Algorithmic Threshold for Multi-Species Spin Glasses

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University of Waterloo Statistics and Actuarial Science Seminar

Joint work with Brice Huang (MIT)

Motivating Example: Tensor PCA

Fix $p \geq 2$. Recover signal $\boldsymbol{x}_0 \in S_N = \sqrt{N}\mathbb{S}^{N-1}$ from noisy tensor observation

$$\boldsymbol{T} = \lambda \boldsymbol{x}_0^{\otimes p} + \boldsymbol{G}^{(p)}, \qquad \boldsymbol{G}^{(p)} \in (\mathbb{R}^N)^{\otimes p} \text{ has i.i.d. } \mathcal{N}(0,1) \text{ entries}$$

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- Null model MLE is precisely optimization of a **spin glass**:

$$\boldsymbol{x}^{null} = \arg\max_{\boldsymbol{x} \in S_N} \langle \boldsymbol{G}^{(p)}, \boldsymbol{x}^{\otimes p} \rangle$$

Mean Field Spin Glasses

Polynomials $H_N : \mathbb{R}^N \to \mathbb{R}$ with **random** coefficients, e.g. random cubic

$$H_N(\boldsymbol{\sigma}) = \frac{1}{N} \sum_{i_1, i_2, i_3 = 1}^{N} g_{i_1, i_2, i_3} \cdot \sigma_{i_1} \sigma_{i_2} \sigma_{i_3} \qquad g_{i_1, i_2, i_3} \underset{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$$

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More generally, mix different degrees. For $\gamma_2, \gamma_3, \ldots \geq 0$,

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Gaussian process on $\mathbb{R}^N$ with covariance

$$\mathbb{E}[H_N(\boldsymbol{\sigma})H_N(\boldsymbol{\rho})] = N\xi(\langle \boldsymbol{\sigma}, \boldsymbol{\rho}\rangle/N), \qquad \xi(q) = \sum_{p=2}^{P} \gamma_p^2 q^p$$

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Goal: optimize H_N over sphere $S_N = \sqrt{N}\mathbb{S}^{N-1}$

Motivations and Connections

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- Neural networks, high-dimensional statistics (Hopfield 82, Gardner-Derrida 87/88, Talagrand 00/02, Choromanska-Henaff-Mathieu-Ben Arous-LeCun 15, Ding-Sun 18, Fan-Mei-Montanari 21)

The maximum of H_N

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- OPT: maximum value that **exists**?
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Theorem (Parisi 82, Talagrand 06/10, Panchenko 14, Auffinger-Chen 17)

The limiting maximum value

$$\mathrm{OPT} = \operatorname*{p-lim}_{N\to\infty} \frac{1}{N} \max_{\boldsymbol{\sigma}\in S_N} H_N(\boldsymbol{\sigma})$$

*exists and is given by the **Parisi formula*** $\mathsf{P}(\xi)$.

Efficient Optimization

- Today's goal: understand power of **efficient** algorithms $\mathcal{A}$ to optimize H_N. For $\boldsymbol{\sigma} = \mathcal{A}(H_N)$, what is max of

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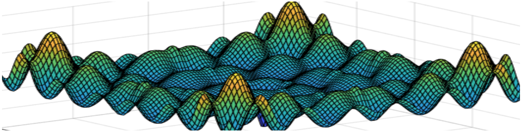
- Gradient descent, convex optimization don't cut it ☹
  - Rich landscapes, e^{cN} bad local maxima well below OPT (ABAČ 13, Subag 17)



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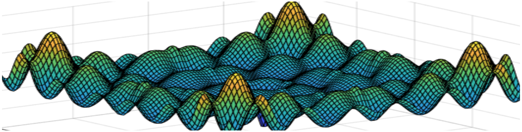

- Worst-case lower bounds overly pessimistic ☹
  - Adversarial H_N: $(\log^c N)$-approximation NP-hard (ABHKS 05, BBHKSZ 12)

Efficient Optimization: Some Approaches

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Can study **critical points** of H_N

- Pure p-spin models ($p \geq 3$): e^{cN} local maxima appear at value $E_\infty < \mathrm{OPT}$ (Auffinger-Ben Arous-Černý 13, Subag 17)
- Conjectured to obstruct e.g. gradient descent
- But no rigorous hardness implications

Informal Result

We determine sharp threshold ALG for a class of **Lipschitz** algorithms

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Result holds for yet more general **multi-species spin glasses**

Overlap Gap Property

💡 solution geometry **clustering** $\Rightarrow$ rigorous hardness for **stable** algorithms

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- Max independent set in random sparse graphs (Gamarnik-Sudan 14, Rahman-Virág 17, Gamarnik-Jagannath-Wein 20, Wein 20)
- Random (NAE-)k-SAT (Gamarnik-Sudan 17, Bresler-Huang 21)
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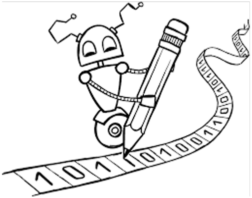
Overlap: $\langle \boldsymbol{\sigma}, \boldsymbol{\rho} \rangle / N \in [-1, 1]$

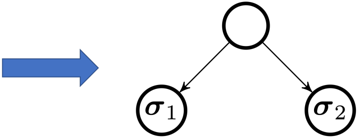
Overlap gap: no high-value $\boldsymbol{\sigma}, \boldsymbol{\rho}$ have **medium** overlap $\in [\nu_1, \nu_2]$

- Means high-value points are either close together or far apart

Classic OGP (Gamarnik-Sudan 14)

