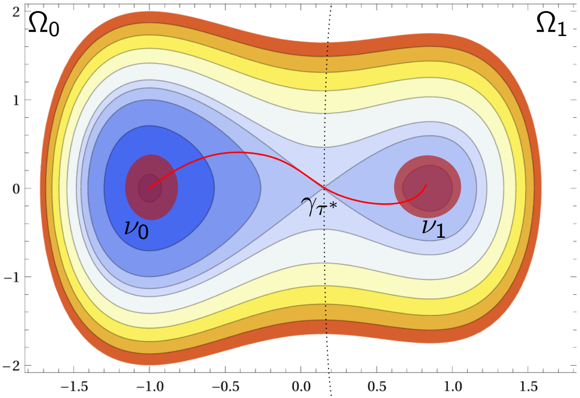

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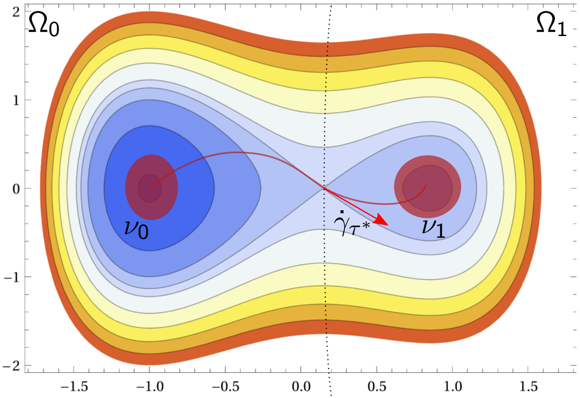

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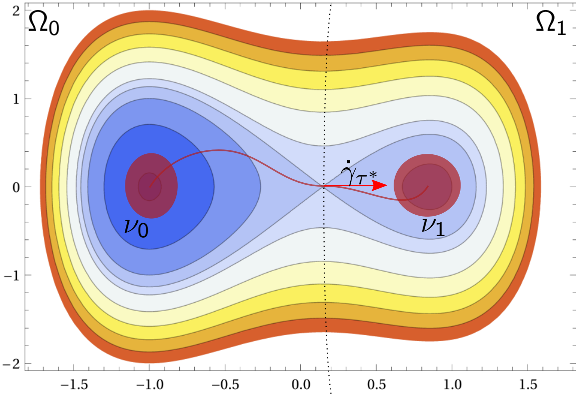

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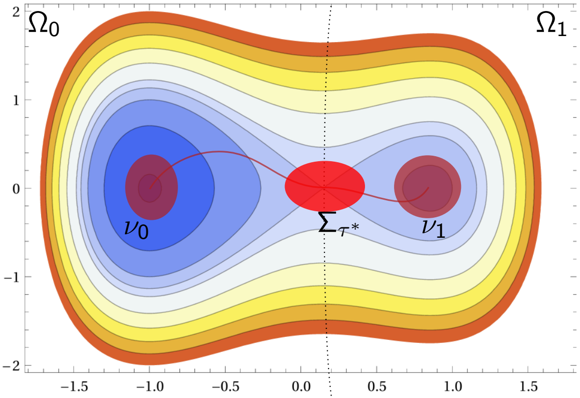

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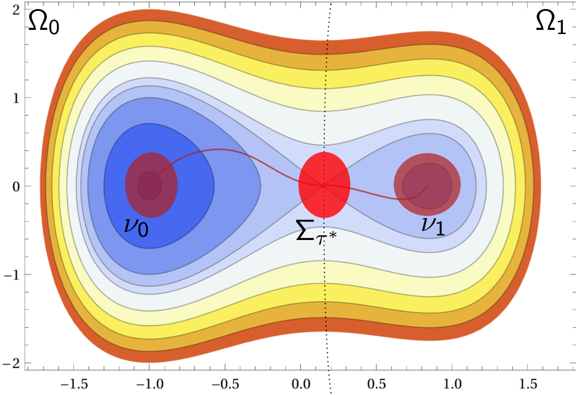

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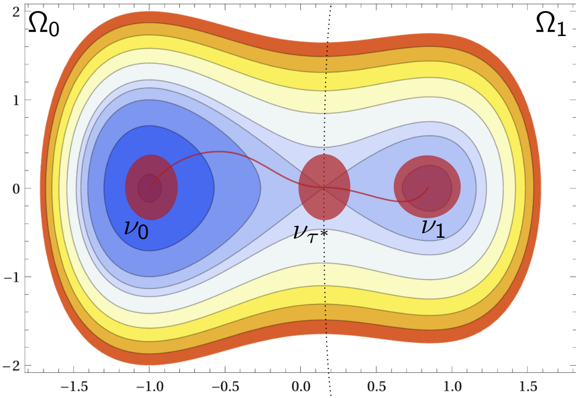
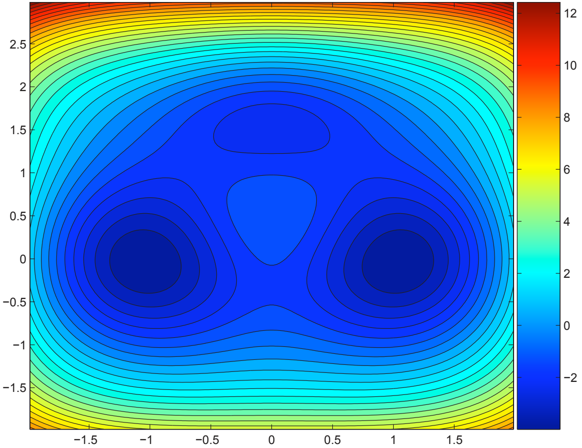


