A Positivity-First Approach to Sum-of-Squares (Lower Bounds) Over the Hypercube

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I. Problem Setting

$$\mathsf{OPT}(\boldsymbol{W}) := \max_{\boldsymbol{x} \in \{\pm 1\}^N} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}$$

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But is it easy or hard to **compute** $\mathsf{OPT}(\boldsymbol{W})$?

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- Local search
- Relax & round
- Message passing (Ahmed's talk—can get near-equality!)

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2. Certification: Compute $c(\boldsymbol{W}) \in \mathbb{R}$ with $\mathsf{OPT}(\boldsymbol{W}) \leq c(\boldsymbol{W})$ *for all* $\boldsymbol{W}$, and as small as possible.

- LP relaxations (Sherali-Adams)
- SDP relaxations (Goemans-Williamson, sum-of-squares)

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↑

This talk—what happens here?

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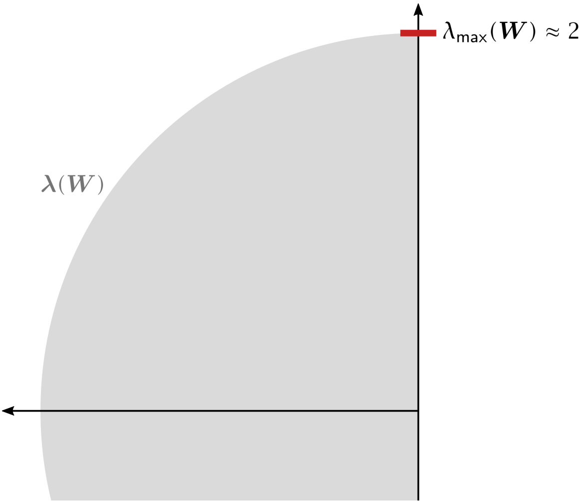
\end{aligned}$$

Afonso's talk (sort of)—indirect evidence suggests among poly(N)-time certificates this is **optimal!**

Search-Certification Gap in SK Hamiltonian



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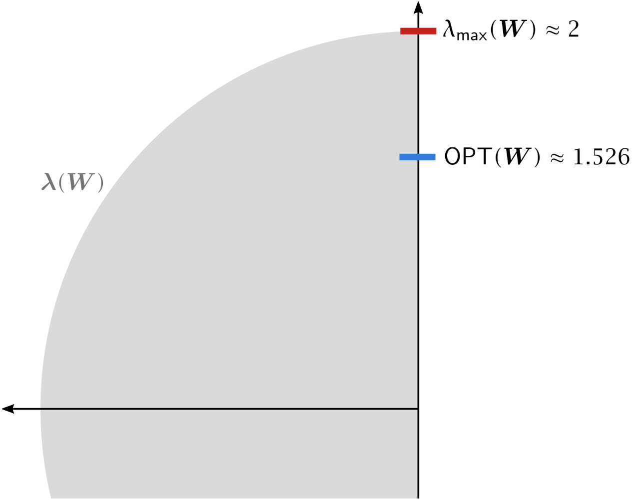

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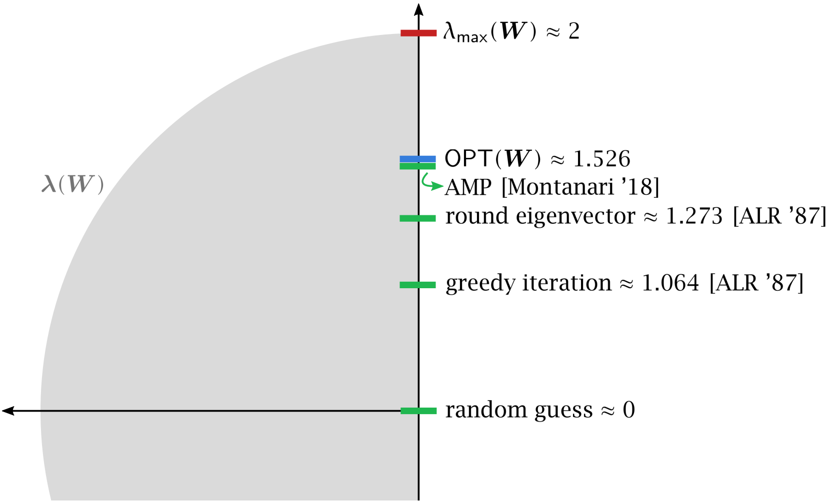

