

Diffusion-Based Sampling for Spin Glasses

Mark Sellke (Harvard Statistics)

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Collaborators

Ahmed El Alaoui (Cornell)



Andrea Montanari (Stanford)



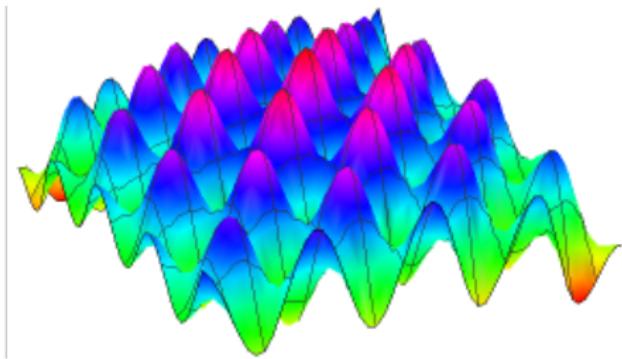
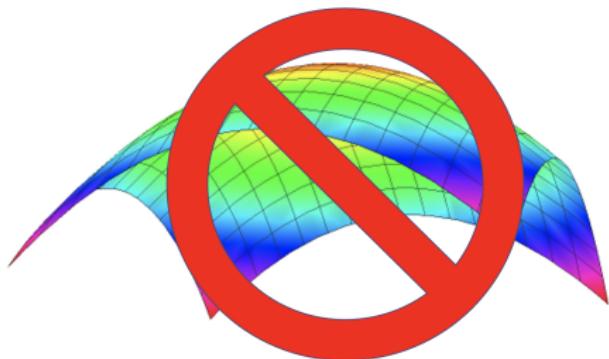
- ➊ Background on High-Dimensional Sampling
 - Sequential sampling
 - Stochastic localization
 - Connection to diffusion models
 - Goal for today: the Sherrington–Kirkpatrick model
- ➋ Main Results
 - Algorithm: approximate message passing and more
 - Stability of the algorithm; hardness from chaos.
 - p -spin generalizations; another source of chaos.

Sampling

Goal: generate

$$x^* \sim \mu(dx) \quad \text{given} \quad \mu \in \mathcal{P}(\mathbb{R}^n).$$

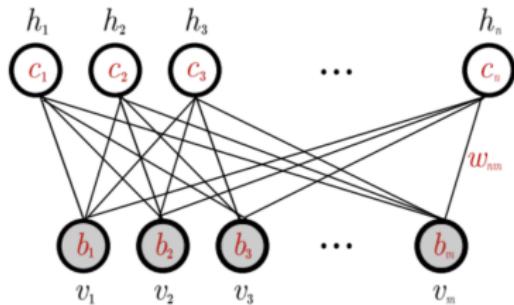
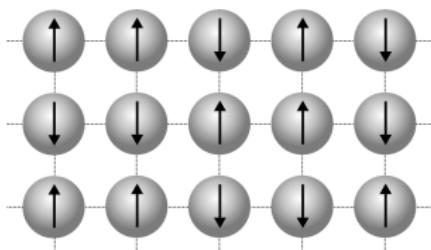
For μ high-dimensional and NOT log-concave.



Sampling

In this talk, focus on Ising models:

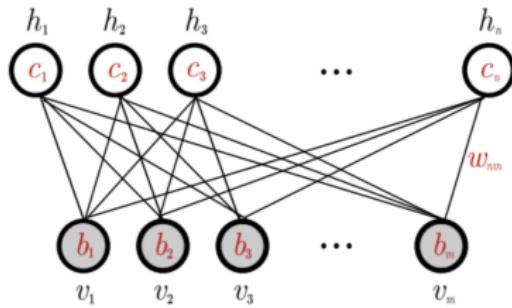
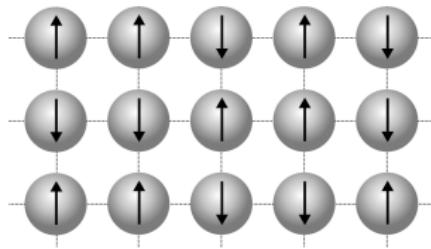
$$\mu_{A,\beta}(x) = \frac{1}{Z(\beta)} e^{\beta \langle x, Ax \rangle / 2}, \quad x \in \{-1, +1\}^n.$$



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Glauber dynamics

- Repeatedly choose $i \in [n]$ and resample x_i given other coordinates.
- Mixes rapidly if βA is small. In general, mixing can be very slow.

