

# Tight Algorithmic Thresholds for Optimizing Mean Field Spin Glass Hamiltonians

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Simons Workshop on Rigorous Evidence for  
Information-Computation Trade-offs

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Joint work with Brice Huang (MIT)

- 1 Problem setup: optimizing a mean field spin glass Hamiltonian.

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- 2 Background: Parisi formula, AMP, overlap gap property.
- 3 New result: a tight characterization of the best value achieved by a class of efficient algorithms.
- 4 Some key ideas: ultrametricity and a branching OGP.

Definition (Sherrington-Kirkpatrick 75,...)

Fix constants  $\gamma_1, \gamma_2, \dots, \gamma_K \geq 0$ . The mixed  $p$ -spin Hamiltonian  $H_N : \mathbb{R}^N \rightarrow \mathbb{R}$  is a random degree  $K$  polynomial defined by

$$H_N(\sigma_1, \dots, \sigma_N) = \sum_{k=1}^K N^{-\frac{k-1}{2}} \gamma_k \sum_{1 \leq i_1, \dots, i_k \leq N} J_{i_1, \dots, i_k} \sigma_{i_1} \dots \sigma_{i_k}.$$

Here  $J_{i_1, \dots, i_k}$  are IID standard gaussians.

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Here  $J_{i_1, \dots, i_k}$  are IID standard Gaussians.

- Equivalently: let  $\xi(t) = \sum_{k=1}^K \gamma_k^2 t^k$ . Then  $H_N$  is the centered Gaussian process with covariance

$$\mathbb{E}[H_N(\sigma)H_N(\sigma')] = N\xi(\langle \sigma, \sigma' \rangle / N).$$

- Two input sets will be considered:
  - Ising –  $\sigma \in \{-1, 1\}^N$
  - Spherical –  $\|\sigma\| = \sqrt{N}$ .

# Motivations for the Model

- The Sherrington-Kirkpatrick model ( $K = 2$ ) was introduced to study diluted magnetic alloys such as Copper Manganese.
- Magnetic interaction rapidly oscillates with distance, so use an Ising model with **random weights**:  $H_N = \sum_{i,j} J_{i,j} \sigma_i \sigma_j$ .



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- Higher degree interactions and spherical inputs are mathematically natural extensions.
- Also arises as high-degree limit of random MaxCut, MaxSAT (Dembo-Montanari-Sen 17, Panchenko 18).
- Rich source of random non-convex functions, related to some neural network models (Gardner-Derrida 80s, Amit-Gutfreund-Sompolinsky 85, Choromanska-Henaff-Mathieu-Ben Arous-LeCun 15).

Theorem (Parisi 82, Talagrand 06/10, Panchenko 14, Auffinger-Chen 17)

*In both the Ising and spherical settings, the limit*

$$\text{OPT} \equiv \text{p-lim}_{N \rightarrow \infty} \max_x \frac{H_N(x)}{N} = \inf_{\zeta \in \mathcal{U}} \mathcal{P}_\xi(\zeta)$$

*holds for explicit Parisi functionals  $\mathcal{P}_\xi^{\text{Is}}$ ,  $\mathcal{P}_\xi^{\text{Sp}}$ . Here  $\mathcal{U}$  is the set of **non-decreasing** functions  $\zeta : [0, 1] \rightarrow \mathbb{R}^+$ .*

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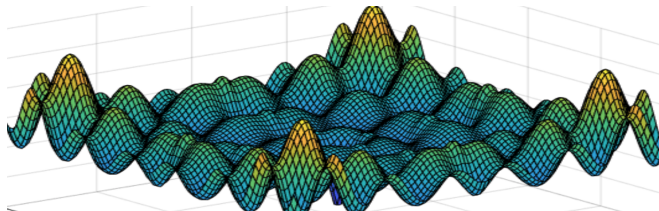
- Question: can efficient algorithms reach  $(\text{OPT} - \varepsilon)N$ ?
- If not, what can be done efficiently?
- Goal: compute  $\sigma = \mathcal{A}(H_N)$  with  $H_N(\sigma)$  as large as possible.