1. Stable algorithm $\mathcal{A}$ reaching $E \Rightarrow$ 2 points of value E with **medium overlap**





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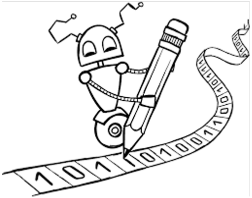
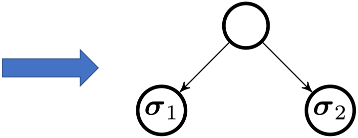
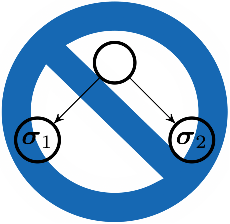


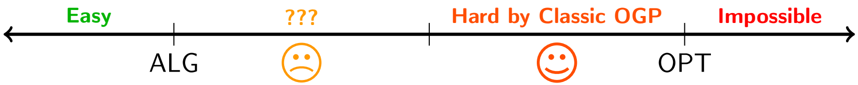


   Construct by partially rerandomizing $\mathcal{A}$

2. **Overlap gap** $\Rightarrow$ this pair does not exist. So $\mathcal{A}$ cannot reach E



Classic OGP to Multi-OGP



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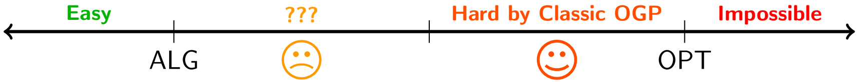

Multi-OGP: more complex forbidden structure

Classic OGP to Multi-OGP

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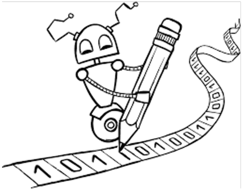
Multi-OGP: more complex forbidden structure

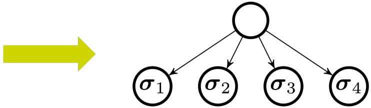
Can we push hardness all the way to ALG?

Star OGP (Rahman-Virág 17)

For max independent set

1. Stable algorithm $\mathcal{A}$ reaching $E \Rightarrow$ constellation of points of value E





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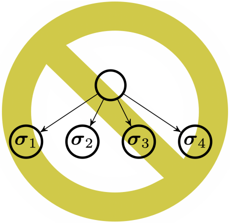

Ladder OGP (Wein 20, Bresler-Huang 21)

For max independent set, random k-SAT

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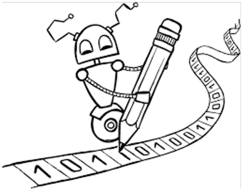
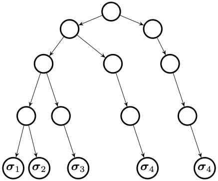
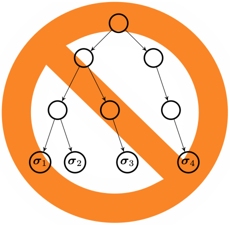




2. Such a constellation does not exist. So $\mathcal{A}$ cannot reach E



Overview of Main Result (Huang-**S** 21, 23+)

- We show that for spin glasses, **Branching OGP** gives tight hardness
  - Matches value ALG of best algorithm

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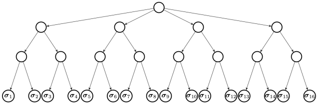

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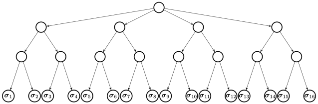

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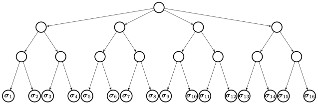

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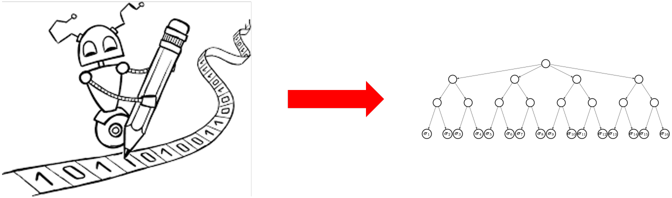
  - View $\mathcal{A}$ as map from $(g_{1,1}, \ldots, g_{N,N}, g_{1,1,1}, \ldots)$ to $\mathbb{R}^N$ (with L^2 distance)
  - Includes:
    - $O(1)$ rounds of gradient descent or any constant order method
    - Langevin dynamics for $e^{\beta H_N}$ for $O(1)$ time
    - The algorithm attaining ALG

1. $O(1)$-Lipschitz algorithm $\mathcal{A}$ reaching E $\Rightarrow$ ultrametric of points of value E



Construct from correlated Hamiltonian ensemble (more later)

Branching OGP (Huang-**S** 21)

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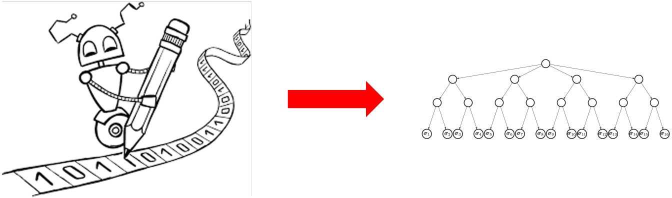

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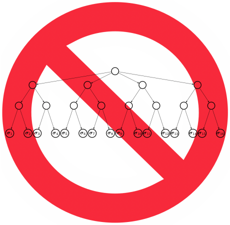

The Algorithmic Threshold

Theorem (Subag 18)

An efficient algorithm finds $\boldsymbol{\sigma}$ such that

$$\frac{1}{N} H_N(\boldsymbol{\sigma}) \geq \mathsf{ALG} \equiv \int_0^1 \xi''(q)^{1/2} \mathrm{d}q.$$

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Tight answer for even models, but brittle proof using **Guerra's interpolation**

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- New proof avoids Guerra's interpolation
- Same method works for multi-species spin glasses (described later)
  - In these models, OPT not always known! (Because Guerra's interpolation fails)

Subag's Algorithm (Hessian Ascent)