Sequential Sampling

Given a distribution $\mu \in \mathcal{P}(\{-1, +1\}^n)$, suppose we have a conditional expectation **oracle** to evaluate

$$m^t = \mathbb{E}_{x \sim \mu}[x \mid (x_1 = x_1^*, \dots, x_t = x_t^*)], \quad t \in \{0, 1, \dots, n-1\}.$$

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Then we can directly sample x , one coordinate at a time. Namely,

$$\mathbb{P}^t[x_{t+1} = 1 \mid x_1, \dots, x_t] = \frac{m_{t+1}^t + 1}{2}.$$

This is the foundation for equivalence between counting and sampling.

Sequential Sampling

Directly implementing sequential sampling may be too much to hope for.

- Requires a strong oracle, especially for continuous variables.
- Maybe estimating m^t is no easier than sampling.
- Unclear how to choose a good order for the coordinates.

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The high-level idea is to reveal x^* **gradually**. This is fundamentally different from a Markov chain!

And, information can be gradually revealed in other ways.

Sampling via Stochastic Localization

Given $\mu \in \mathcal{P}(\mathbb{R}^n)$, consider a **Brownian motion with unknown drift**:

$$y_t = tx^* + B_t \sim \mathcal{N}(tx^*, tI_n).$$

$x^* \sim \mu$ is independent of Brownian motion B_t and **only y_t is observed**.

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Our sampling algorithm takes the following form:

- ① **Simulate y_t** for a long time $t \in [0, T]$ without knowing x^* .
- ② **Read off**

$$x^* \approx \frac{y_T}{T}.$$

Equivalently, increments $y_{(k+1)\delta} - y_{k\delta}$ are IID noisy observations of x^* .

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This process has been popularized in high-dimensional convex geometry
[Eldan 13, Lee-Vempala 17, Chen 21, Klartag-Lehec 22, Jambulapati-Lee-Vempala 22].

Simulating y_t

Our goal is to sample a random path

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This law on paths is actually Markovian. The instantaneous drift is the **current conditional expectation** of the unknown drift:

$$\begin{aligned} dy_t &= m_t dt + dW_t; \\ m_t &= \mathbb{E}[x^* \mid \mathcal{F}_t] = \mathbb{E}[x^* \mid y_t] \end{aligned}$$

for W_t a (separate) Brownian motion.

Markov property: y_t is a sufficient statistic for $y_{[0,t]}$.

Parallels with Pólya's Urn

Pólya's urn gives an indirect way to sample $p \sim \text{Unif}([0, 1])$. Stochastic localization sampling is a continuous-time parallel.

Goal	Pólya's Urn	Stoch. Loc.
Want to sample	$p \sim \text{Unif}([0, 1])$	$x^* \sim \mu \in \mathcal{P}(\mathbb{R}^n)$
Observation process	$a_1, a_2, \dots \stackrel{\text{IID}}{\sim} \text{Ber}(p)$	$y_t = tx^* + B_t$
Process w/o sample	$a_t \sim \text{Ber}(\mathbb{E}^t[p])$	$dy_t = \mathbb{E}^t[x^*] + dB_t$
Process \rightarrow sample	$p \approx (a_1 + \dots + a_T)/T$	$x^* \approx y_T/T$

In this case, $\mathbb{E}^t[p] = \frac{N_t(1)+1}{N_t(0)+N_t(1)+2}$ by Laplace's rule of succession.

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$S_N = a_1 + \dots + a_T$ plays the role of y_T .

- Given p : S_T is a discrete walk with drift p .
- Given x^* : y_t is a continuous walk with drift x^* .
- Increments $y_{(j+1)\delta} - y_{j\delta}$ play the role of a_j .