# A Look at the Landscape

- If  $H_N$  is close to convex, maybe gradient descent works.
- Not the case! On the sphere,  $H_N$  can have:

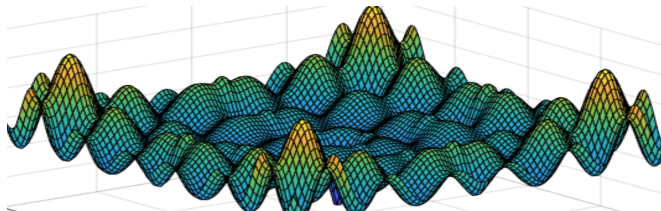
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    - Exponentially many near-optimal local maxima. 😊
    - Exponentially *more* suboptimal local maxima. 😞
    - Exponentially *more* suboptimal saddle points. 😞
- (Auffinger-Ben Arous 13, A-BA-Černý 13, Subag 17,  
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- **Adversarial  $H_N$ :** reaching  $\frac{\text{OPT}}{\log(N)^c}$  is hard (Arora-Berger-Hazan-Kindler-Safra 05, Barak-Brandao-Harrow-Kelner-Steurer-Zhou 12).

# AMP Algorithms Succeed under No Overlap Gap

Theorem (Subag 18, Montanari 19, El Alaoui-Montanari-S 20, S 21)

*The asymptotic value*

$$\text{ALG} = \inf_{\zeta \in \mathcal{L}} \mathcal{P}_\xi(\zeta)$$

*is achievable by AMP (assuming a minimizer  $\zeta_* \in \mathcal{L}$  exists).*

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- Approximate message passing (AMP) is really efficient.
  - Uses only  $O(1)$  queries of  $\nabla H_N$ . Great for tons of problems.
  - (Bolthausen 14, Donoho-Maleki-Montanari 09, Bayati-Montanari 11, Javanmard-Montanari 13, Bayati-Lelarge-Montanari 15, Rush-Venkataramanan 18, Montanari-Venkataramanan 21, . . .)

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- In brief: take small steps to simulate an SDE related to  $\mathcal{P}_\xi$ .
  - (AMS 20, roughly): No SDE-based AMP can reach  $\text{ALG} + \varepsilon$ .
- Equality case  $\text{ALG} = \text{OPT}$  corresponds to *no overlap gap*.

Theorem (Gamarnik-Jagannath 20, G-J-Wein 20&21, S 21)

*No **stable** algorithm can achieve OPT unless aforementioned AMP algorithms succeed (in even models with  $\gamma_3 = \gamma_5 = \dots = 0$ ).*

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- Stable algorithms include:
  - $O(1)$  iterations of gradient descent or AMP
  - ... or *any* “constant-order method” querying  $\nabla^{O(1)} H_N$
  - Langevin dynamics run for  $O(1)$  time
  - Low degree polynomials
  - Poly-size circuits with depth at most  $\frac{\log N}{2 \log \log N}$ .

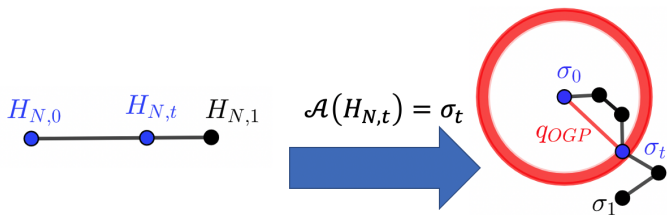
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- Proof based on overlap gap property (OGP): a family of topological hardness criteria.  
(Achlioptas-Coja Oghlan 08, Gamarnik-Sudan 14, Gamarnik-Sudan 17 Rahman-Virag 17, Gamarnik-Zadik 17, Chen-Gamarnik-Panchenko-Rahman 17, Gamarnik-Jagannath-Sen 19, Wein 20, ...)

