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...

Example distribution: strongly log-concave distribution

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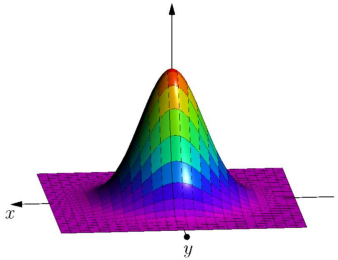

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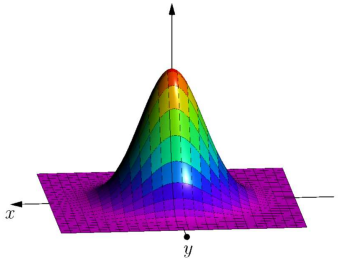
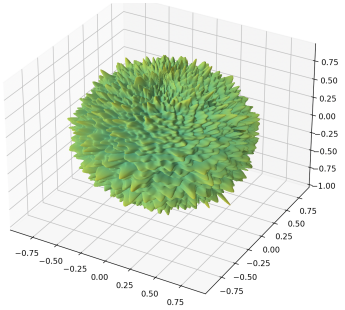


Classical result that such distributions can be efficiently sampled from. (see [Che23])

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

Example distribution: Spherical 4-spin glass



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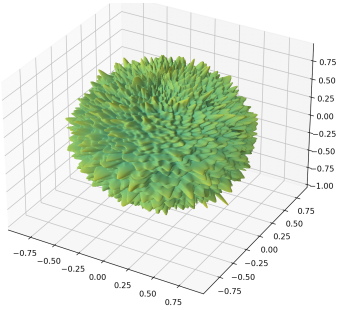
Set

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

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



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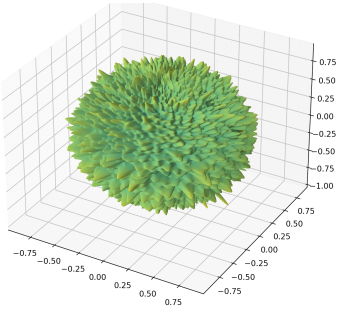
Extremely well-studied in statistical physics. Subject of 2021 Nobel Prize in Physics!



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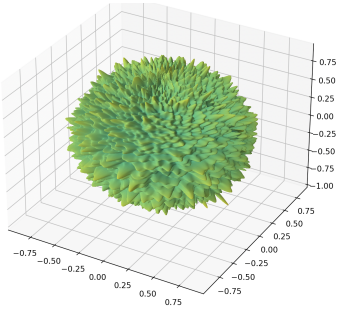
Highly non-convex, unclear that it can be sampled from.



How do we sample?

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Markov Chain Monte Carlo!

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

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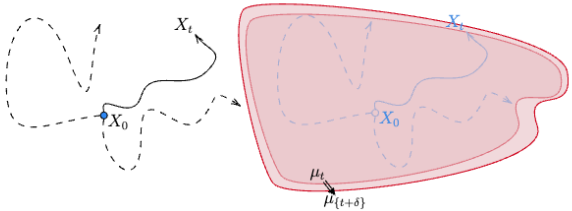

Figure from Yuansi Chen

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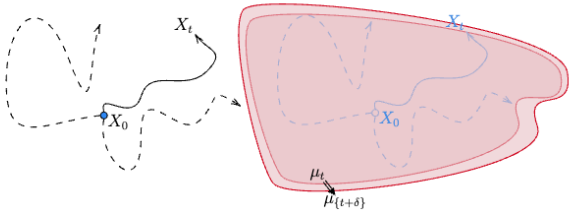

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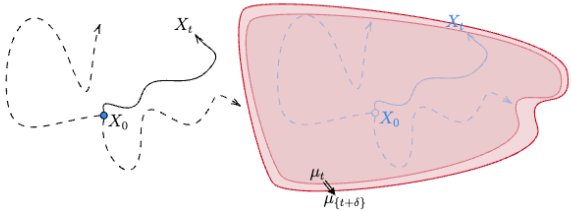
Definition can be modified for distributions supported on the sphere, say.



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Mixing times

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

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- Canonical paths [JS89, JSV04, HMMR05]
- Curvature considerations/Bakry–Émery theory [BÉ06, Vil09, EHMT17, CMS24]
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- Correlation decay [DSVW04, Wei04, Wei06, CLV21, CLMM23]
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} Localization schemes [CE22b]

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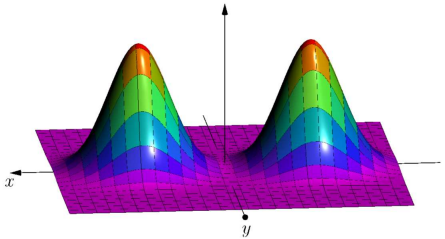

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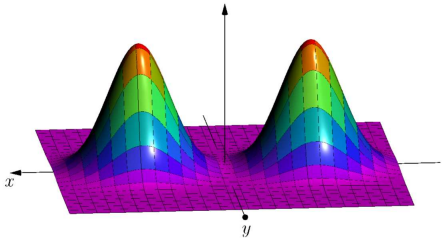

Maybe if I initialize with equal mass in each cluster, I do mix.