The Resulting Algorithm

$$dy_t = m_t dt + dW_t,$$

A continuous-time stochastic process is not really an algorithm.

Of course, we should discretize time.

The Resulting Algorithm

$$dy_t = m_t dt + dW_t,$$

Input: Data: Probability measure μ

Input: Result: Sample $x^* \sim \mu$

for $t \in [0, \delta, \dots, T - \delta]$ **do**

 Sample $g_t \sim \mathcal{N}(0, I_n)$

 Set $\hat{y}_{t+\delta} = \hat{y}_t + \delta \hat{m}_t(y_t) + \sqrt{\delta} g_t$

end

Set $\hat{x}^* = Round(\hat{y}_T / T) \in \{-1, +1\}^n$

return \hat{x}^*

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Set $\hat{x}^* = Round(\hat{y}_T / T) \in \{-1, +1\}^n$

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Main requirement: a good approximation

$$\hat{m}_t(\hat{y}_t) \approx m_t(\hat{y}_t) \equiv \mathbb{E}[x^* | \hat{y}_t].$$

Where Do We Stand?

So far:

- General sampling procedure.
- Requires repeatedly estimating $m_t(\hat{y}_t) \approx \mathbb{E}[x^* | \hat{y}_t]$.

We have replaced the need for one oracle with another...is it any better?

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Main result for this talk: example where the answer is yes.

- SK model: coupling matrix A is GOE.
- Computing $m_t(y_t)$ falls into the wheelhouse of high-dimensional statistics/optimization.
- But, provable hardness for “stable” sampling at large β .

Connection to Diffusion Models



Connection to Diffusion Models

Modern diffusion-based sampling has two main processes:

- Forward: turn **sample** $X_0 \sim \mu$ into **noise** via OU flow

$$dX_T = -X_T dT + \sqrt{2} dW_T.$$

- Backward: time-reverse the forward process, i.e. **noise** \rightarrow **sample**.
- The backward process gains a μ -dependent drift.

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Given X_S for $S < T$: $e^T X_T \stackrel{d}{=} e^S X_S + \sqrt{e^{2T} - e^{2S}} \mathcal{N}(0, I_n)$.

Given y_s for $s > t$: $y_t/t \stackrel{d}{=} y_s/s + \sqrt{\frac{s-t}{t}} \mathcal{N}(0, I_n)$.

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Stochastic localization is a reparametrization of the backward process!

- Diffusion models learn SDE coefficients from forward process on samples. Provable guarantees from good estimates (ask Sitan!)
- This talk: no samples, but a formula for μ .

Sherrington-Kirkpatrick Model

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Ising model with random couplings:

$$\mu_{G,\beta}(x) = \frac{1}{Z_n(\beta)} e^{\beta \langle x, Gx \rangle / 2}.$$

Random symmetric matrix $G \sim GOE(n)$:

- $G = G^\top$. Entries otherwise independent.
- $G_{i,j} \sim \mathcal{N}(0, 1/n)$ for $i < j$.

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Goal: given $G \sim GOE(n)$, generate a sample from $\mu_{G,\beta}$.

Dobrushin's condition for fast mixing of Glauber works if $\beta \leq cn^{-1/2}$.
But we would like β to be constant size.

Brief History of the SK Model

[Ising 1925]: Ising model for ferromagnets.

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[Talagrand 2006] proves the Parisi formula.

- Huge amount of other important work including
[Aizenman-Ruelle-Lebowitz 82, Ruelle 87, Guerra 03, Chatterjee 09,
Panchenko 14, Ding-Sly-Sun 15, Auffinger-Chen 17,...].

SK model is a prototype for disordered, random probability measures.

- Random MaxCut and K -SAT.
- Coloring random graphs.
- Posteriors in high-dimensional statistics.

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E.g. optimal MaxCut in a random sparse graph ([Dembo-Montanari-Sen 17]).

For $G \sim G\left(n, \frac{\lambda}{n}\right)$:

$$\text{MaxCut}(G) = n \left(\frac{\lambda}{4} + C_* \sqrt{\frac{\lambda}{4}} + o(\sqrt{\lambda}) \right) + o(n).$$

Rigorous Results on Sampling

$$\mu_{G,\beta}(x) = \frac{1}{Z_n(\beta)} e^{\beta \langle x, Gx \rangle / 2}.$$

Expect: efficient sampling possible for $\beta < 1$, impossible for $\beta > 1$.

