Weak Poincaré Inequalities and Simulated Annealing

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Motivation

Motivating Problem

Given a high-dimensional probability distribution μ, efficiently sample a point from μ.

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Useful in various downstream tasks:

- optimization
- inference
- integration…

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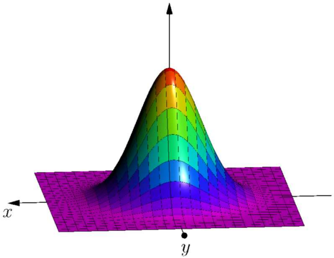

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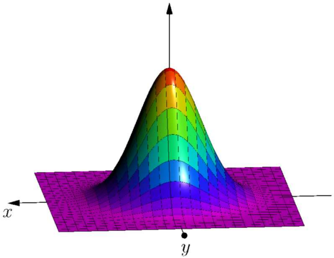

Classical result that such distributions can be efficiently sampled from. (see Chewi [Che23])

[Che23]: S Chewi. Log-concave sampling.

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P *mixes* (from x_0) in time T if $d_{\mathrm{TV}}\left(x_T, \mu\right)$ is tiny.

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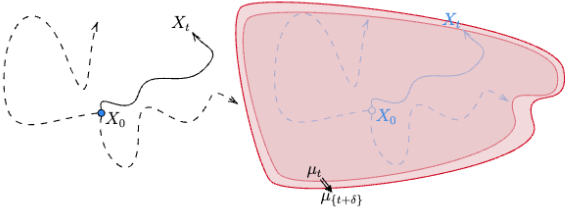

Figure from Yuansi Chen

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Definition can be modified for distributions supported on the sphere, say.

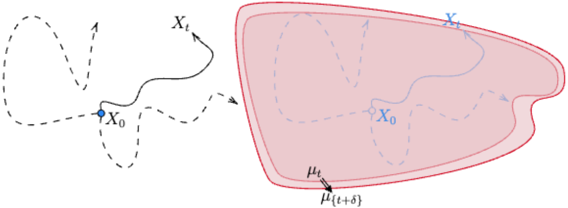

Figure from Yuansi Chen

Mixing times

Mixing is shown by proving that for *any* distribution ν,

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There are now many many ways to show this:

- Coupling [BDJ96, BD97a]
- Path coupling [Jer95, BD97b, BD97c]
- Canonical paths [JS89, JSV04, HMMR05]
- Curvature considerations/Bakry–Émery theory [BÉ06, Vil09, EHMT17, CMS24]
- Zerofreeness [LY52, Bar16a, Bar16b, CLV24]
- Correlation decay [DSVW04, Wei04, Wei06, CLV21, CLMM23]
- Spectral independence [ALGV19, ALG21, Liu23, AJK^{+}24]
- Entropic independence [AJK^{+}21a, AJK^{+}21b, CCYZ24]
- Stochastic localization [EKZ22, CE22, AKV24, LMRW24]

Reevaluating the basics

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[LS93]: L Lovász and M Simonovits. Random walks in a convex body and an improved volume algorithm.
[Lov99]: L Lovász. Hit-and-run mixes fast.
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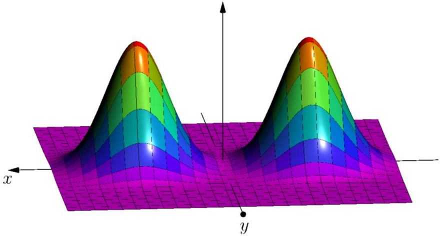

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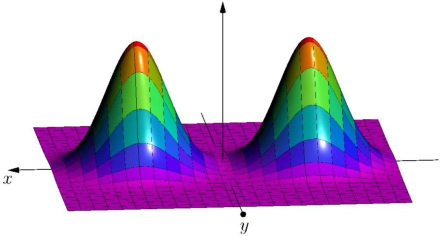

Maybe if I initialize with equal mass in each cluster, I do mix.