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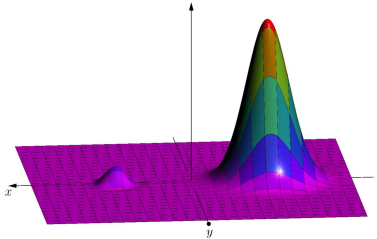

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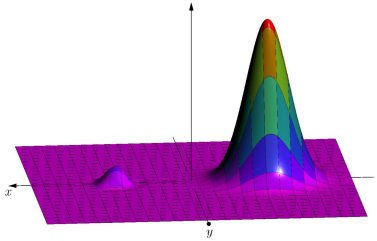

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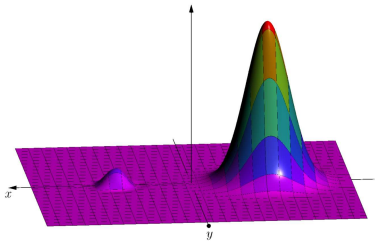

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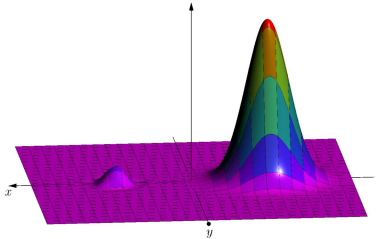

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How do we prove rapid mixing from non-worst-case initializations?

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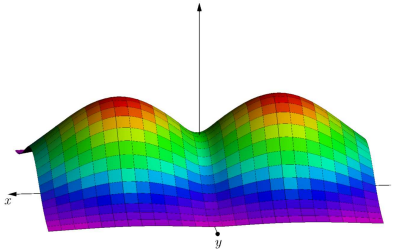

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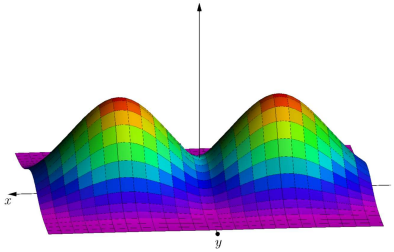

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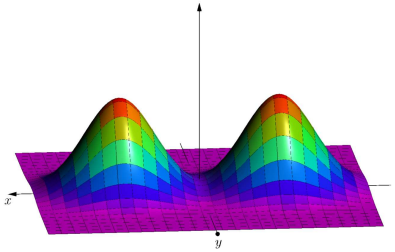

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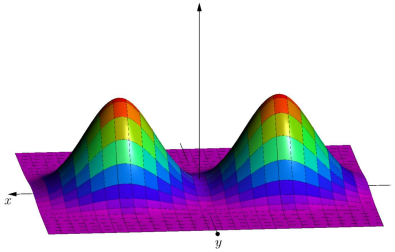
Slowly increase β from 0 to 1, so μ_β provides a good initialization for the Markov chain at $\mu_{\beta+\delta}$.



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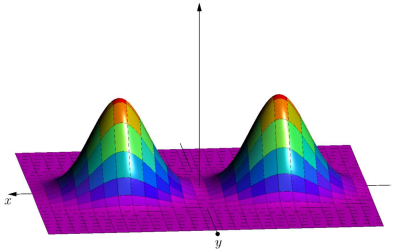

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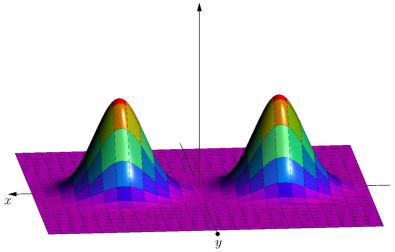

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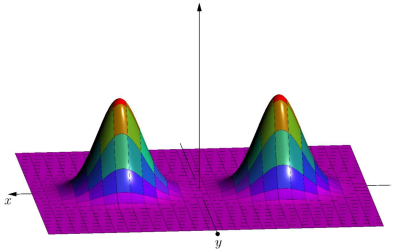

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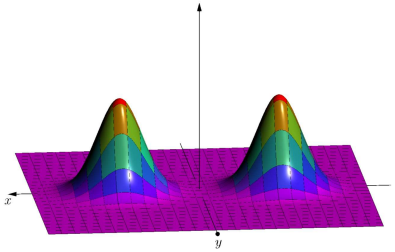
Used very often in practice!