- “Replica symmetric” for $\beta < 1$. For independent $x, x' \sim \mu_{G,\beta}$,

$$\mathbb{E}[|\langle x, x' \rangle|/n] \approx 0.$$

- “Replica symmetry breaking” for $\beta > 1$. Here

$$\mathbb{E}[|\langle x, x' \rangle|/n] \geq c(\beta) > 0.$$

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Recent progress: Glauber mixes in $O(n \log n)$ steps for $\beta < 1/4$.

[Bodineau-Bauerschmidt 20, Eldan-Koehler-Zeitouni 21, Anari-Jain-Koehler-Pham-Vuong 21].

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Our result: stochastic localization succeeds (in a weaker sense) for $\beta < 1$.
(Originally $\beta < 1/2$, improvement by [Celentano 22].)

Normalized Wasserstein Metric

Given $\mu_1, \mu_2 \in \mathcal{P}(\{-1, 1\}^n)$, define the normalized Wasserstein metric

$$W_{1,n}(\mu_1, \mu_2) = \inf_{(x_1, x_2) \sim \text{Coupling}(\mu_1, \mu_2)} \frac{\mathbb{E}[\|x_1 - x_2\|_{\ell^1}]}{n}.$$

$W_{1,n}(\mu_1, \mu_2) \leq o(1)$ means that x_1, x_2 differ by $o(n)$ coordinates under an optimal coupling. We will consider such pairs of points to be close.

Theorem (Alaoui-Montanari-S 22, Celentano 22)

For any $\beta < 1$ and $\varepsilon > 0$, there exists a randomized algorithm with complexity $O(n^2)$ which given G outputs $x \sim \mu_{G,\beta}^{\text{alg}}$ such that

$$\mathbb{E}[W_{1,n}(\mu_{G,\beta}^{\text{alg}}, \mu_{G,\beta})] \leq \varepsilon.$$

Estimating the Mean

Estimating the Mean

To sample for $\beta < 1$, our main goal is to estimate $m_t = \mathbb{E}[x^* | y_t]$ for

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The solution goes through several ideas in high-dimensional statistics and optimization.

Estimating the Mean

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Two phase procedure:

- Rough estimate for m_t using approximate message passing.
- High-accuracy estimate for m_t using gradient descent on a well-chosen potential.

For now, assume perfect simulation until time t . Observe

$$y_t \sim \mathcal{N}(tx^*, tl_n),$$

estimate $m_t(y_t)$.

Step 1: Rough Estimate of m_t

Self-consistent “naive mean-field” equation for $m_t = \mathbb{E}[x | y_t]$:

$$m_t \approx \tanh(\beta G m_t + y_t)$$

- Intuitively, $(\beta G m_t + y_t)_i$ is the effective field on x_i .
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Revised Thouless-Anderson-Palmer (TAP) equation:

$$m_t \approx \tanh \left(\beta G m_t + y_t - \beta^2 \left(1 - \frac{\|m_t\|_2^2}{n} \right) m_t \right).$$

Step 1: Rough Estimate of m_t

Turn the TAP equation into a **recursion** and repeat until convergence to an approximate **fixed point**:

$$\begin{aligned}\hat{m}_t^{(k+1)} &= \tanh \left(\beta G \hat{m}_t^{(k)} + y_t - b_k \hat{m}_t^{(k-1)} \right), \\ b_k &= \beta^2 \left(1 - \frac{\|\hat{m}_t^{(k)}\|_2^2}{n} \right).\end{aligned}$$

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This is an **approximate message passing** algorithm. Generalizes belief propagation to dense matrices G .

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This is an **approximate message passing** algorithm. Generalizes belief propagation to dense matrices G .

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- By now, a major tool in high-dimensional statistics.