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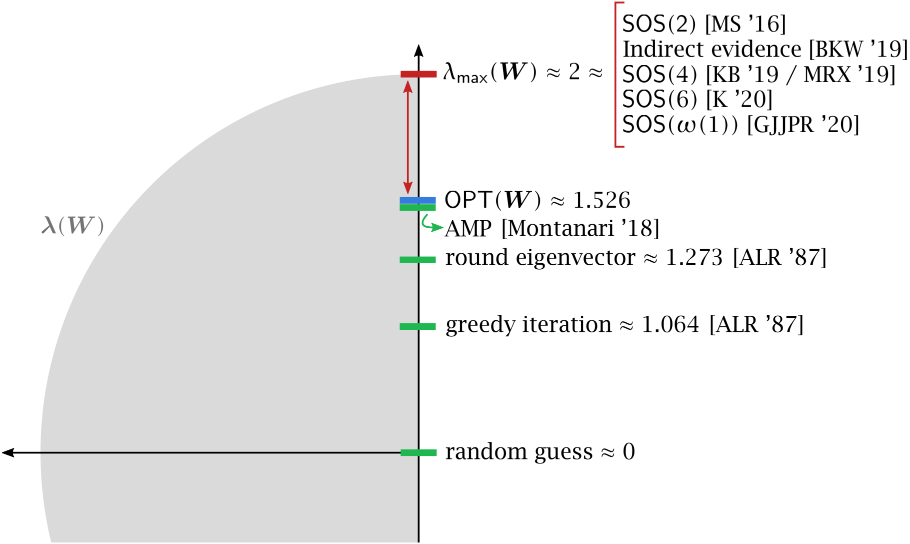

II. Sum-of-Squares Lower Bounds

Sum-of-Squares (SOS) Relaxations

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$\widetilde{\mathbb{E}} : \mathbb{R}[\boldsymbol{x}]_{\leq 2d} \to \mathbb{R}$ is a degree $2d$ pseudoexpectation if

- Linear
- $\widetilde{\mathbb{E}}[1] = 1$ ("normalization")
- $\widetilde{\mathbb{E}}[(x_i^2 - 1)p(\boldsymbol{x})] = 0$ ("ideal annihilation")
- $\widetilde{\mathbb{E}}[p(\boldsymbol{x})^2] \geq 0$ ("positivity")

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Optimizing over these gives a certificate:

$$\mathsf{OPT}(\boldsymbol{W}) \leq \mathsf{SOS}_{2d}(\boldsymbol{W}) := \max_{\substack{\widetilde{\mathbb{E}} \text{ degree } 2d \\ \text{pseudoexpectation}}} \widetilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}]$$

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Optimizing over these gives a **very powerful** certificate:

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To *prove* this, we need to build $\widetilde{\mathbb{E}}$ with

$$\lambda_{\mathsf{max}}(\boldsymbol{W}) \cdot N \approx \widetilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}] \approx \langle \widetilde{\mathbb{E}}[\boldsymbol{x}\boldsymbol{x}^\top], \boldsymbol{W} \rangle$$

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Since $\mathsf{Tr}(\widetilde{\mathbb{E}}[\boldsymbol{x}\boldsymbol{x}^\top]) = N$, $\widetilde{\mathbb{E}}[\boldsymbol{x}\boldsymbol{x}^\top]$ needs most of its mass near the top few eigenvectors of $\boldsymbol{W}$. Roughly:

$\widetilde{\mathbb{E}}[\boldsymbol{x}\boldsymbol{x}^\top] \underset{\sim}{\propto}$ uniformly random low-dimensional projection

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Argue using Bayesian ideas (pseudocalibration ~ Jess' talk), symmetry, or whatever else to predict for each monomial,

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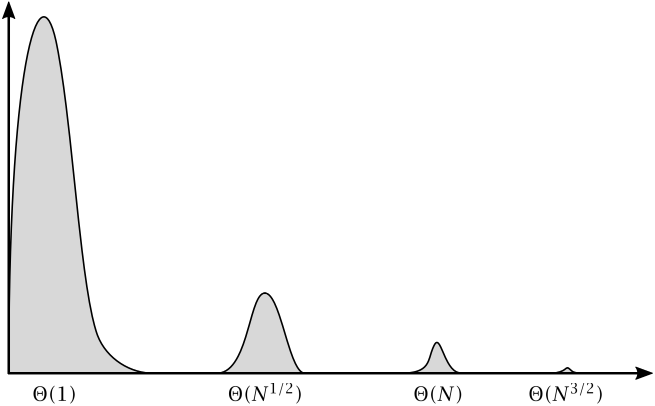
That leaves just one little detail...

$$\text{positivity} \iff \underbrace{\left(\widetilde{\mathbb{E}}[\boldsymbol{x}^S \boldsymbol{x}^T]\right)_{S,T \in \binom{[N]}{\leq d}}}_{\text{pseudomoment matrix}} \succeq \boldsymbol{0}$$

These arguments are hard!