Application to entropic switching

Observation of Eric Vanden-Eijden:
Compare flux between global minima at low and very low temperature



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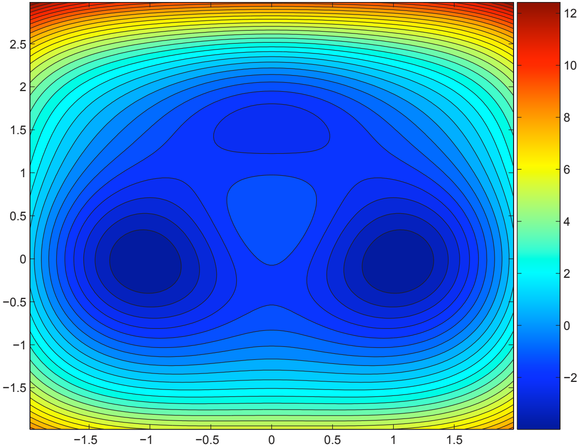

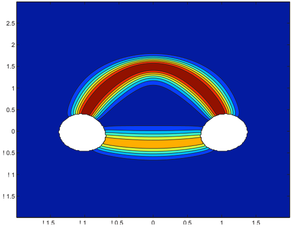

Very low temperature:
$\varepsilon = 0.15$

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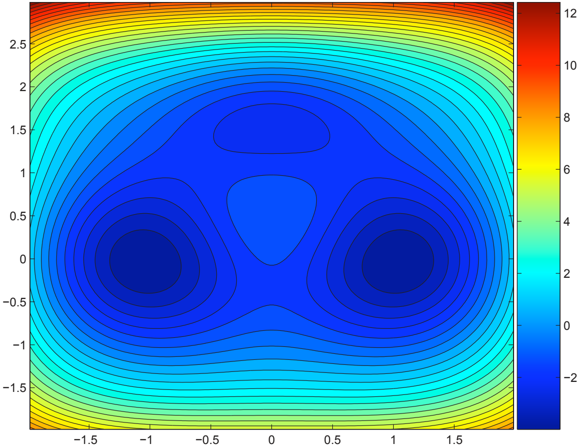
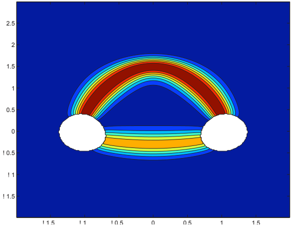
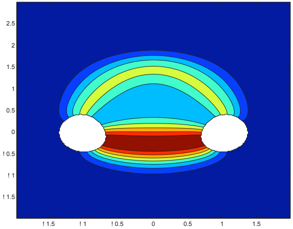
Compare flux between global minima at low and very low temperature





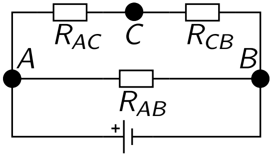
Very low temperature: $\varepsilon = 0.15$



Low temperature: $\varepsilon = 0.6$

Translation to electrical networks

- minima A, B, C become nodes
- saddle points become resistors
- *reaction rate* k_{AB} becomes the total conductance $R_{\text{tot}}^{-1}(A,B)$ between A, B.



This identification can be justified using the weighted transport distance

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

where

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

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

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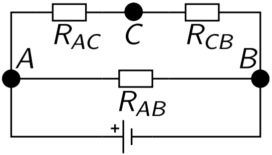

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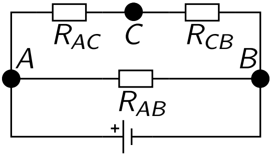

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Comparison of numerical data

	$\varepsilon = 0.15$	$\varepsilon = 0.6$
[MSVE06] TPT, flux	9.47×10^{-8}	1.912×10^{-2}
[MSVE06] TPT, committor	9.22×10^{-8}	1.924×10^{-2}
numerical simulation		$(1.918 \pm 0.052) \times 10^{-2}$
$\mathcal{T}(\nu_A, \nu_B)$, Z_μ Gaussian	9.63×10^{-8}	2.373×10^{-2}
$\mathcal{T}(\nu_A, \nu_B)$, Z_μ numerical	9.33×10^{-8}	1.926×10^{-2}

Table : Numerical estimates on $k_{A,B}$

[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.

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
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