[Bolthausen 14, Donoho-Maleki-Montanari 09, Bayati-Montanari 11, Javanmard-Montanari 12,
Rush-Venkatesan 18, Chen-Lam 20, Fan 20, Dudeja-Lu-Sen 22]

For large n and $k = O(1)$ iterations, **state evolution** describes AMP.

State Evolution for AMP

$$\hat{m}_t^{(k+1)} = \tanh \left(\beta G \hat{m}_t^{(k)} + y_t - b_k \hat{m}_t^{(k-1)} \right)$$

Idea of AMP: for deterministic v, w , the vectors

$$Gv, Gw$$

each have i.i.d. Gaussian coordinates. Covariance between $(Gv)_i$ and $(Gw)_i$ equals $\langle v, w \rangle$.

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- **Onsager term** lets us apply this recursively to each $\hat{m}_t^{(k+1)}$, despite re-using the same G many times.

State evolution: from **simple initialization** (\hat{m}_t^0, y_t) , choose uniform $i \in [n]$. Tells us the $n \rightarrow \infty$ limiting distribution of

$$\left((\hat{m}_t^0)_i, (\hat{m}_t^1)_i, \dots, (\hat{m}_t^k)_i \right) \in \mathbb{R}^{k+1}.$$

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Problem: $x^* \sim \mu_{G,\beta}$ is NOT SIMPLE. So neither is $y_t \sim \mathcal{N}(tx^*, tI_n)$.

Contiguity with a Simpler Spiked Model

To analyze the AMP recursion, we switch to a **spiked joint distribution** \mathbb{Q} over (G, x^*, y_t) . Under \mathbb{Q} :

$$x^* \sim \text{Unif}(\{-1, 1\}^n), \quad y_t = tx^* + B_t,$$
$$\mathbf{G} \sim \text{GOE}(n) + \frac{\beta x^*(x^*)^\top}{n}.$$

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$$\mathbf{G} \sim \text{GOE}(n) + \frac{\beta x^*(x^*)^\top}{n}.$$

The conditional law $\mathbb{Q}[G \mid x^*]$ looks similar to $\mathbb{P}[x^* \mid G]$ in SK:

$$\mathbb{Q}[G \mid x^*] \propto e^{\beta \langle x^*, G x^* \rangle / 2} v_{\text{GOE}(n)}(G).$$

Contiguity with a Simpler Spiked Model

To analyze the AMP recursion, we switch to a **spiked** joint distribution \mathbb{Q} over (G, x^*, y_t) . Under \mathbb{Q} :

$$x^* \sim \text{Unif}(\{-1, 1\}^n), \quad y_t = tx^* + B_t,$$
$$\mathbf{G} \sim \text{GOE}(n) + \frac{\beta x^*(x^*)^\top}{n}.$$

The conditional law $\mathbb{Q}[G \mid x^*]$ looks similar to $\mathbb{P}[x^* \mid G]$ in SK:

$$\mathbb{Q}[G \mid x^*] \propto e^{\beta \langle x^*, Gx^* \rangle / 2} v_{\text{GOE}(n)}(G).$$

Swapping the order distorts probabilities by a partition function factor

$$Z_{SK}(G) = \sum_{v \in \{-1, +1\}^n} e^{\beta \langle v, Gv \rangle / 2}.$$

- $Z_{SK}(G)$ fluctuates **mildly** for $\beta < 1$ [Aizenman-Ruelle-Lebowitz 82]. Yields **contiguity**; estimating m_t w.h.p. is **equivalent**.

State Evolution for AMP

State evolution: i -th coordinate of $\hat{m}_t^{(k)}$ behaves like

$$\tanh(a_t^{(k)}x_i + b_t^{(k)}Z), \quad Z \sim \mathcal{N}(0, 1).$$

Limits (a_t^∞, b_t^∞) yield the asymptotic mean-squared error (MSE)

$$E_*(t) = \lim_{k \rightarrow \infty} \text{p-lim}_{n \rightarrow \infty} \mathbb{E} \|\hat{m}_t^{(k)} - x\|_2^2.$$

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I-MMSE Area Law [Guo-Shamai-Verdu 04, Deshpande-Abbe-Montanari 15]:

$$\frac{1}{2} \int_0^\infty \text{MMSE}(t) dt = \text{Ent}(x^*).$$

- We verify explicitly that $\int_0^\infty E_*(t) dt \approx \text{Ent}(x^*)$ for large n .