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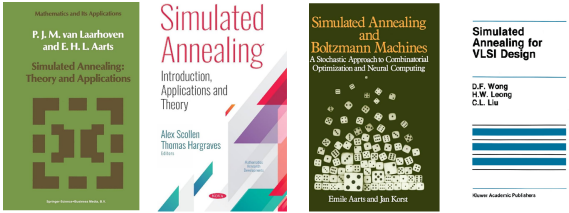
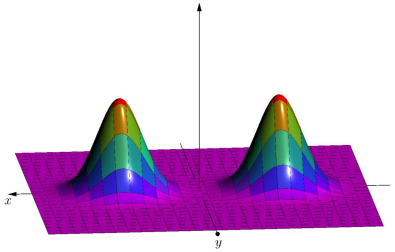


Simulated annealing

Say I have distribution $\mu(x) \propto e^{-V(x)}$. In simulated annealing, consider $\mu_\beta(x) \propto e^{-\beta V(x)}$. Sampling is easy at small β, possibly difficult at $\beta = 1$.
Slowly increase β from 0 to 1, so μ_β provides a good initialization for the Markov chain at $\mu_{\beta+\delta}$.
Used very often in practice!



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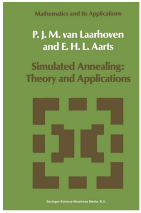

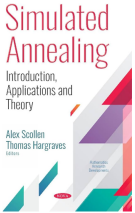

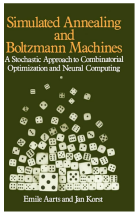

How do we prove rapid mixing from non-worst-case initializations?

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

Results: Sampling from spherical 4-spin models

$H(\sigma) = \frac{1}{N^{3/2}} \langle G, \sigma^{\otimes 4} \rangle$

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

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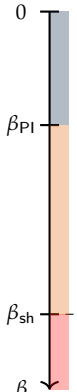

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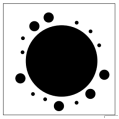

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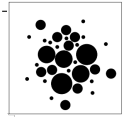

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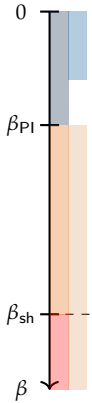

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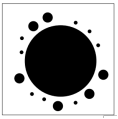

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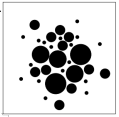

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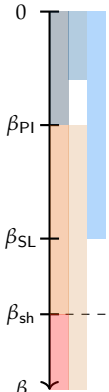

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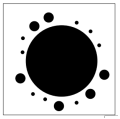

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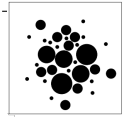

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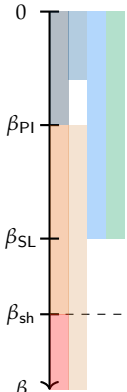

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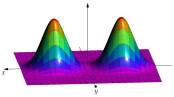

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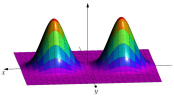

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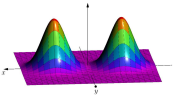

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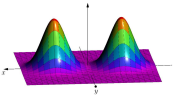

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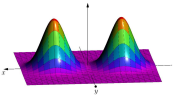

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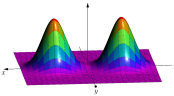

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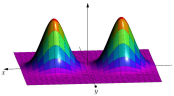

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This problem is studied in more detail in parallel independent work by Koehler–Lee–Vuong [KLV23].

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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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An observation

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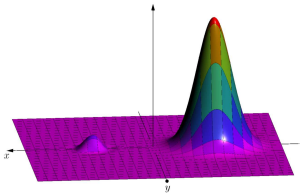

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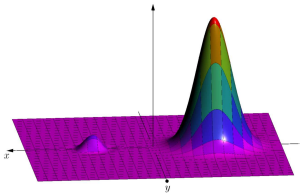

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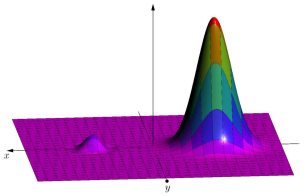

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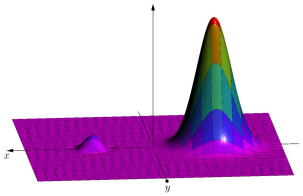

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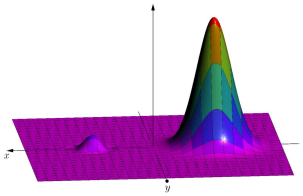

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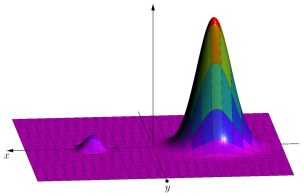

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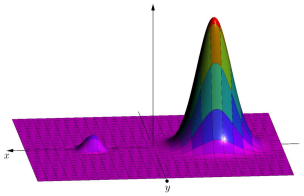

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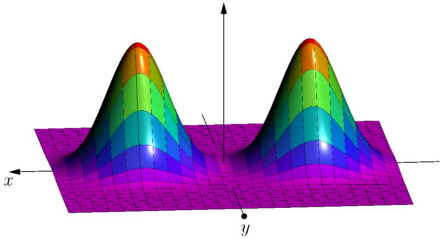
Bounded influence for *most* pinnings/control on *most* localization paths $\implies$ weak Poincaré inequality