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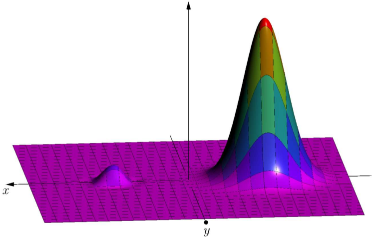

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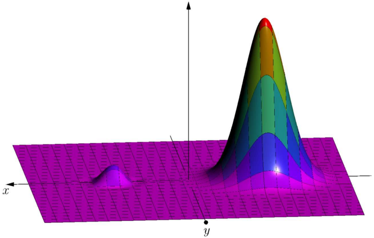

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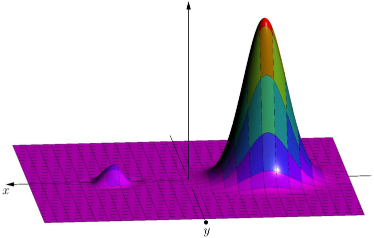

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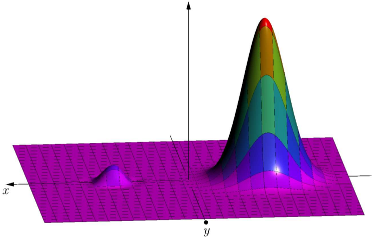

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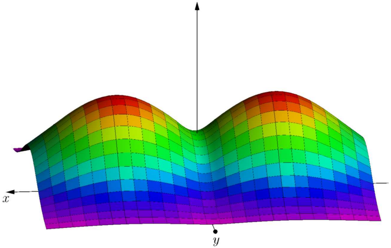

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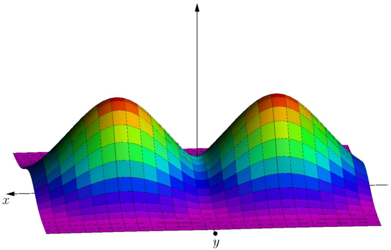

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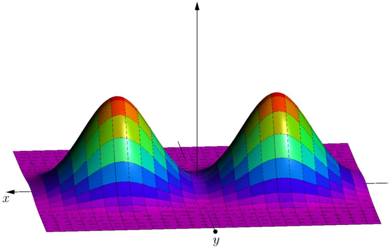

$\beta = 0.4$

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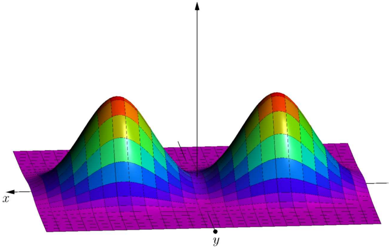
Slowly increase β from 0 to 1, so μ_β provides a good initialization for the Markov chain at $\mu_{\beta+\delta}$.



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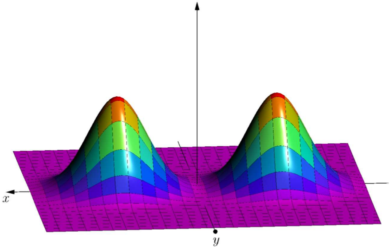

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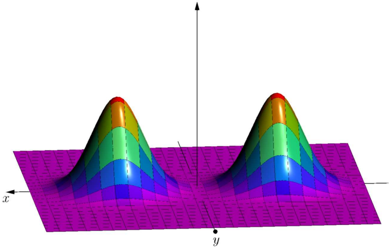

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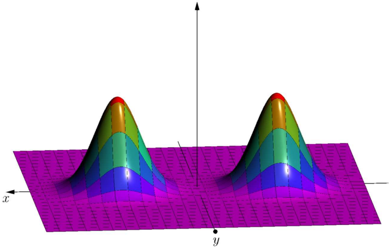

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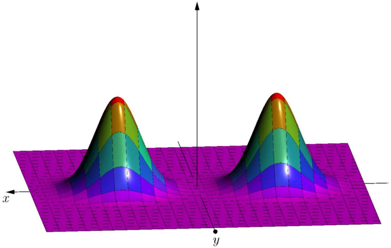
Used very often in practice!



