Gramian constructions of SOS lower bounds and the spectra of pseudomoments

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I. Introduction

Certifying Bounds on Quadratic Forms

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Goal: Build efficient algorithms taking in $\boldsymbol{W} \in \mathbb{R}^{n \times n}_{\mathsf{sym}}$ and outputting upper bounds on

$$\mathsf{opt}(\boldsymbol{W}) := \max_{\boldsymbol{x} \in \{\pm 1\}^n} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}.$$

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Applications and motivations:

- Maximum cut in graphs
- Community detection in graphs
- Statistical physics: ground states of Ising models (Sherrington-Kirkpatrick model especially prominent)
- Statistics toy problems:
  - Spiked matrix models
  - "Planted" vector in a random subspace

Sum-of-Squares: Algebraic Proof Formulation

Familiar to this audience: in time $n^{O(D)}$, can efficiently solve the (even) degree D SOS relaxation:

$$
\begin{aligned}
\text{minimize} \quad & c \\
\text{subject to} \quad & c - \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x} = \sum_{i=1}^{n} p_i(x)(x_i^2 - 1) + \sum_j s_j(x)^2, \\
& \deg(p_i) \leq D - 2, \\
& \deg(s_j) \leq D/2.
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Can be written as a semidefinite program by relating polynomials $q(\boldsymbol{x})$ to representing matrices $\boldsymbol{Q}$ with

$$q(\boldsymbol{x}) = \boldsymbol{m}(\boldsymbol{x})^\top \boldsymbol{Q}\, \boldsymbol{m}(\boldsymbol{x}),$$

for $\boldsymbol{m}(\boldsymbol{x})$ the vector of low-degree monomials in $x_1, \dots, x_n$.

Sum-of-Squares: Pseudomoment Formulation

Maybe slightly less familiar: a formulation of the convex dual popular in theoretical computer science,

$$\begin{array}{ll} \text{maximize} & \widetilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}] \\ \text{subject to} & \widetilde{\mathbb{E}} : \mathbb{R}[x_1, \dots, x_n]_{\leq D} \to \mathbb{R} \\ & \widetilde{\mathbb{E}} \text{ linear}, \\ & \widetilde{\mathbb{E}}[1] = 1, \\ & \widetilde{\mathbb{E}}[(x_i^2 - 1)p(x)] = 0 \text{ for all } i \in [n], \\ & \widetilde{\mathbb{E}}[s(x)^2] \geq 0. \end{array}$$

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By linearity, enough to give **pseudomoments** $\widetilde{\mathbb{E}}[x_{i_1} \cdots x_{i_d}]$, and positivity $\Leftrightarrow$ pseudomoment matrix $\boldsymbol{M} \succeq \boldsymbol{0}$, where

$$M_{(i_1,\dots,i_{d_1}),(j_1,\dots,j_{d_2})} := \widetilde{\mathbb{E}}[x_{i_1} \cdots x_{i_{d_1}} x_{j_1} \cdots x_{j_{d_2}}].$$

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General questions: How large do we need to take D for SOS to work well? What properties of $\boldsymbol{W}$ control this?

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Proof strategy: Construct a $\widetilde{\mathbb{E}}$, or equivalently a pseudomoment matrix $\boldsymbol{M}$, that is feasible for high-degree SOS but gives a poor bound:

$$\widetilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}] \gg \mathsf{opt}(\boldsymbol{W}) = \max_{\boldsymbol{x} \in \{\pm 1\}^n} \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}.$$

Boils down to understanding the **spectra** of large **patterned** matrix functions of various $\boldsymbol{W}$—can be very technical!

II. A Mystery in SOS Lower Bounds

Grigoriev-Laurent Lower Bound

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Let n be odd. Pin down the degree needed for **exactness**:

Theorem: [Grigoriev '01, Laurent '03] For some $\boldsymbol{W}$,

$$\max_{\tilde{\mathbb{E}} \text{ of degree } n-1} \tilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}] > \mathrm{opt}(\boldsymbol{W}).$$

Theorem: [Fawzi, Saunderson, Parrilo '16] For all $\boldsymbol{W}$,

$$\max_{\tilde{\mathbb{E}} \text{ of degree } n+1} \tilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}] = \mathrm{opt}(\boldsymbol{W}).$$

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Bad W is $\boldsymbol{W} := \boldsymbol{I} - \frac{1}{n}\boldsymbol{1}\boldsymbol{1}^\top$ = projection to $\mathsf{span}(\boldsymbol{1})^\perp$. By parity,

$$\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x} = n - \frac{1}{n}\left(\sum_{i=1}^n x_i\right)^2 \leq n - \frac{1}{n},$$

but can find $\tilde{\mathbb{E}}$ such that

$$\tilde{\mathbb{E}}[\boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}] = n.$$