Weak Poincaré inequalities from symmetry



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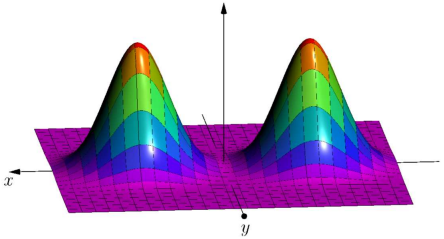

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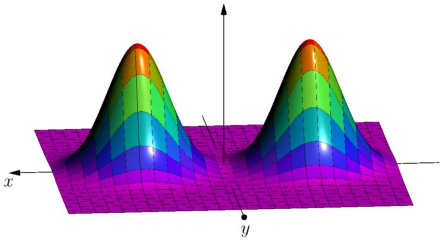

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Proof: Sampling from data-based initializations

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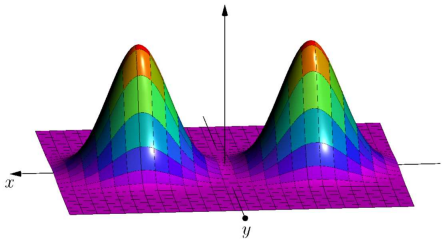

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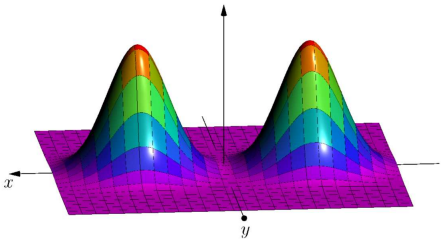
Let $\pi = \sum_{i=1}^K p_i \pi_i$ be a mixture of strongly log-concave distributions.

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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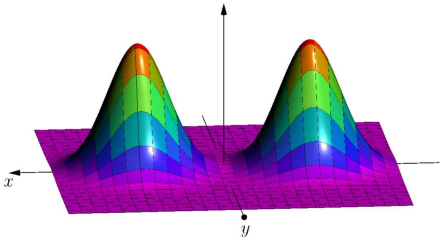

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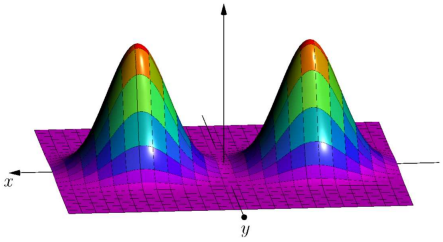

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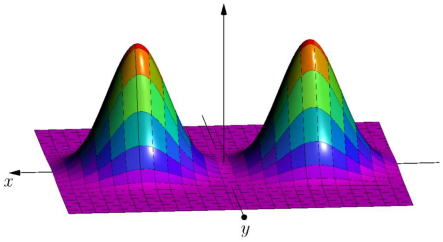

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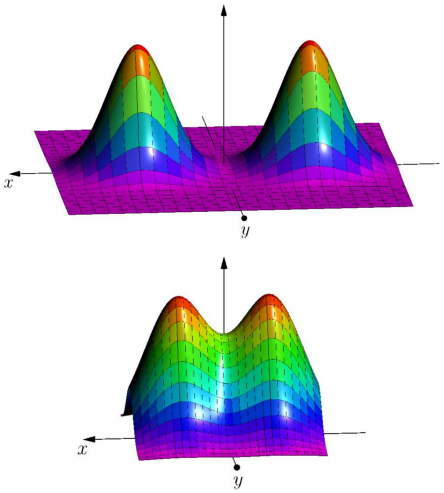

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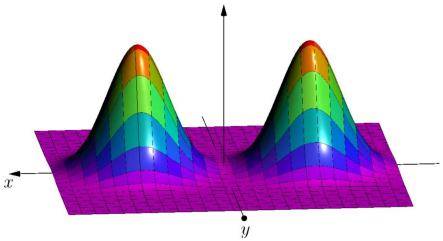

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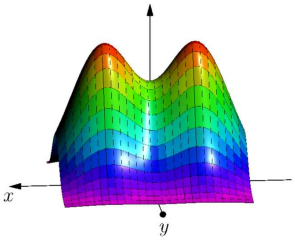

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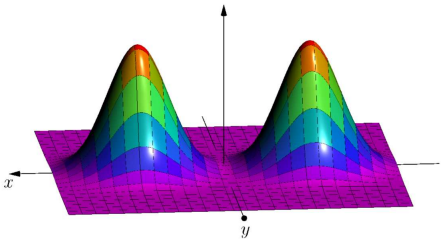

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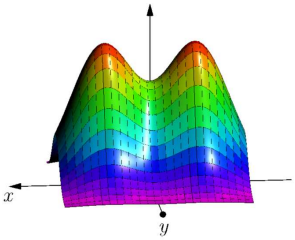