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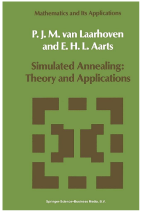
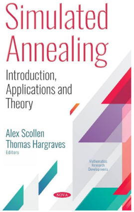


Mathematics and Its Applications

P. J. M. van Laarhoven
and E. H. L. Aarts

Simulated Annealing:
Theory and Applications

Springer-Science+Business Media, B.V.



Simulated
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Introduction,
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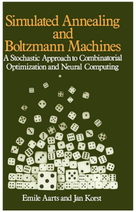
Thomas Hargraves
Editors

Mathematics
Research
Developments

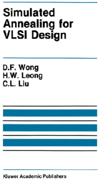
NOVA



Simulated Annealing
and
Boltzmann Machines

A Stochastic Approach to Combinatorial
Optimization and Neural Computing

Emile Aarts and Jan Korst



Simulated
Annealing for
VLSI Design

D.F. Wong
H.W. Leong
C.L. Liu

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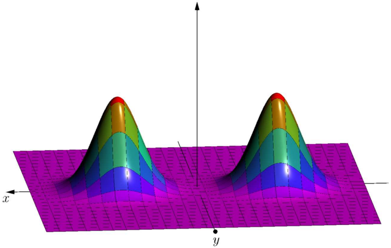

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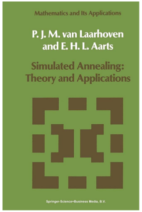
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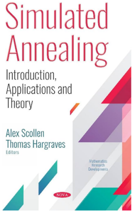
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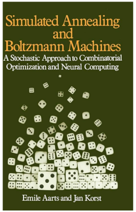
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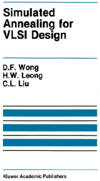
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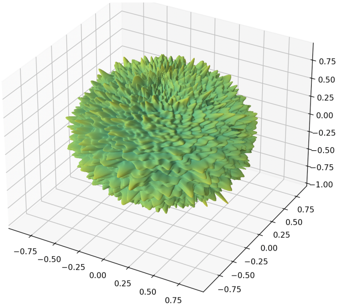
How do we prove rapid mixing from non-worst-case initializations?

1. Results
    - Sampling from spherical spin glasses
    - Sampling from data-based initializations
2. Techniques

Spherical 4-spin glass

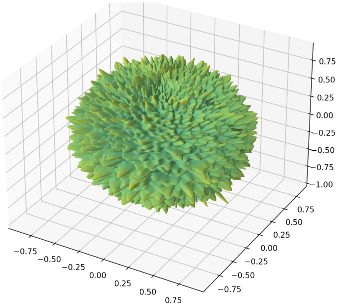


Spherical 4-spin glass

Set

$$H(\sigma) = \frac{\gamma}{N^{3/2}} \langle G, \sigma^{\otimes 4} \rangle$$

for $\sigma \in \sqrt{N} \cdot \mathbb{S}^{N-1}$ for G a random rank-4 tensor ($G_{i_1,\ldots,i_4} \sim \mathcal{N}(0,1)$), and set $\mu(\sigma) \propto e^{H(\sigma)}$.



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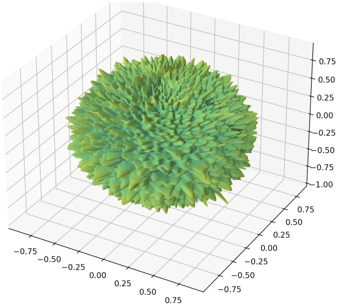
Extremely well-studied in statistical physics. Subject of 2021 Nobel Prize in Physics!