Conclusion of Step 1: Rough Estimate for m_t

$$\hat{m}_t^{(k+1)} = \tanh \left(\beta G \hat{m}_t^{(k)} + y_t - b_k \hat{m}_t^{(k-1)} \right),$$

Proposition (Alaoui-Montanari-S 22)

For $\beta < 1$ and any $\varepsilon, t \geq 0$ there exists $k_0(t, \varepsilon)$ such that for all $k \geq k_0$,

$$\lim_{n \rightarrow \infty} \mathbb{P} \left[\|\hat{m}_t^{(k)}(y_t) - m_t(y_t)\| \leq \varepsilon \sqrt{n} \right] = 1.$$

Here y_t is perfect stochastic localization at time t . The algorithm can only use an estimate \hat{y}_t .

We still must bound $\|\hat{m}_t^{(k)}(y_t) - \hat{m}_t^{(k)}(\hat{y}_t)\|$ to control **error accumulation across time**.

Step 2: Refined Estimate of m_t

Surprisingly, finishing the proof is non-obvious.

- Two types of error: SDE δ -discretization and $\hat{m}_t^{(k)} \approx m_t$.
- Sending $(\delta, k) \rightarrow (0, \infty)$ does not suffice.
 - Lipschitz constant of $\hat{m}_t^{(k)}$ diverges with k .

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Second step: by construction, $\hat{m}_t^{(k)}$ is an approximate stationary point for the “TAP free energy”:

$$F_{TAP}(m, y_t) = -\frac{\beta}{2} \langle m, Gm \rangle - \langle \hat{y}_t, m \rangle - \sum_{i=1}^n h(m_i).$$

- With gradient descent, refine $\hat{m}_t^{(k)}$ to

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- [Celentano 22]: F_{TAP} is **strongly convex** near \hat{m}_t^∞ for $\beta < 1$.
Hence \hat{m}_t^∞ is C_β -Lipschitz in \hat{y}_t . No blow-up with AMP accuracy.

Algorithmic Stability

Our algorithm is **stable** with respect to (G, β) : just uses $O_{\beta, \varepsilon}(1)$ matrix-vector products, and some 1-dimensional non-linearities.

Concretely, from i.i.d. $G = G_0$ and G_1 , consider perturbation path

$$G_s = \sqrt{1-s^2}G_0 + sG_1.$$

Stability of the algorithm tells us:

$$\lim_{s \rightarrow 0} \lim_{n \rightarrow \infty} \mathbb{E}[W_{1,n}(\mu_{G_0, \beta}^{\text{alg}}, \mu_{G_s, \beta}^{\text{alg}})] = 0.$$

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A purely structural consequence with an algorithmic proof:

Theorem (Alaoui-Montanari-S 22; Celentano 22)

The true SK Gibbs measures are stable when $\beta < 1$:

$$\lim_{s \rightarrow 0} \lim_{n \rightarrow \infty} \mathbb{E}[W_{1,n}(\mu_{G_0, \beta}, \mu_{G_s, \beta})] = 0.$$

Similar stability holds for small perturbations in β .

The stability property

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Hardness via Chaos

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Theorem (Chatterjee 09; Disorder Chaos)

Let $(x_0, x_s) \sim \mu_{G_0, \beta} \times \mu_{G_s, \beta}$. For all $\beta \in \mathbb{R}$ and $s > 0$,

$$\lim_{n \rightarrow \infty} \mathbb{E}[|\langle x_0, x_s \rangle|/n] = 0.$$

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Theorem (Replica Symmetry Breaking)

Let $x_0, x'_0 \sim \mu_{G_0, \beta}$ be independent. For all $\beta > 1$,

$$\liminf_{n \rightarrow \infty} \mathbb{E}[|\langle x_0, x'_0 \rangle|/n] \geq c(\beta) > 0.$$