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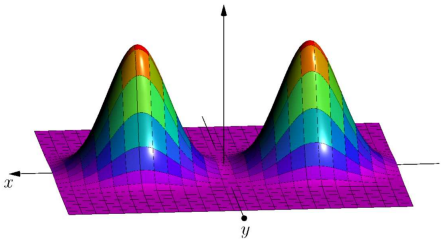

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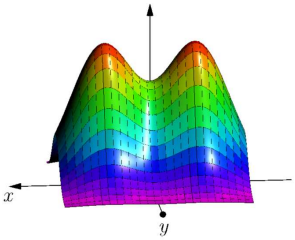

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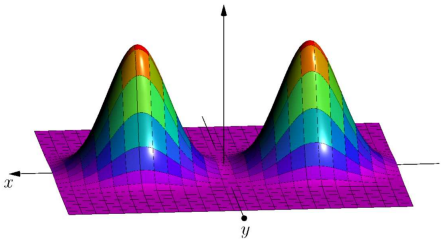

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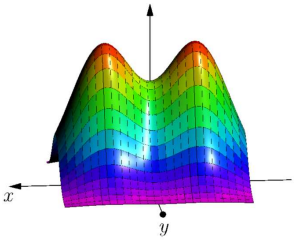

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Proving a weak Poincaré inequality

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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

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

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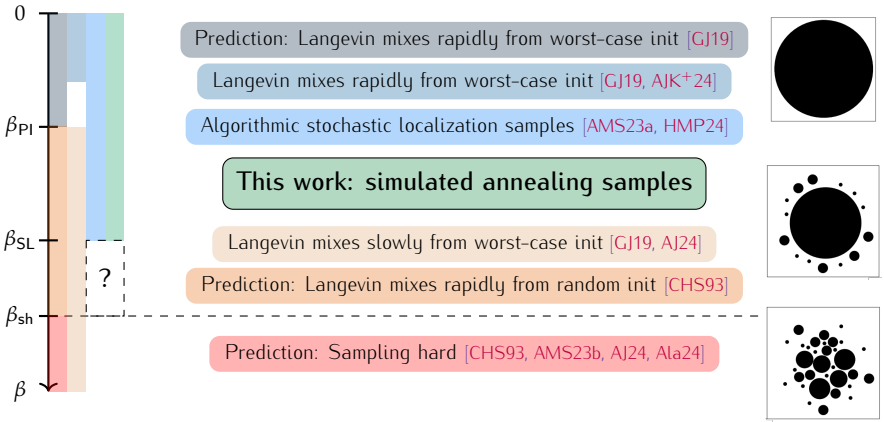
So $\mathbf{Error}(f_t)$ is small with high probability! We are done!

Open Questions I: Sampling down to the shattering threshold



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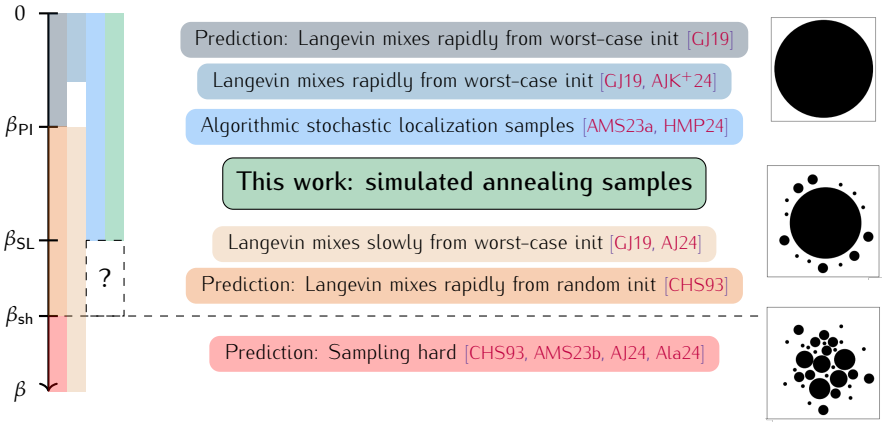

How do we close this gap? It seems like our proof strategy gets stuck...

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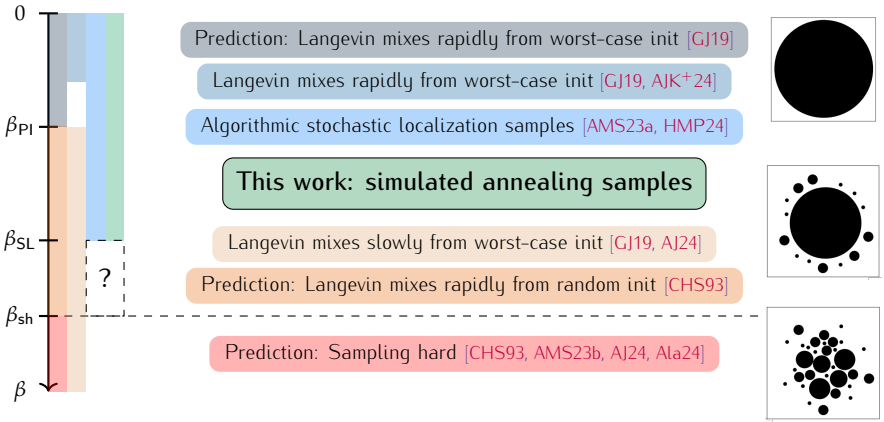
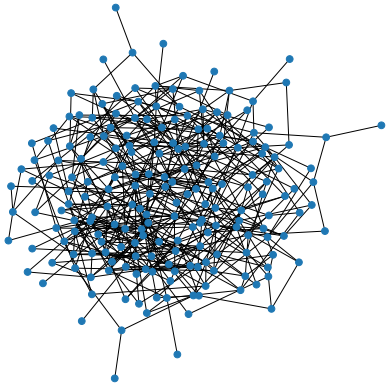