Results: Sampling from spherical 4-spin models

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$\mu(\sigma) \propto e^{\gamma H(\sigma)}$ for $\sigma \in \sqrt{N} \cdot \mathbb{S}^{N-1}$

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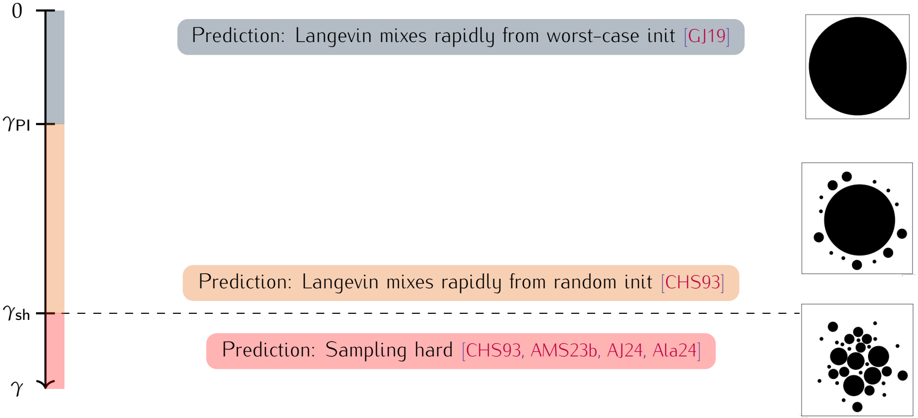

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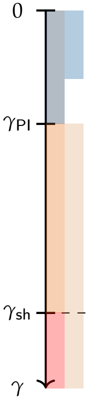

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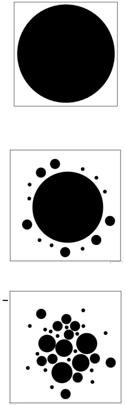

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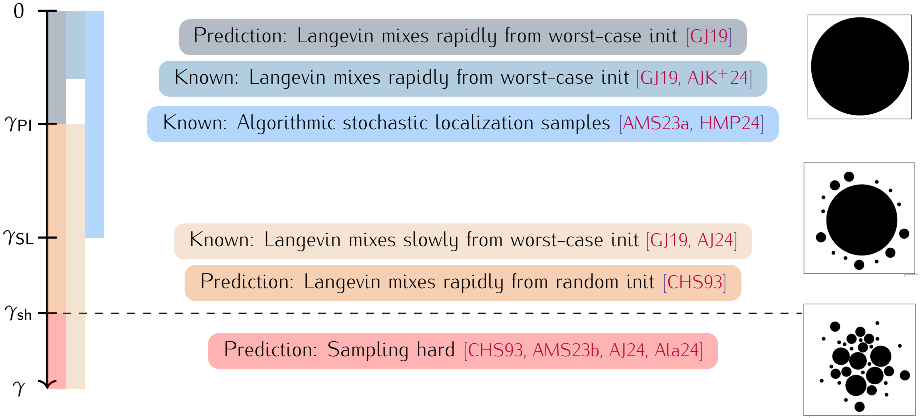

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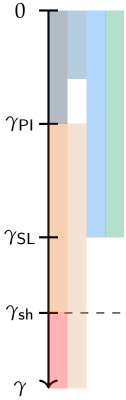

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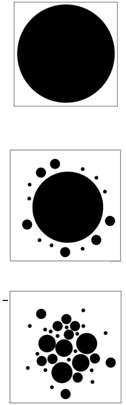

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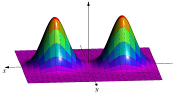
Results: Sampling from data-based initializations



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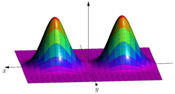

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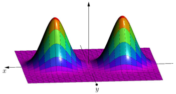

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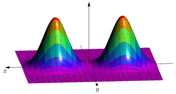

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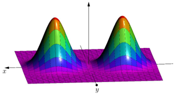

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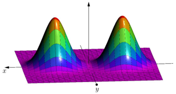

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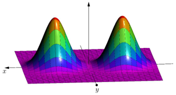

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This problem is studied in more detail in parallel independent work by Koehler–Lee–Vuong [KLV23].

[KV23]: F Koehler and TD Vuong. Sampling multimodal distributions with the vanilla score: Benefits of data-based initialization.
[KLV23]: F Koehler, H Lee, and TD Vuong. Efficiently learning and sampling multimodal distributions with data-based initialization.

Techniques

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Lemma

Turns out that for Langevin, $-\frac{\mathrm{d}}{\mathrm{d}t}\operatorname{Var}_\mu[f_t] = \mathbb{E}_\mu\|\nabla f_t\|_2^2$!