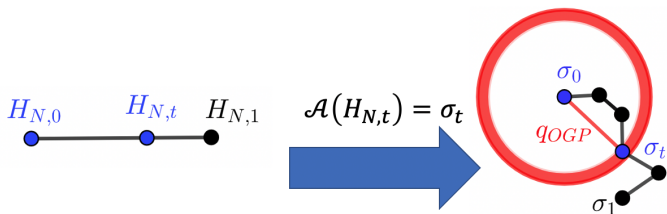
# Overlap Gap Property for Spin Glasses: A Cartoon

- Consider path  $H_{N,t} = \sqrt{1-t}H_{N,0} + \sqrt{t}H_{N,1}$ .
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- Overlap gap property: for some  $q_{\text{OGP}} \in (0, 1)$ , if  $\|\sigma_0 - \sigma_t\| \approx q_{\text{OGP}}\sqrt{N}$ , then either  $\sigma_0$  or  $\sigma_t$  is suboptimal.

$$\min(H_{N,0}(\sigma_0), H_{N,t}(\sigma_t)) \leq (\text{OPT} - \varepsilon)N.$$

- “Continuity” implies  $\|\sigma_t - \sigma_0\| \approx q_{\text{OGP}}\sqrt{N}$  for some  $t \in [0, 1]$ .

# New Result: An Algorithmic Threshold

Theorem (Huang-S. 21+)

No **overlap concentrated** algorithm can **beat ALG** (in even models).

- Overlap concentrated algorithms include:
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- For the algorithms listed above, result holds in a strong sense:

$$\mathbb{P}[H_N(\mathcal{A}(H_N)) \geq (\text{ALG} + \varepsilon)N] \leq O(e^{-c(\varepsilon)N}).$$

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- Proof relies on a new **branching OGP**.
- In spherical models, branching OGP is in some sense **necessary** to rule out  $\text{ALG} + \varepsilon$ . Simpler OGPs cannot.

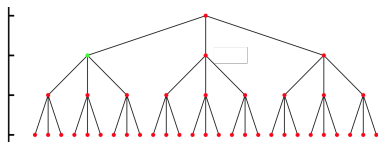
# Ultrametric Spaces and Trees

- Recall: ultrametric spaces  $X$  satisfy the ultrametric triangle inequality

$$d(x, y) \leq \max(d(x, z), d(y, z)), \quad \forall x, y, z \in X.$$

Equivalent to hierarchical clustering, or graph metrics of leaves of a rooted tree.

(All ultrametrics will be finite with sensible diameter.)



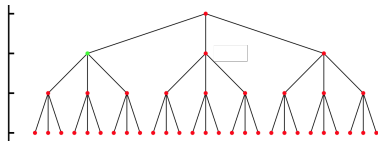
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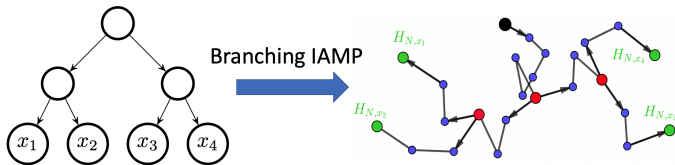
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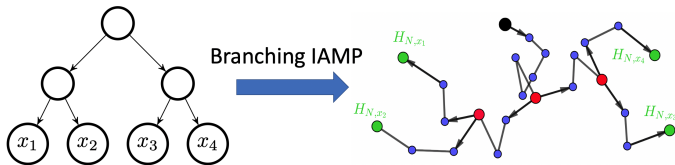
- For all  $\beta > 0$ , Gibbs measure  $e^{\beta H_N(\sigma)} d\sigma / Z$  is “ $\approx$  ultrametric”. (Parisi 82, Mézard-Parisi-Soullas-Toulouse-Virasoro 84, Derrida 85, Ruelle 87, Panchenko 13, Jagannath 17, Chatterjee-Sloman 20, . . .)

# Algorithms and Ultrametrics

- Turns out algorithms can build ultrametric spaces!
- AMP algorithms for this problem explore using many small steps. **Branch** to get a multi-valued algorithm.



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- AMP algorithms for this problem explore using many small steps. **Branch** to get a multi-valued algorithm.