How do we close this gap? It seems like our proof strategy gets stuck...
Can we extend our results to the state space being $\{\pm 1\}^N$?

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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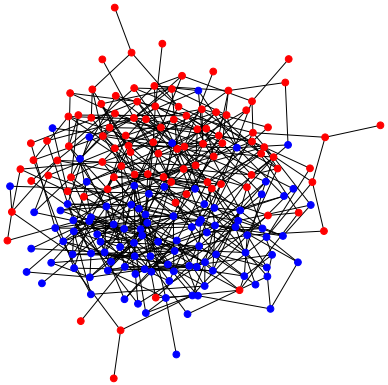
Connect vertices with probability $\frac{d+\lambda\sqrt{d}}{n}$ if + + or − −



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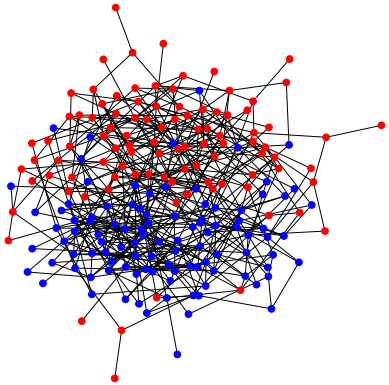

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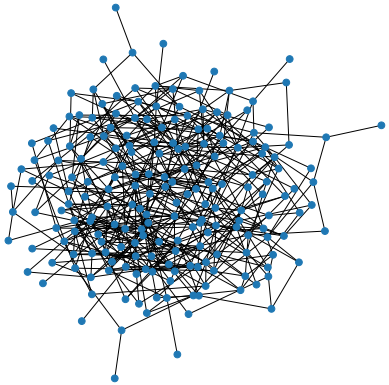

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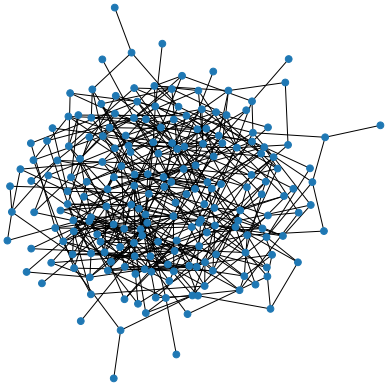
Annealing run on the posterior of the stochastic block model appears to perform optimally... why?



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

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Does running MCMC initialized at the SDP solution do anything?
Our framework describes how to get sampling guarantees from non-worst-case initializations... can we say anything about inference/optimization guarantees? (Recent work [LMR+24] describes how to do this from worst-case initializations)

[HK22]: JT Hsieh and P Kothari. Approximating Max-Cut on Bounded Degree Graphs: Tighter Analysis of the FKL Algorithm.
[LMR+24]: K Liu, S Mohanty, P Raghavendra, AR, and DX Wu. Locally Stationary Distributions: A Framework for Analyzing Slow-Mixing Markov Chains

Thank you! Questions?

Feel free to email at amit_r@mit.edu.

Bibliography I

[AEGP23] Ahmed El Alaoui, Ronen Eldan, Reza Gheissari, and Arianna Piana. Fast relaxation of the random field Ising dynamics. *arXiv preprint arXiv:2311.06171*, 2023.

[Aid98] Shigeki Aida. Uniform positivity improving property, Sobolev inequalities, and spectral gaps. *Journal of functional analysis*, 158(1):152–185, 1998.

[AJ24] Gérard Ben Arous and Aukosh Jagannath. Shattering versus metastability in spin glasses. *Communications on Pure and Applied Mathematics*, 77(1):139–176, 2024.

[AJK+21a] Nima Anari, Vishesh Jain, Frederic Koehler, Huy Tuan Pham, and Thuy-Duong Vuong. Entropic independence i: Modified log-sobolev inequalities for fractionally log-concave distributions and high-temperature ising models. *arXiv preprint arXiv:2106.04105*, 2021.

[AJK+21b] Nima Anari, Vishesh Jain, Frederic Koehler, Huy Tuan Pham, and Thuy-Duong Vuong. Entropic independence ii: optimal sampling and concentration via restricted modified log-sobolev inequalities. *arXiv preprint arXiv:2111.03247*, 2021.