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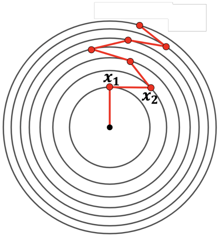

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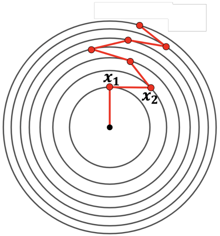

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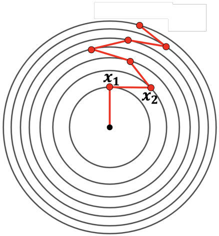

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Can be implemented as $O(1)$-Lipschitz algorithm (El Alaoui-Montanari-Sellke 20)

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- If $\|\boldsymbol{x}\|_2 = \sqrt{qN}$, tangential Hessian $\nabla^2 H_N(\boldsymbol{x})_{\boldsymbol{x}^\perp}$ has law $\xi''(q)^{1/2} \times GOE_{N-1}$

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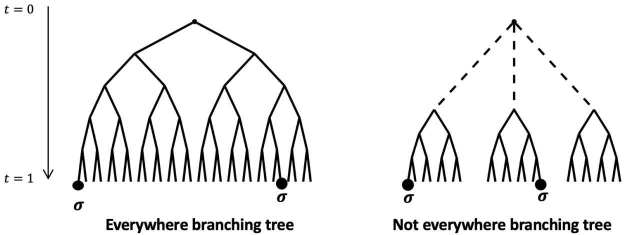
- Although $\boldsymbol{x}^t$ depends on H_N, ok by **uniform** lower bound on $\lambda_{\max}(H_N(\boldsymbol{x})_{\boldsymbol{x}^\perp})$ for all $\|\boldsymbol{x}\|_2 = \sqrt{qN}$

Connection to Physics Theory

- Approximate maxima of H_N are **ultrametric**, i.e. isometric to a tree



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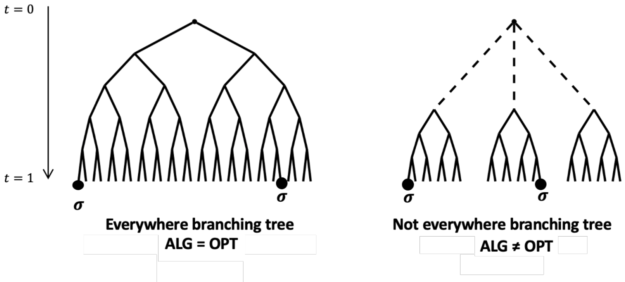
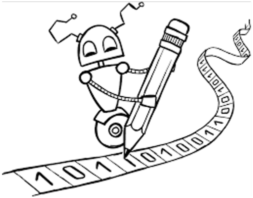


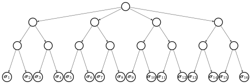
Subag's algorithm attains OPT iff branching occurs at all depths

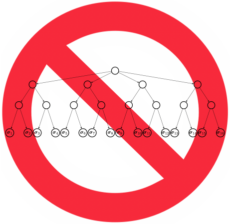
- Intuition: algorithm traces root-to-leaf path of tree

Branching OGP

Subag's algorithm reaches ALG. We next see how to show hardness beyond ALG

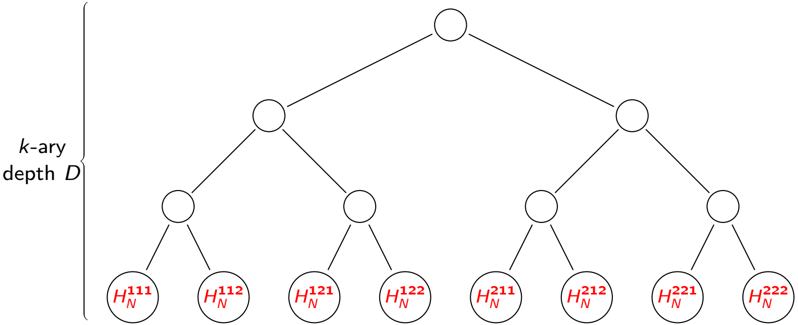






Hierarchically Correlated Hamiltonians

Generate tree of Hamiltonians $(H_N^u)_{u\in[k]^D}$



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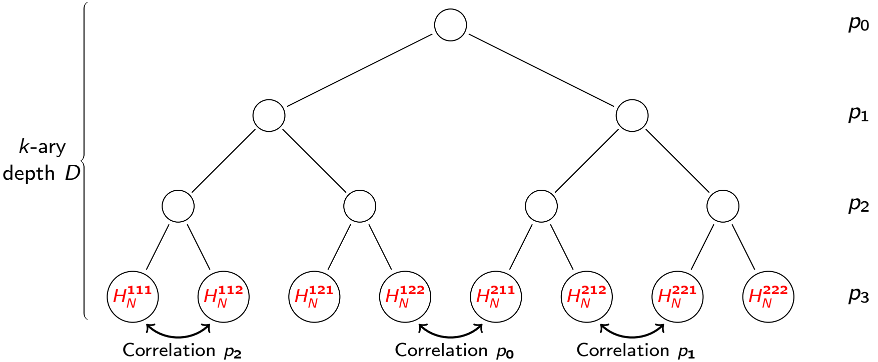