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Poincaré inequalities are equivalent to the more familiar spectral gaps. All the techniques from earlier show rapid mixing by proving Poincaré inequalities/showing large spectral gaps.

An observation

This only cares about functions f_t encountered along the trajectory of the chain!

Weak Poincaré inequalities

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So far, not new [Aid98], even for sampling guarantees [RW01].

[Aid98]: S Aida. Uniform positivity improving property, Sobolev inequalities, and spectral gaps.
[RW01]: M Röckner and FY Wang. Weak Poincaré inequalities and L^2-convergence rates of Markov semigroups

Weak Poincaré inequalities for simulated annealing

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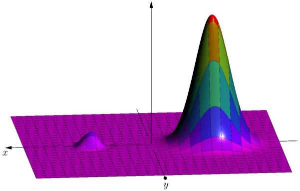

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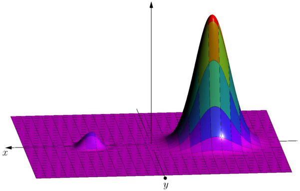

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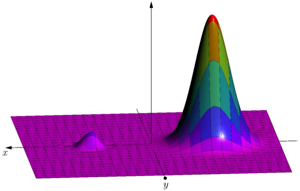

TV-close to true Poincaré $\Longrightarrow$ $\mathbf{Defect} = \varepsilon \cdot \mathrm{osc}(f)^2$.
Weak Poincaré inequalities can be proved using localization schemes! (generalizations of spectral independence, stochastic localization...)

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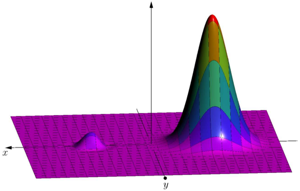

TV-close to true Poincaré $\implies$ $\mathbf{Defect} = \varepsilon \cdot \mathrm{osc}(f)^2$.
Weak Poincaré inequalities can be proved using localization schemes! (generalizations of spectral independence, stochastic localization...)

A quick jargon-infested elaboration for the expert.

Weak Poincaré inequalities for simulated annealing

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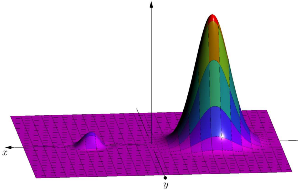

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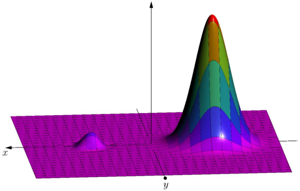

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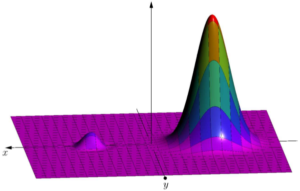

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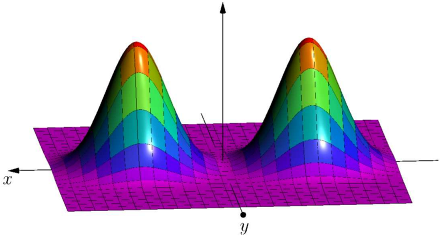
- Bounded influence for **all** pinnings/control on **all** localization paths $\implies$ Poincaré
- Bounded influence for **most** pinnings/control on **most** localization paths $\implies$ weak Poincaré

Weak Poincaré inequalities from symmetry



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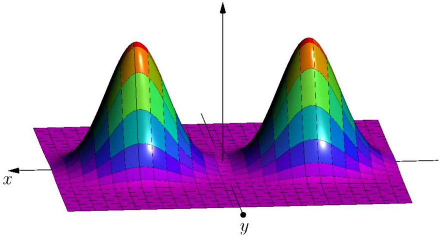

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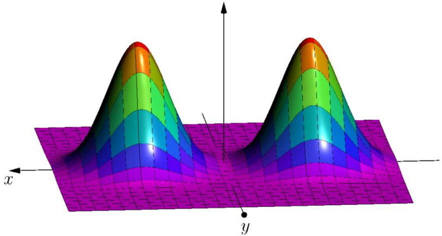

Symmetric function $\implies$ **Defect** $= 0$.
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Proof: Sampling from data-based initializations