- Result: for any finite ultrametric  $X$ , branching IAMP can output a configuration  $(\sigma_x)_{x \in X}$  approximating  $X$ :

$$H_N(\sigma_x) \approx \text{ALG} \cdot N, \quad \forall x \in X,$$
$$\|\sigma_x - \sigma_y\| \approx d_X(x, y) \sqrt{N}, \quad \forall x, y \in X.$$

(Subag 18, El Alaoui-Montanari 20, **S** 21)

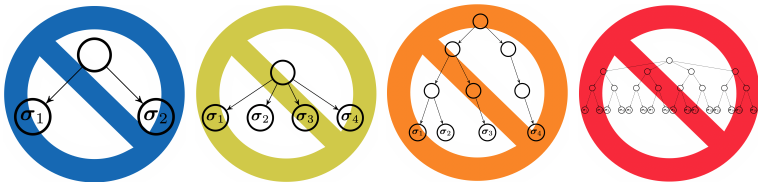
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- **1 layer** OGP: tuples  $(\sigma_1, \dots, \sigma_m)$  with all distances  $q_{\text{OGP}}\sqrt{N}$ .
- **Ladder** OGP:  $\text{Dist}(\sigma_{i+1}, \text{span}(\sigma_1, \dots, \sigma_i)) = \delta\sqrt{N}$ .



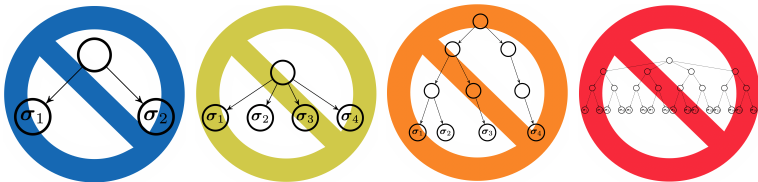
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- But...why would branching OGP imply hardness?

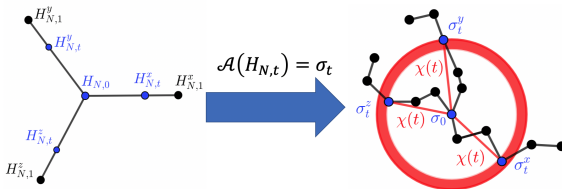
# Overlap Concentrated Algorithms

## Definition

An algorithm  $\mathcal{A}$  is **overlap concentrated** if the random distance

$$\frac{\|\mathcal{A}(H_{N,0}) - \mathcal{A}(H_{N,t})\|}{\sqrt{N}}$$

tightly concentrates around its mean  $\chi(t)$ , uniformly over  $t \in [0, 1]$ .



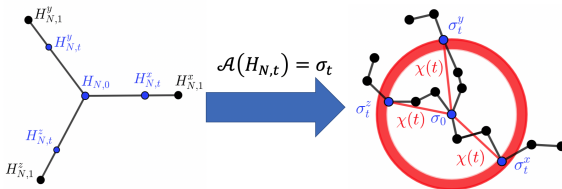
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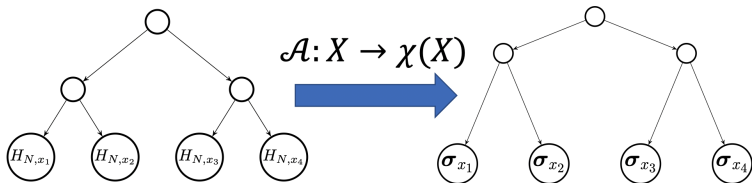


- Holds by concentration of measure if  $\mathcal{A}$  is Lipschitz in  $H_N$ .
- $\implies$  gradient descent, AMP, ... are overlap concentrated.

# Ultrametric Transformations from Overlap Concentration

- For ultrametric  $X$ , create correlated Hamiltonians  $(H_{N,x})_{x \in X}$ .
- Outputs  $\sigma_x = \mathcal{A}(H_{N,x})$  form a new ultrametric space  $\chi(X)$ :