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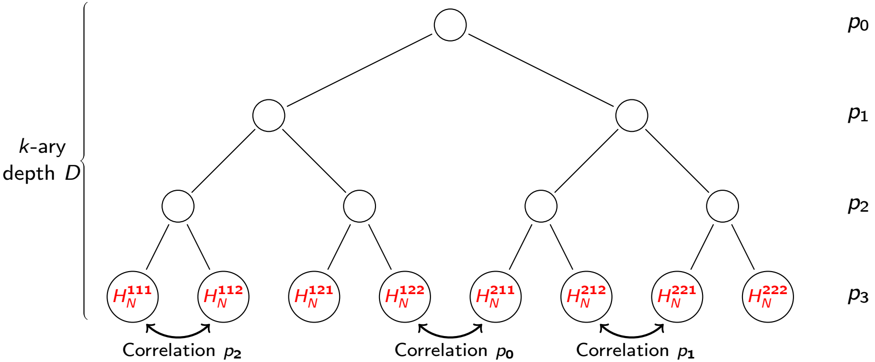

$$k, D \in \mathbb{N} \text{ large, } 0 \le p_0 < p_1 < \cdots < p_D = 1$$

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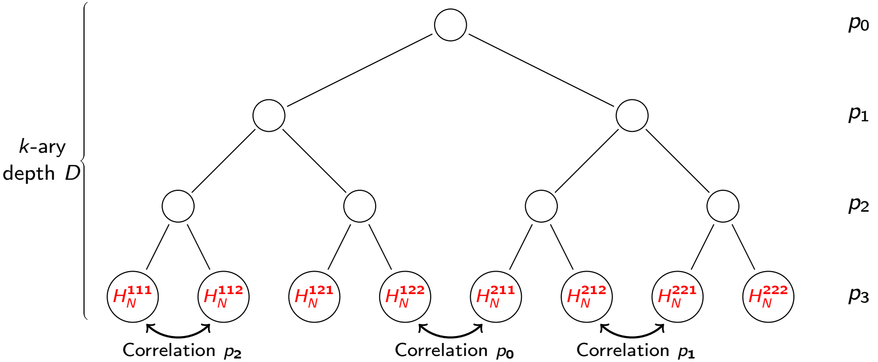

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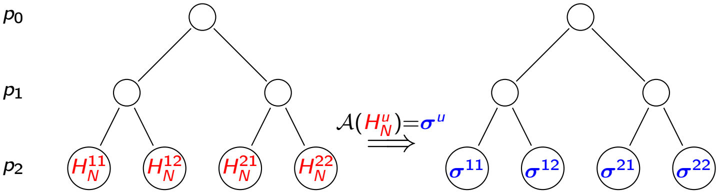
Vocab: "$(H_N^u)_{u\in[k]^D}$ has correlation $\vec{p} = (p_0, \dots, p_D)$"

Lipschitz Algorithms to Ultrametric Trees

Let $\mathcal{A}$ be $O(1)$-Lipschitz



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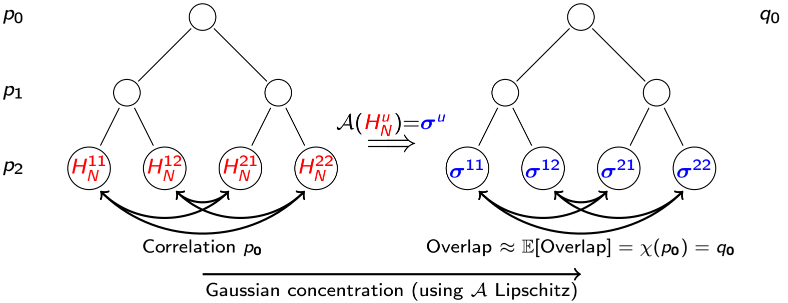

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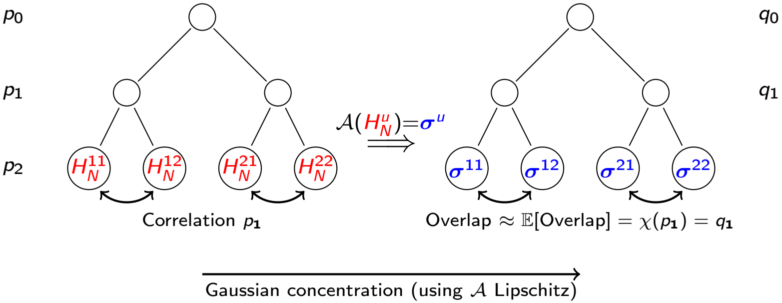

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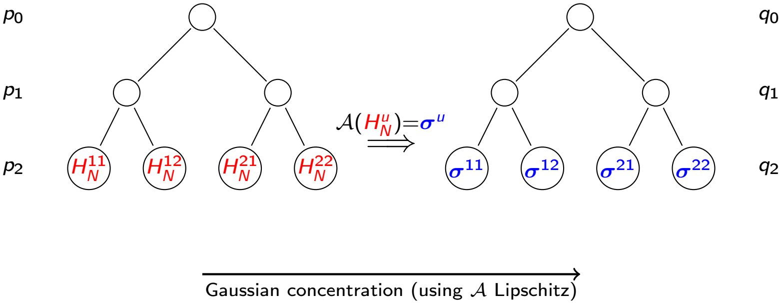

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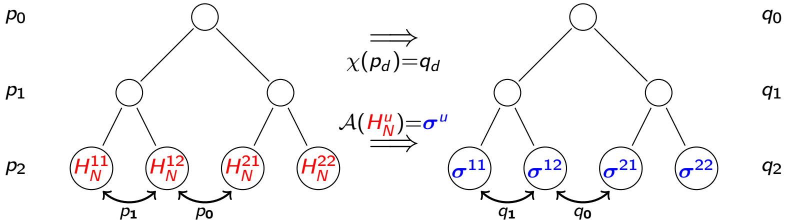

$\longrightarrow$
Gaussian concentration (using $\mathcal{A}$ Lipschitz)