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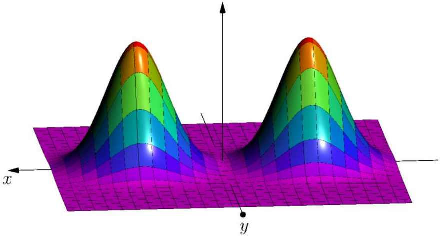

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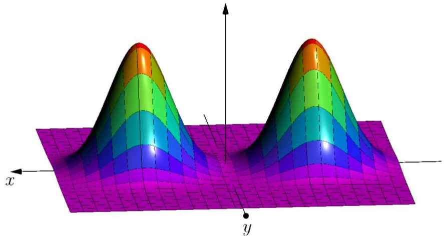
Let $\pi = \sum_{i=1}^K p_i\pi_i$ be a mixture of strongly log-concave distributions.

Theorem (HMRW)

Suppose $\min p_i \geqslant p_*$. Let $x_1, x_2, \ldots, x_m$ be sampled according to π. For $m = \Omega\left(\frac{1}{p_*\varepsilon^2}\right)$, with high probability over the samples, Langevin diffusion initialized at $\frac{1}{m}\sum \delta_{x_i}$ run for $\mathbf{poly}(n)$ time samples from π to TV distance ε.

Intuition



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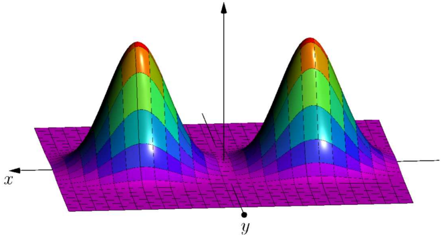

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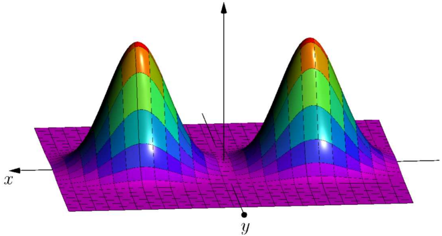

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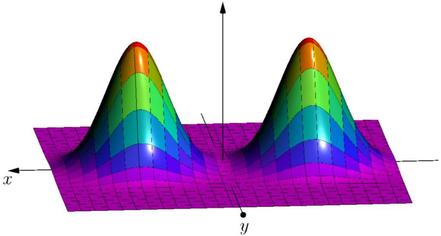

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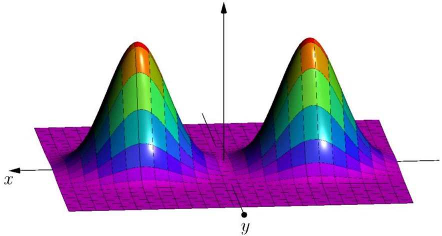

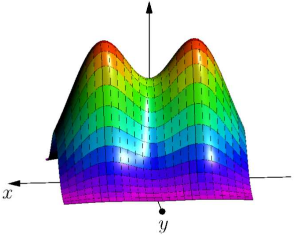

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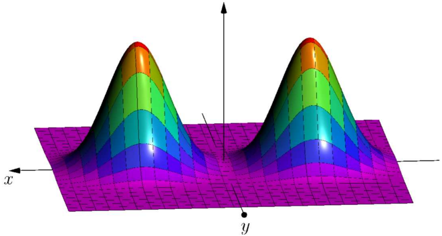

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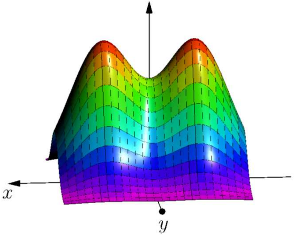

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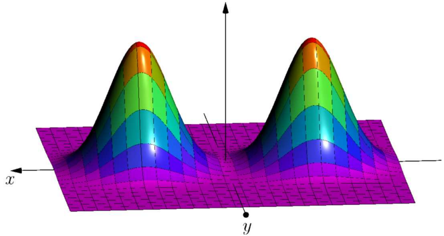