Bibliography II

[AJK+24] Nima Anari, Vishesh Jain, Frederic Koehler, Huy Tuan Pham, and Thuy-Duong Vuong. Universality of spectral independence with applications to fast mixing in spin glasses. In *Proceedings of the 2024 Annual ACM-SIAM Symposium on Discrete Algorithms (SODA)*, pages 5029–5056. SIAM, 2024.

[AKV24] Nima Anari, Frederic Koehler, and Thuy-Duong Vuong. Trickle-down in localization schemes and applications. In *Proceedings of the 56th Annual ACM Symposium on Theory of Computing*, pages 1094–1105, 2024.

[Ala24] Ahmed El Alaoui. Near-optimal shattering in the ising pure p-spin and rarity of solutions returned by stable algorithms. *arXiv preprint arXiv:2412.03511*, 2024.

[ALG21] Nima Anari, Kuikui Liu, and Shayan Oveis Gharan. Spectral independence in high-dimensional expanders and applications to the hardcore model. *SIAM Journal on Computing*, (0):FOCS20–1, 2021.

[ALGV19] Nima Anari, Kuikui Liu, Shayan Oveis Gharan, and Cynthia Vinzant. Log-concave polynomials ii: high-dimensional walks and an fpras for counting bases of a matroid. In *Proceedings of the 51st Annual ACM SIGACT Symposium on Theory of Computing*, pages 1–12, 2019.

Bibliography III

[AMS23a] Ahmed El Alaoui, Andrea Montanari, and Mark Sellke. Sampling from mean-field gibbs measures via diffusion processes. *arXiv preprint arXiv:2310.08912*, 2023.

[AMS23b] Ahmed El Alaoui, Andrea Montanari, and Mark Sellke. Shattering in pure spherical spin glasses. *arXiv preprint arXiv:2307.04659*, 2023.

[Bar16a] Alexander Barvinok. Approximating permanents and hafnians. *arXiv preprint arXiv:1601.07518*, 2016.

[Bar16b] Alexander Barvinok. *Combinatorics and complexity of partition functions*, volume 30. Springer, 2016.

[BD97a] Russ Bubley and Martin Dyer. Graph orientations with no sink and an approximation for a hard case of# sat. In *Proceedings of the Eighth Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 248–257, 1997.

[BD97b] Russ Bubley and Martin Dyer. Path coupling: A technique for proving rapid mixing in markov chains. In *Proceedings 38th Annual Symposium on Foundations of Computer Science*, pages 223–231. IEEE, 1997.

Bibliography IV

[BD97c] Russ Bubley and ME Dyer. Path coupling, dobrushin uniqueness, and approximate counting. *RESEARCH REPORT SERIES-UNIVERSITY OF LEEDS SCHOOL OF COMPUTER STUDIES LU SCS RR*, 1997.

[BDJ96] Russ Bubley, Martin Dyer, and Mark Jerrum. *A new approach to polynomial-time generation of random points in convex bodies*. University of Edinburgh. Laboratory for Foundations of Computer Science, 1996.

[BÉ06] Dominique Bakry and Michel Émery. Diffusions hypercontractives. In *Séminaire de Probabilités XIX 1983/84: Proceedings*, pages 177–206. Springer, 2006.

[CCYZ24] Xiaoyu Chen, Zongchen Chen, Yitong Yin, and Xinyuan Zhang. Rapid mixing at the uniqueness threshold. *arXiv preprint arXiv:2411.03413*, 2024.

[CE22a] Yuansi Chen and Ronen Eldan. Hit-and-run mixing via localization schemes. *arXiv preprint arXiv:2212.00297*, 2022.

[CE22b] Yuansi Chen and Ronen Eldan. Localization schemes: A framework for proving mixing bounds for markov chains. In *2022 IEEE 63rd Annual Symposium on Foundations of Computer Science (FOCS)*, pages 110–122. IEEE, 2022.

Bibliography V

[Che23] Sinho Chewi. Log-concave sampling. *Book draft available at https://chewisinho. github. io*, 2023.

[CHS93] Alessandro Crisanti, Herbert Horner, and H-J Sommers. The spherical p-spin interaction spin-glass model: the dynamics. *Zeitschrift für Physik B Condensed Matter*, 92:257–271, 1993.

[CLMM23] Zongchen Chen, Kuikui Liu, Nitya Mani, and Ankur Moitra. Strong spatial mixing for colorings on trees and its algorithmic applications. In *2023 IEEE 64th Annual Symposium on Foundations of Computer Science (FOCS)*, pages 810–845. IEEE, 2023.

[CLV21] Zongchen Chen, Kuikui Liu, and Eric Vigoda. Optimal mixing of glauber dynamics: Entropy factorization via high-dimensional expansion. In *Proceedings of the 53rd Annual ACM SIGACT Symposium on Theory of Computing*, pages 1537–1550, 2021.