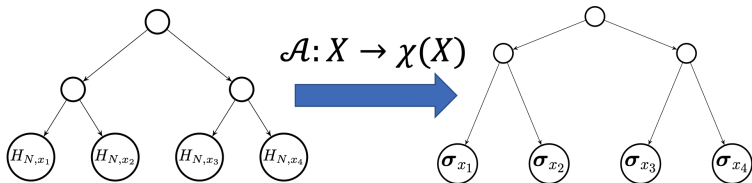
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- $\chi$  is continuous, so we can make  $\chi(X)$  **any ultrametric**.
- $\implies$  if  $\mathcal{A}$  achieves  $(\text{ALG} + \varepsilon)N$ , then there is a configuration  $(\sigma_x)_{x \in X}$  approximating **any desired ultrametric**  $\chi(X)$  with

$$H_{N,x}(\sigma_x) \geq (\text{ALG} + \varepsilon)N, \quad \forall x \in X.$$

# Ruling Out a Complicated Ultrametric

- Take  $\chi(X)$  a  $k$ -ary tree branching at depths  $[0, \delta, 2\delta, \dots, 1]$ .
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- Parisi formula upper bound generalizes to richer settings.  
Control average of  $H_{N,x}(\sigma_x)$  over all  $\chi(X)$ -configurations:

$$\max_{(\sigma_x)_{x \in X}} \left\{ \frac{1}{|X|} \sum_{x \in X} H_{N,x}(\sigma_x) : \frac{\|\sigma_{x_1} - \sigma_{x_2}\|}{\sqrt{N}} \approx d_{\chi(X)}(x_1, x_2) \quad \forall x_1, x_2 \in X \right\}.$$

- Upper bounds from any **increasing** function  $\zeta : [0, 1] \rightarrow \mathbb{R}^+$ , expressed as multi-dimensional generalizations  $\mathcal{P}_\xi^X$  of  $\mathcal{P}_\xi$ .



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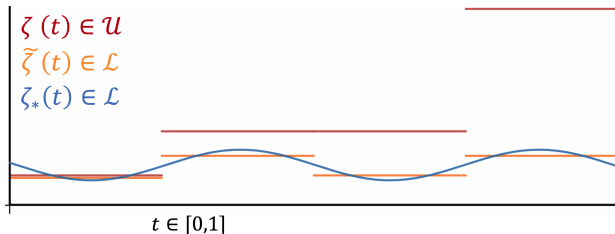
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- Eventually, obtain upper bound  $\mathcal{P}_\xi(\tilde{\zeta})$  in terms of the original Parisi functional.
- **Increasing**  $\zeta$  transforms into **no-longer increasing**  $\tilde{\zeta}$ .

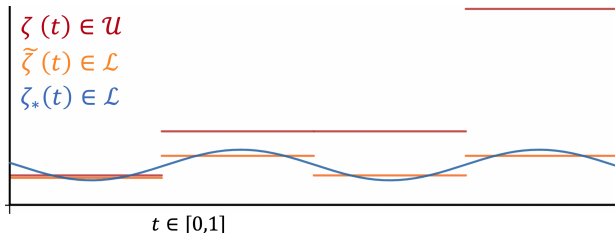
# Ruling Out a Complicated Ultrametric

- The ratio  $\tilde{\zeta}/\zeta$  is piece-wise constant, shrinks at each  $j\delta$ .
- Hence  $\tilde{\zeta}$  approximates any  $\zeta_* \in \mathcal{L}$ , get upper bound  $\text{ALG} + \varepsilon$ .



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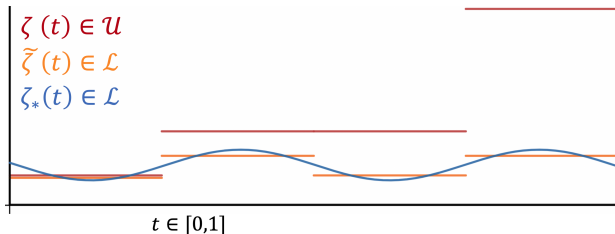
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## Theorem (Huang-S 21+)

*On the sphere, to rule out  $(\text{ALG} + \varepsilon)$  with forbidden ultrametric trees, the trees must contain full binary subtrees of unbounded size (as  $\varepsilon \rightarrow 0$ ).*

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- Result: ALG is the best asymptotic value achievable by overlap concentrated algorithms, so existing AMP algorithms are optimal within this class (modulo technical points).

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- Proof uses a **branching** OGP based on general ultrametric trees, which is in some sense necessary.
- A natural open direction: how generally does branching OGP identify the exact algorithmic threshold?