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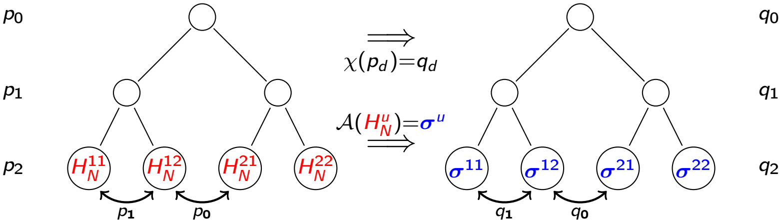

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Vocab: "$(\boldsymbol{\sigma}^u)_{u\in[k]^D}$ has geometry $\vec{q} = (q_0, \ldots, q_D)$"

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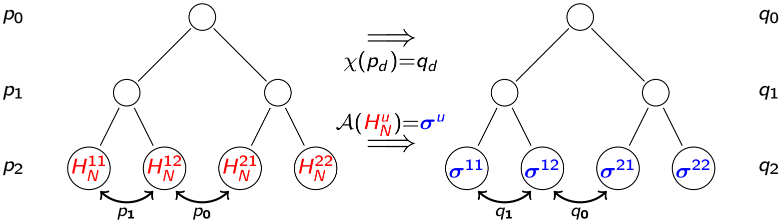

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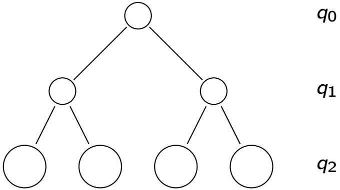
χ continuous. Can choose $\vec{p}$ to achieve **any** $0 \le q_0 < \cdots < q_D = 1$

Lipschitz Algorithms to Ultrametric Trees



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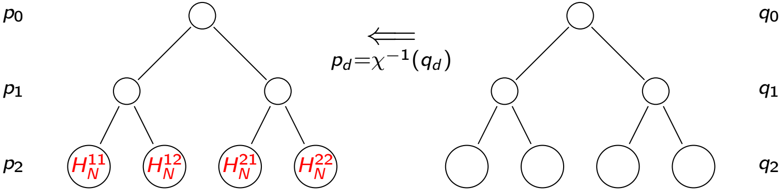

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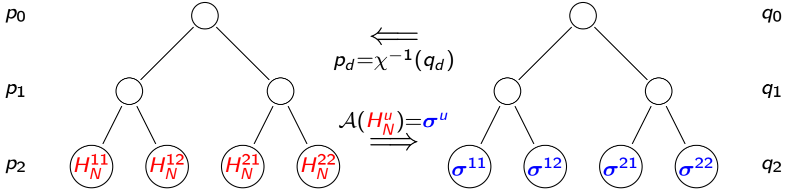

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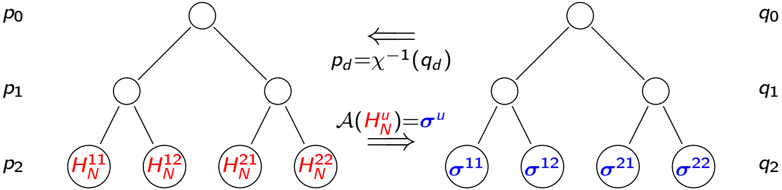

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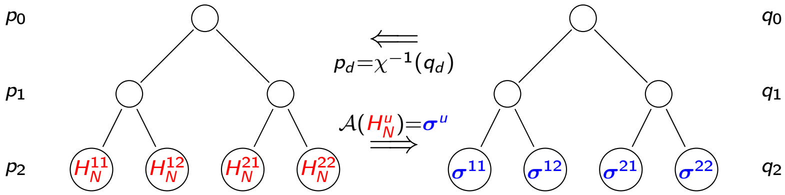

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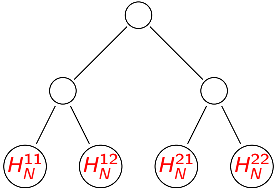
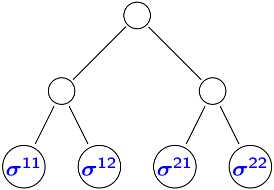
- *For* ***some*** $\vec{p}$, *there is a tree constellation with value* E *and geometry* $\vec{q}$

The value BOGP





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$\delta = 1/D$

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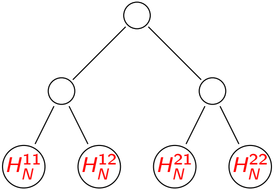

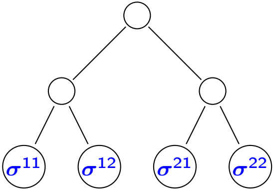

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$$\text{TreeValue}(\vec{p}) = \operatorname*{p-lim}_{N \to \infty} \max_{\substack{(\boldsymbol{\sigma}^u)_{u \in [k]^D} \\ \text{geometry } \vec{q}}} \frac{1}{k^D} \sum_{u \in [k]^D} \frac{1}{N} H_N^u(\boldsymbol{\sigma}^u)$$

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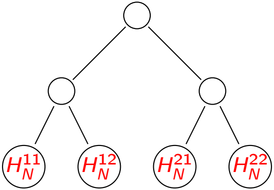

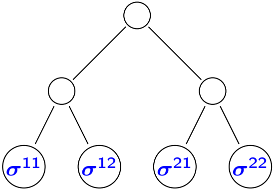

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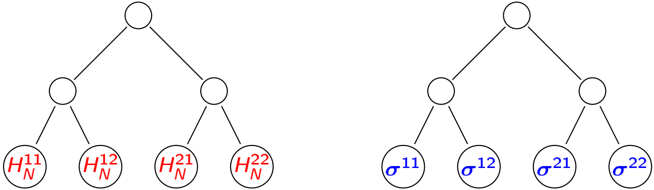