The previous results show that $\mu_{G_0, \beta}$ and $\mu_{G_s, \beta}$ must be significantly different. Therefore:

Theorem (Alaoui-Montanari-S 22)

Let $\mu_{G, \beta}^{\text{alg}}$ be the law of $\text{ALG}_n(G, \beta, \omega)$ conditional on G . If ALG_n is stable, then for all $\beta > 1$,

$$\liminf_{n \rightarrow \infty} \mathbb{E}[W_{1,n}(\mu_{G, \beta}^{\text{alg}}, \mu_{G, \beta})] > c(\beta) > 0.$$

Stability holds for gradient-based methods such as Langevin dynamics and AMP, at least on **dimension-independent** time-scales.

Extension to p -spin Models

Instead of a random matrix, start with a Gaussian **tensor**

$$G^{(p)} \sim N^{-(p-1)/2} \cdot \mathcal{N}(0, I_{n^p}).$$

The pure p -spin glass distribution is:

$$\mu_{p,\beta}(x) = \frac{1}{Z_{p,n}(\beta)} e^{\beta \langle x^{\otimes p}, G^{(p)} \rangle}.$$

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Physics belief: sampleable for $\beta = \beta_{dyn}(p) \approx \sqrt{\frac{1}{p}}$.

[ABXY 22, AJKPV 23]: Glauber mixes fast for $\beta \ll p^{-3/2}$.

[Alaoui-Montanari-**S** 23]: stochastic localization succeeds for $\beta \ll \frac{1}{p}$.

However, replica-symmetric below $\beta_c(p) \approx \sqrt{2 \log 2} \gg \beta_{dyn}(p)$.

Shattering

$\beta_c(p) \gg \beta_{dyn}(p)$ is expected for large p due to **shattering**.

This means there are disjoint clusters $\mathcal{C}_1, \dots, \mathcal{C}_M \subseteq \{-1, +1\}^n$ with...

- ① Small diameter and probability:

$$\max_{1 \leq m \leq M} diam(\mathcal{C}_m) \leq \varepsilon \sqrt{N}, \quad \max_{1 \leq m \leq M} \mu_\beta(\mathcal{C}_m) \leq e^{-cN}.$$

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- ③ Together, the clusters account for nearly all the probability:

$$\mu_\beta \left(\bigcup_{m=1}^M \mathcal{C}_m \right) \geq 1 - e^{-cN}.$$

Hardness for p -spin Sampling

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Theorem (Gamarnik-Jagannath-Kizildag 23)

Pure p -spin glasses shatter for $0.51\beta_c(p) < \beta < 0.99\beta_c(p)$ and $p \geq O(1)$.

Theorem (Alaoui-Montanari-S 23b)

For spin glasses, “shattering \implies chaos \implies hardness”.

- Noising $G^{(p)}$ re-randomizes cluster weight ratios $\mu_\beta(\mathcal{C}_i)/\mu_\beta(\mathcal{C}_j)$.

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For spherical analogs: $\beta_{dyn}^{sph}(p) \approx \sqrt{e} \ll \beta_c^{sph}(p) \approx \sqrt{\log p}$.

Theorem (Alaoui-Montanari-S 23b)

Spherical p -spin glasses shatter for $\beta \in [O(1), \beta_c^{sph}(p))$.

Sharp thresholds (algorithmic and mathematical) open beyond SK.

Summary

Stochastic localization sampling for the SK model

$$\mu_{G,\beta}(x) = \frac{1}{Z_n(\beta)} e^{\beta \langle x, Gx \rangle / 2}.$$

Approach: to obtain $x^* \sim \mu$, simulate $y_t = tx^* + B_t$.

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Main result: Wasserstein-approximate samples for $\beta < 1$. For $\beta > 1$, disorder chaos is a natural barrier for stable algorithms.

- For general p -spin models, sharp thresholds will require an understanding of **shattering**.
- Upgrade to TV sampling?
- What other distributions are stochastic localization sampleable?

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Other provable implementations of diffusion sampling:

- [Montanari-Wu 23]: posterior sampling for noisy low-rank matrices.
- [AHLVXY 23]: TV sampling for structured μ , e.g. DPPs.