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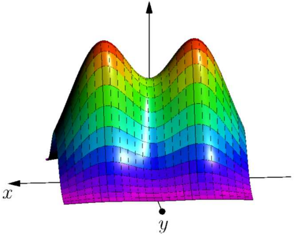

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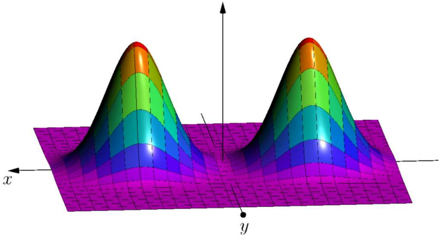

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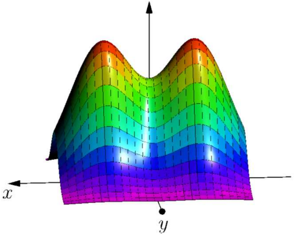

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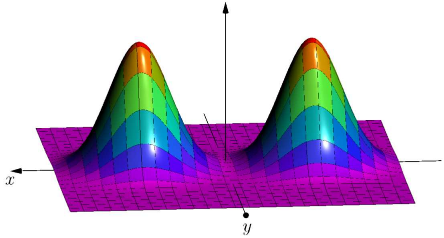

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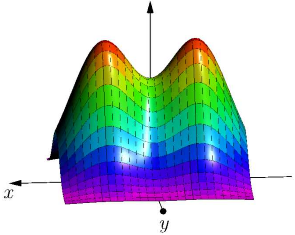

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Mass can travel between clusters, but it should do so in a symmetric fashion.
Defect should stay small? (controlling this is essentially the source of the doubly exponential dependence in previous work)

Proving a weak Poincaré inequality

$$\mathbb{E}\|\nabla f\|_2^2 \geqslant \rho\left(\mathrm{Var}_\mu[f] - \mathrm{Defect}(f)\right)$$
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(proof on board) Will show

$$\mathbb{E}\|\nabla f\|_2^2 \gtrsim \mathrm{Var}[f] - \underbrace{\sum_{i=1}^{K} p_i\left(\mathbb{E}_{\pi_i}[f]^2 - \mathbb{E}_\pi[f]^2\right)}_{\mathrm{Defect}(f)} .$$

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This is a random variable depending on the samples $x_1, \ldots, x_m$. Would like to show that it is small with high probability (over the samples) along the path of the Markov chain.

Controlling the error

$$\mathrm{Defect}(f_t) = \sum_{i=1}^{K} p_i \left(\mathbb{E}_{\pi_i}[f_t]^2 - 1 \right) \; .$$

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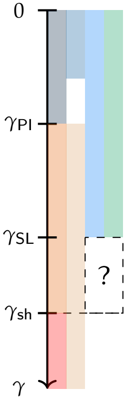
So $\mathbf{Defect}(f_t)$ is small with high probability! We are done!

Open Questions I: Sampling down to the shattering threshold



Prediction: Langevin mixes rapidly from worst-case init [GJ19]

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Algorithmic stochastic localization samples [AMS23a, HMP24]

This work: simulated annealing samples

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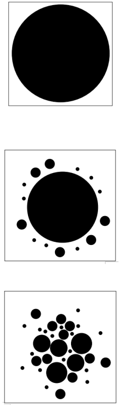
Prediction: Sampling hard [CHS93, AMS23b, AJ24, Ala24]



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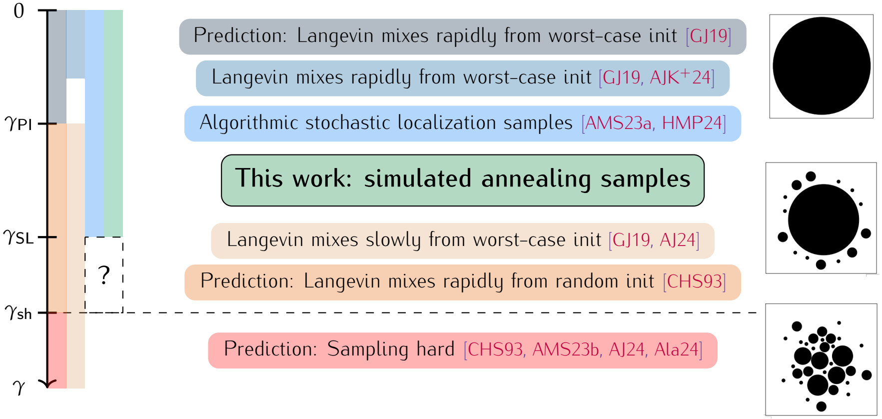