[CLV24] Zongchen Chen, Kuikui Liu, and Eric Vigoda. Spectral independence via stability and applications to holant-type problems. *TheoretiCS*, 3, 2024.

[CMS24] Pietro Caputo, Florentin Münch, and Justin Salez. Entropy and curvature: beyond the peres-tetali conjecture. *arXiv preprint arXiv:2401.17148*, 2024.

Bibliography VI

[DSVW04] Martin Dyer, Alistair Sinclair, Eric Vigoda, and Dror Weitz. Mixing in time and space for lattice spin systems: A combinatorial view. *Random Structures & Algorithms*, 24(4):461–479, 2004.

[EHMT17] Matthias Erbar, Christopher Henderson, Georg Menz, and Prasad Tetali. Ricci curvature bounds for weakly interacting markov chains. 2017.

[EKZ22] Ronen Eldan, Frederic Koehler, and Ofer Zeitouni. A spectral condition for spectral gap: fast mixing in high-temperature ising models. *Probability theory and related fields*, 182(3):1035–1051, 2022.

[GJ19] Reza Gheissari and Aukosh Jagannath. On the spectral gap of spherical spin glass dynamics. *Annales de l'Institut Henri Poincaré, Probabilités et Statistiques*, 55(2):756 – 776, 2019.

[HK22] Jun-Ting Hsieh and Pravesh K Kothari. Approximating max-cut on bounded degree graphs: Tighter analysis of the fkl algorithm. *arXiv preprint arXiv:2206.09204*, 2022.

[HMMR05] Shlomo Hoory, Avner Magen, Steven Myers, and Charles Rackoff. Simple permutations mix well. *Theoretical computer science*, 348(2-3):251–261, 2005.

Bibliography VII

[HMP24] Brice Huang, Andrea Montanari, and Huy Tuan Pham. Sampling from Spherical Spin Glasses in Total Variation via Algorithmic Stochastic Localization. *arXiv preprint arXiv:2404.15651*, 2024.

[Jer95] Mark Jerrum. A very simple algorithm for estimating the number of k-colorings of a low-degree graph. *Random Structures & Algorithms*, 7(2):157–165, 1995.

[JS89] Mark Jerrum and Alistair Sinclair. Approximating the permanent. *SIAM journal on computing*, 18(6):1149–1178, 1989.

[JSV04] Mark Jerrum, Alistair Sinclair, and Eric Vigoda. A polynomial-time approximation algorithm for the permanent of a matrix with nonnegative entries. *Journal of the ACM (JACM)*, 51(4):671–697, 2004.

[KLV23] Frederic Koehler, Holden Lee, and Thuy-Duong Vuong. Efficiently learning and sampling multimodal distributions with data-based initialization. *arXiv preprint arXiv:2411.09117*, 2023.

[KV23] Frederic Koehler and Thuy-Duong Vuong. Sampling multimodal distributions with the vanilla score: Benefits of data-based initialization. *arXiv preprint arXiv:2310.01762*, 2023.

Bibliography VIII

[Liu23] Kuikui Liu. *Spectral Independence a New Tool to Analyze Markov Chains*. PhD thesis, University of Washington, 2023.

[LMR+24] Kuikui Liu, Sidhanth Mohanty, Prasad Raghavendra, Amit Rajaraman, and David X Wu. Locally stationary distributions: A framework for analyzing slow-mixing markov chains. *arXiv preprint arXiv:2405.20849*, 2024.

[LMRW24] Kuikui Liu, Sidhanth Mohanty, Amit Rajaraman, and David X Wu. Fast mixing in sparse random ising models. *arXiv preprint arXiv:2405.06616*, 2024.

[Lov99] László Lovász. Hit-and-run mixes fast. *Mathematical programming*, 86:443–461, 1999.

[LS93] László Lovász and Miklós Simonovits. Random walks in a convex body and an improved volume algorithm. *Random structures & algorithms*, 4(4):359–412, 1993.

[LV23] Aditi Laddha and Santosh S Vempala. Convergence of gibbs sampling: Coordinate hit-and-run mixes fast. *Discrete & Computational Geometry*, 70(2):406–425, 2023.

[LY52] Tsung-Dao Lee and Chen-Ning Yang. Statistical theory of equations of state and phase transitions. ii. lattice gas and ising model. *Physical Review*, 87(3):410, 1952.

Bibliography IX

[RW01] Michael Röckner and Feng-Yu Wang. Weak Poincaré inequalities and L2-convergence rates of Markov semigroups. *Journal of Functional Analysis*, 185(2):564–603, 2001.

[Vil09] Cédric Villani. *Optimal transport: old and new*, volume 338. Springer, 2009.

[Wei04] Dror Weitz. *Mixing in time and space for discrete spin systems*. University of California, Berkeley, 2004.

[Wei06] Dror Weitz. Counting independent sets up to the tree threshold. In *Proceedings of the thirty-eighth annual ACM symposium on Theory of computing*, pages 140–149, 2006.