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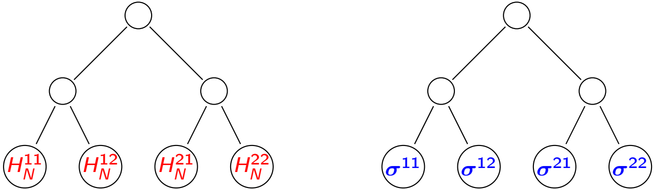

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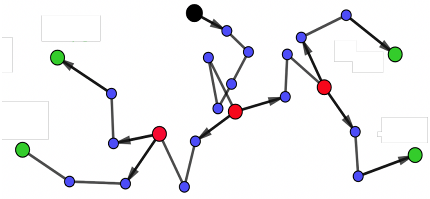

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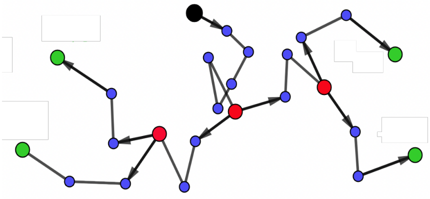

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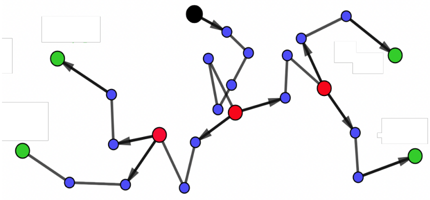
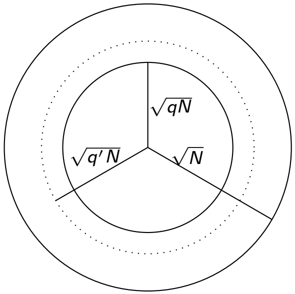


- This tree is built in a greedy way
- Main claim: best way to construct tree is greedy
    - "Can't plan ahead so that my gain at 20th level is unusually big"
    - Proved by **uniform concentration**

Uniform Concentration

Configuration $\boldsymbol{x}, \boldsymbol{x}^1, \dots, \boldsymbol{x}^k$:



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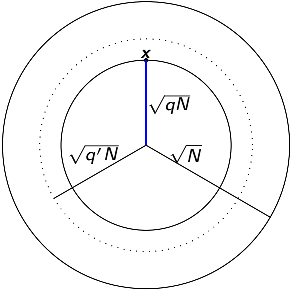

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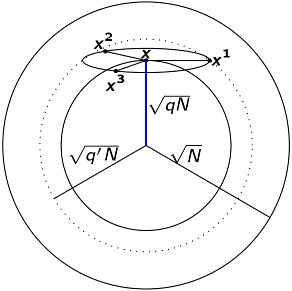

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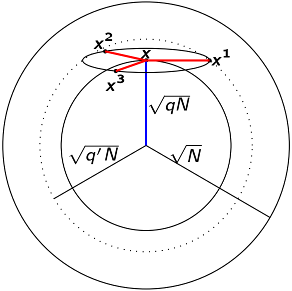

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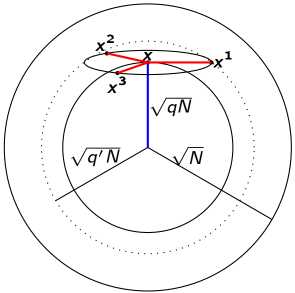

$$F(\boldsymbol{x}) = \max_{\boldsymbol{x}^1,\dots,\boldsymbol{x}^k} \frac{1}{kN} \sum_{i=1}^{k} (H_N(\boldsymbol{x}^i) - H_N(\boldsymbol{x}))$$

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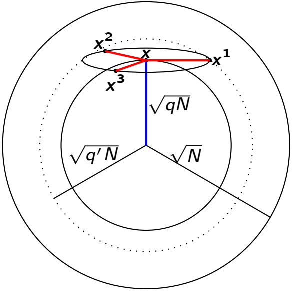

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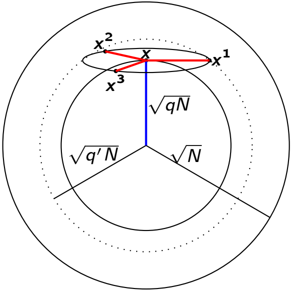

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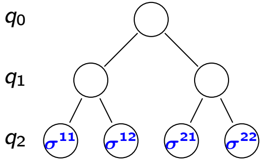
No $\|\boldsymbol{x}\|_2 = \sqrt{qN}$ is unusually good for building a tree, so might as well be greedy.

Upper Bounding the Tree Value

Let interior $\boldsymbol{\sigma}^u$ be recursive barycenters:
$\boldsymbol{\sigma}^u = \frac{1}{k}\sum_{i=1}^{k} \boldsymbol{\sigma}^{ui}$



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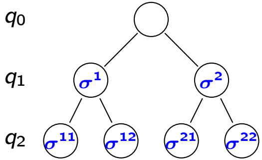

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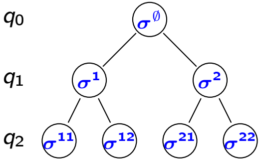

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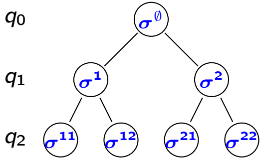

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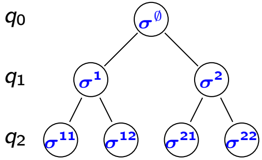

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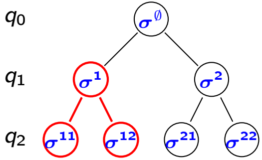

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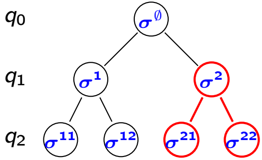

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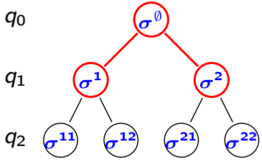