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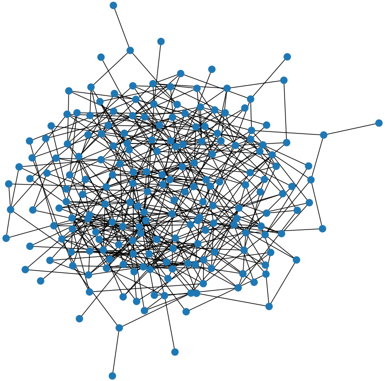
How do we close this gap? It seems like our proof strategy gets stuck...

Open Questions II: Annealing for inference

Inference problem: Infer $\mathbf{x} \sim \{\bullet, \bullet\}^n$ after observing a sparse random graph with "community structure" $\mathbf{x}$.



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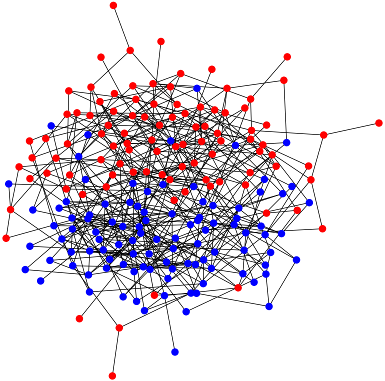

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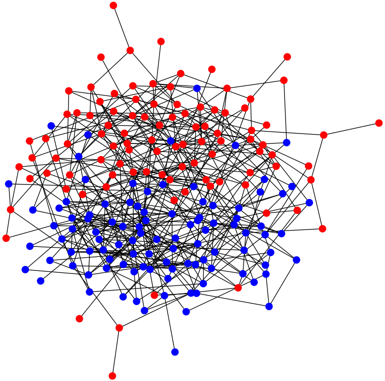

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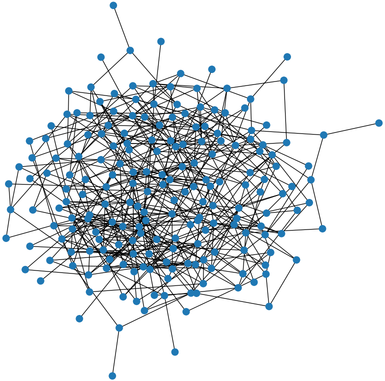

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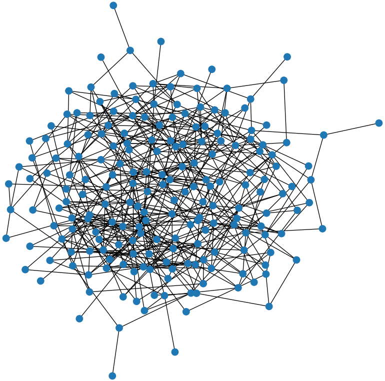
Annealing run on the posterior of the stochastic block model appears to perform optimally... why?



Open Questions III: Worst-case approximation algorithms from non-worst-case initializations

For max-cut in a graph, SDPs provide a 0.878-approximation to the max-cut.

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(Liu–Mohanty–Raghavendra–R–Wu [LMR$^+$24] describes how to do this from worst-case initializations)

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[LMR$^+$24]: K Liu, S Mohanty, P Raghavendra, AR, and DX Wu. Locally Stationary Distributions: A Framework for Analyzing Slow-Mixing Markov Chains
[Tre01]: L Trevisan. Non-approximability results for optimization problems on bounded degree instances.

Thank you! Questions?

Feel free to email at **`amit_r@mit.edu`**.

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