Why Entries-First Makes Things Hard

There is not much intuition for *why* we have positivity, and the matrices involved have complicated *multiscale* spectra:



“Positivity First” Using Surrogate Tensors

A different approach: build a random *surrogate* tensor $\boldsymbol{G}^{(d)} \in (\mathbb{R}^N)^{\otimes d}$ for $\boldsymbol{x}^{\otimes d}$, and take

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Otherwise, take $\boldsymbol{G}^{(d)}$ *as random as possible* $\rightsquigarrow$ condition canonical gaussian symmetric tensor.

What Comes Out

The result, upon squinting the right way, has the joint symmetry in $S + T$ we wanted! This has a diagrammatic interpretation:

$$\mathbb{E}[G_S^{(d)} G_T^{(d)}] \approx \sum_{F \text{ forest on } 2d \text{ leaves}} \mu(F) p_F(\boldsymbol{W}, S + T)$$

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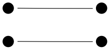
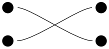
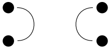
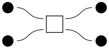
Ex. If $2d = 4$, $S = \{i, j\}$, $T = \{k, \ell\}$, $\boldsymbol{M} \approx \widetilde{\mathbb{E}}[\boldsymbol{x}\boldsymbol{x}^\top]$ is the rescaled projector to top eigenspace of $\boldsymbol{W}$, then

$M_{ik}M_{j\ell}$ $\qquad$ $M_{i\ell}M_{jk}$ $\qquad$ $M_{ij}M_{k\ell}$ $\qquad$ $\sum_{a=1}^{N} M_{ia}M_{ja}M_{ka}M_{\ell a}$

Cancellations for Ideal Constraint: $i = j$

 +  +  − 2 

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Therefore, $\widetilde{\mathbb{E}}[x_i^2 x_k x_\ell] \approx \widetilde{\mathbb{E}}[x_k x_\ell]$.

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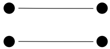

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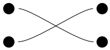

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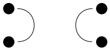

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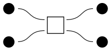

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Therefore, $\widetilde{\mathbb{E}}[x_i^4] \approx 1$.

Remarkably, $\mu(F)$ is a *Möbius function* of a partial ordering of forests, meaning such things always happen!

Actual Results

- If instead of $\widetilde{\mathbb{E}}[\boldsymbol{x}\boldsymbol{x}^\top] \approx$ random *low-rank* projection want *high-rank* $(N - o(N))$ projection, then can build $\widetilde{\mathbb{E}}$ of degree $\sim \log N / \log\log N$.

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- Driving the proofs are the combinatorics relating the conditional distribution of $\boldsymbol{G}^{(d)}$ (positivity constraints) with the Möbius function (ideal constraints).

Thank You!

Sketch of Conditioning Calculations

If $\boldsymbol{P}$ is projection to top eigenspace, $P_{ij} = \langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle$, then amounts to calculating projection to the subspace

$$\mathsf{span}(\{\boldsymbol{v}_1 \odot \boldsymbol{v}_1, \ldots, \boldsymbol{v}_N \odot \boldsymbol{v}_N\}) \odot \mathsf{Sym}^{d-2}(\mathbb{R}^N) \subset \mathsf{Sym}^{d}(\mathbb{R}^N)$$

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In homogeneous polynomials, this is the *ideal* of $\langle \boldsymbol{v}_i, \boldsymbol{z} \rangle^2$.

The Frobenius inner product becomes the *apolar inner product*, and, remarkably, the orthogonal complement is the *multiharmonic polynomials* $\langle \boldsymbol{v}_i, \boldsymbol{\partial} \rangle^2 p(\boldsymbol{z}) = 0$.

Sketch of Conditioning Calculations

If $\boldsymbol{P}$ is projection to top eigenspace, $P_{ij} = \langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle$, then amounts to calculating projection to the subspace

$$\mathsf{span}(\{\boldsymbol{v}_1 \odot \boldsymbol{v}_1, \ldots, \boldsymbol{v}_N \odot \boldsymbol{v}_N\}) \odot \mathsf{Sym}^{d-2}(\mathbb{R}^N) \subset \mathsf{Sym}^{d}(\mathbb{R}^N)$$

In homogeneous polynomials, this is the *ideal* of $\langle \boldsymbol{v}_i, \boldsymbol{z} \rangle^2$.

The Frobenius inner product becomes the *apolar inner product*, and, remarkably, the orthogonal complement is the *multiharmonic polynomials* $\langle \boldsymbol{v}_i, \boldsymbol{\partial} \rangle^2 p(\boldsymbol{z}) = 0$.

Using an analogy with harmonic polynomials, we can heuristically calculate by suggesting a “Green’s function” for this system.