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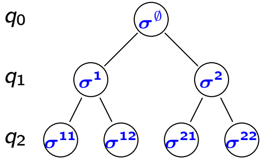

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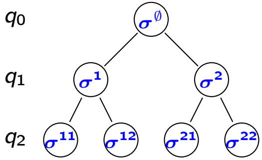

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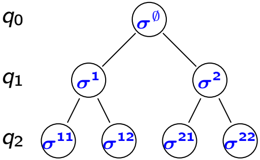

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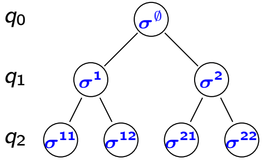

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Theorem (Huang-S 21)

If an ultrametric constellation is forbidden at value $\mathrm{ALG} + \varepsilon$*, it must contain a complete binary subtree of diverging depth as* $\varepsilon \to 0$*.*

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- Example: **bipartite SK model**

$$H_N(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{\sqrt{N}} \langle \boldsymbol{G}\boldsymbol{x}, \boldsymbol{y} \rangle, \qquad \boldsymbol{G} \in \mathbb{R}^{N \times N} \text{ i.i.d. } \mathcal{N}(0,1) \text{ entries}$$

or higher-order polynomials

$$H_N(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{N} \langle \boldsymbol{G}, \boldsymbol{x}^{\otimes 3} \rangle + \frac{1}{N} \langle \boldsymbol{G}', \boldsymbol{x} \otimes \boldsymbol{y}^{\otimes 2} \rangle, \qquad \boldsymbol{G}, \boldsymbol{G}' \in (\mathbb{R}^N)^{\otimes 3}$$

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- Interaction weights $\gamma_2, \gamma_3, \ldots$ now $(\gamma_{s_1,s_2})_{s_1,s_2 \in \mathscr{S}}, (\gamma_{s_1,s_2,s_3})_{s_1,s_2,s_3 \in \mathscr{S}}, \ldots$

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$$[N] = \mathcal{I}_1 \cup \cdots \cup \mathcal{I}_r, \qquad |\mathcal{I}_s| = \lambda_s N$$

- Interaction weights $\gamma_2, \gamma_3, \ldots$ now $(\gamma_{s_1,s_2})_{s_1,s_2 \in \mathscr{S}}, (\gamma_{s_1,s_2,s_3})_{s_1,s_2,s_3 \in \mathscr{S}}, \ldots$
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- ALG has richer behavior than in one species

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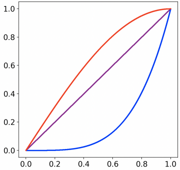

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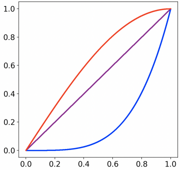

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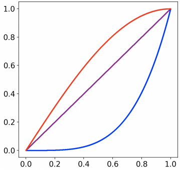

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- Each Φ gives algorithm taking small orthogonal steps **in each species**
- Algorithm value

$$\mathbb{A}(\Phi) \equiv \sum_{s \in \mathscr{S}} \lambda_s \int_0^1 \sqrt{(\partial_{q_s}\xi \circ \Phi)'(q)\Phi_s'(q)}\, \mathrm{d}q$$

Multi-Species Algorithmic Threshold

Theorem (Huang-**S** 23+)

Define

$$\mathrm{ALG} = \sup_{\substack{\Phi:[0,1]\to[0,1]^{\mathscr{S}} \\ \textit{increasing, differentiable}}} \sum_{s\in\mathscr{S}} \lambda_s \int_0^1 \sqrt{(\partial_{q_s}\xi \circ \Phi)'(q)\Phi_s'(q)}\,\mathrm{d}q$$

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- *An explicit $O(1)$-Lipschitz algorithm achieves* ALG *w.h.p.*
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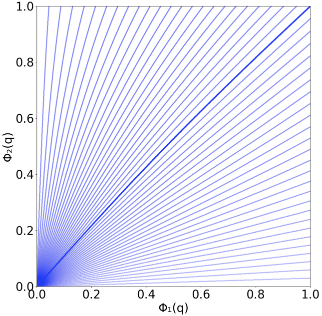
Theorem (Huang-**S** 23+)

The variational formula has a maximizer Φ, which solves an explicit ODE.

Variational Problem Example

Consider $(\lambda_1, \lambda_2) = (1/3, 2/3)$ and

$$\xi(q_1, q_2) = (\lambda_1 q_1)^2 + (\lambda_1 q_1)(\lambda_2 q_1) + (\lambda_2 q_1)^2 + (\lambda_1 q_1)^4 + (\lambda_1 q_1)(\lambda_2 q_2)^3$$

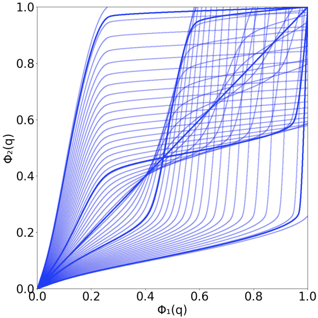


Some ODE solutions. Optimal $\Phi : [0, 1] \to [0, 1]^2$ in bold

Algorithmic Symmetry Breaking

Optimal Φ may be asymmetric, even when model is symmetric!

$$\lambda_1 = \lambda_2 = \frac{1}{2}, \quad \xi(q_1, q_2) = (3q_1)^2 + (3q_1)(3q_2) + (3q_2)^2 + (3q_1)^4 + (3q_2)^4$$



The plot thickens...

Pure Multi-Species Models

- Models where
$$\xi(q_1, \dots, q_r) = q_1^{a_1} q_2^{a_2} \cdots q_r^{a_r}$$
- Example: bipartite SK $\xi(q_1, q_2) = q_1 q_2$

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- Optimal Φ is **polynomial**

$$\Phi(q) = (q^{b_1}, \dots, q^{b_r})$$

- In this case, $\text{ALG} = E_\infty$ has explicit non-variational formula.
- Langevin dynamics is believed to reach the same threshold!

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- We determine algorithmic threshold of $O(1)$-Lipschitz algorithms for optimizing multi-species spherical spin glasses

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Thank you!

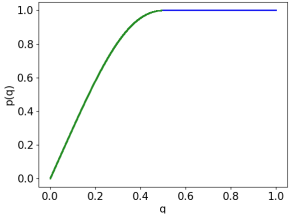
Models with Linear Terms

Suppose model has 1-spin interaction (external field)

$$H_N(\boldsymbol{\sigma}) = \sum_{p=\color{red}{1}}^{P} \frac{\gamma_p}{N^{(p-1)/2}} \langle \boldsymbol{G}^{(p)}, \boldsymbol{\sigma}^{\otimes p} \rangle \qquad \xi(q) = \sum_{p=\color{red}{1}}^{P} \gamma_p^2 q^p$$

Then

$$\mathrm{ALG} = \mathrm{BOGP} = \sup_{\substack{p:[0,1]\to[0,1] \\ \text{increasing, differentiable}}} \int_0^1 \sqrt{(p\xi')'(q)}\,\mathrm{d}q$$



Optimal p for $\xi(q) = q^4 + q$

Multi-Species Algorithmic Threshold with Linear Terms

Theorem (Huang-S 23+)

Define

$$\mathsf{ALG} = \sup_{\substack{p:[0,1]\to[0,1] \\ \Phi:[0,1]\to[0,1]^{\mathscr{S}} \\ \textit{increasing, differentiable}}} \sum_{s\in\mathscr{S}} \lambda_s \int_0^1 \sqrt{(p \times \partial_{q_s}\xi \circ \Phi)'(q)\Phi_s'(q)}\, \mathrm{d}q$$

- *An explicit $O(1)$-Lipschitz algorithm achieves* ALG *w.h.p.*
- *No $O(1)$-Lipschitz algorithm beats* ALG *with probability e^{-cN}*

Theorem (Huang-S 23+)

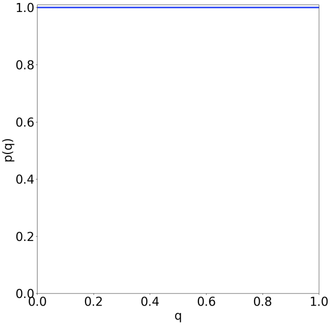
This variational problem has a maximizer (p, Φ).

- *The maximizer solves an explicit ODE.*
- *If ξ has no 1-spin interactions, then $p \equiv 1$.*

Variational Problem Example: No Linear Term

Consider $(\lambda_1, \lambda_2) = (1/3, 2/3)$

$$\xi(q_1, q_2) = (\lambda_1 q_1)^2 + (\lambda_1 q_1)(\lambda_2 q_1) + (\lambda_2 q_1)^2 + (\lambda_1 q_1)^4 + (\lambda_1 q_1)(\lambda_2 q_2)^3$$



Optimal $p : [0,1] \to [0,1]$

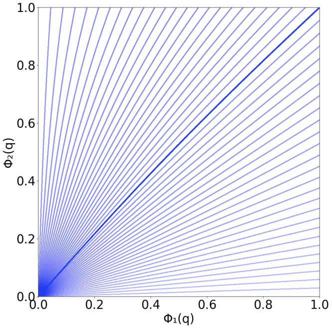
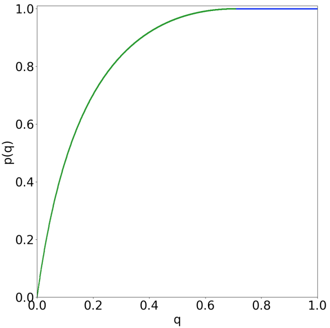


Image of optimal $\Phi : [0,1] \to [0,1]^2$ in bold

Variational Problem Example: Small Linear Term

Consider $(\lambda_1, \lambda_2) = (1/3, 2/3)$

$$\xi(q_1, q_2) = (\lambda_1 q_1)^2 + (\lambda_1 q_1)(\lambda_2 q_1) + (\lambda_2 q_1)^2 + (\lambda_1 q_1)^4 + (\lambda_1 q_1)(\lambda_2 q_2)^3 + 0.05(\lambda_1 q_1) + 0.5(\lambda_2 q_2)$$



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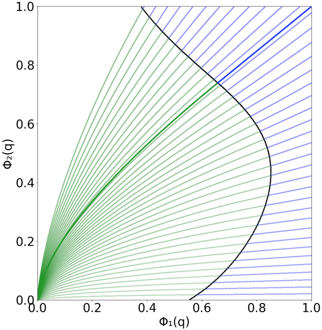

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Variational Problem Example: Large Linear Term

Consider $(\lambda_1, \lambda_2) = (1/3, 2/3)$

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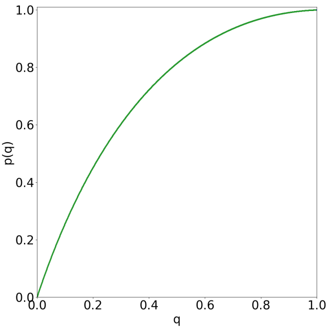
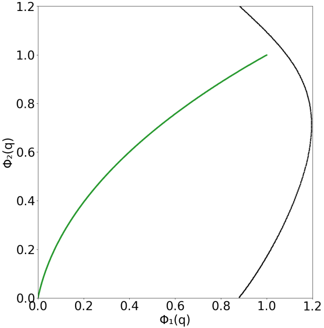


Optimal $p : [0,1] \to [0,1]$



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