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For even pseudomoments, guess:

$$\begin{aligned} 0 &= \widetilde{\mathbb{E}}\left[\left(\sum_{i=1}^n x_i\right)^2\right] \\ &= \sum_{i=1}^n \widetilde{\mathbb{E}}[x_i^2] + 2\sum_{1\le i<j\le n} \widetilde{\mathbb{E}}[x_i x_j] \\ &= n + n(n-1)a_2. \qquad \text{(constraint + symmetry)} \end{aligned}$$

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Solving leads to predict, for all $i \neq j$,

$$\widetilde{\mathbb{E}}[x_i x_j] := a_2 = -\frac{1}{n-1}.$$

Choosing $\widetilde{\mathbb{E}}$: Finishing the Job

Symmetrize over $(x_1, \ldots, x_n) \mapsto (x_{\sigma(1)}, \ldots, x_{\sigma(n)}) \rightsquigarrow$

$$\widetilde{\mathbb{E}}[x_{i_1} \cdots x_{i_{2k}}] := a_{2k},$$

and expect these to satisfy

$$\begin{aligned} 0 &= \widetilde{\mathbb{E}}\left[\left(\sum_{i=1}^n x_i\right)^{2k}\right] \\ &= \text{constant} + \text{linear combination of } a_2, \ldots, a_{2k-2}, a_{2k}. \end{aligned}$$

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Solving simple combinatorial recursion gives the **Grigoriev-Laurent pseudomoments**,

$$\widetilde{\mathbb{E}}[x_{i_1} \cdots x_{i_d}] = a_d = \mathbb{1}\{d \text{ even}\} \cdot (-1)^{d/2} \prod_{i=0}^{d/2-1} \frac{2i+1}{n-2i-1}.$$

Laurent's Proof

Must check positivity of $\widetilde{\mathbb{E}} \Leftrightarrow \mathbf{0} \preceq \boldsymbol{M} \in \mathbb{R}^{\binom{[n]}{\leq D/2} \times \binom{[n]}{\leq D/2}}$ with

$$M_{S,T} := a_{|S \triangle T|}.$$

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Observation: The eigenvalues of $\boldsymbol{M}$ have interesting structure and high multiplicity. More direct proof possible?

Mystery: Eigenvalues of Pseudomoments

Read across the diagonals to see Laurent's recursion:

$$n = \cdots$$

1	3	5	7	9	11
	0	0	0	0	0
1	1	$\frac{13}{8}$	$\frac{19}{12}$	$\frac{263}{128}$	$\frac{1289}{640}$
	$\frac{3}{2} \cdot 1$	$\frac{5}{4} \cdot 1$	$\frac{7}{6} \cdot \frac{13}{8}$	$\frac{9}{8} \cdot \frac{19}{12}$	$\frac{11}{10} \cdot \frac{263}{128}$
		$\frac{5 \cdot 3}{4 \cdot 2} \cdot 1$	$\frac{7 \cdot 5}{6 \cdot 4} \cdot 1$	$\frac{9 \cdot 7}{8 \cdot 6} \cdot \frac{13}{8}$	$\frac{11 \cdot 9}{10 \cdot 8} \cdot \frac{19}{12}$
			$\frac{7 \cdot 5 \cdot 3}{6 \cdot 4 \cdot 2} \cdot 1$	$\frac{9 \cdot 7 \cdot 5}{8 \cdot 6 \cdot 4} \cdot 1$	$\frac{11 \cdot 9 \cdot 7}{10 \cdot 8 \cdot 6} \cdot \frac{13}{8}$
				$\frac{9 \cdot 7 \cdot 5 \cdot 3}{8 \cdot 6 \cdot 4 \cdot 2} \cdot 1$	$\frac{11 \cdot 9 \cdot 7 \cdot 5}{10 \cdot 8 \cdot 6 \cdot 4} \cdot 1$
					$\frac{11 \cdot 9 \cdot 7 \cdot 5 \cdot 3}{10 \cdot 8 \cdot 6 \cdot 4 \cdot 2} \cdot 1$

Not hard to predict multiplicities also.

Bigger Mystery: Explaining Positivity

Philosophical comment: our process was to

1. Build M to satisfy the entrywise constraints, and...
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This work: A rederivation of the pseudomoments that swaps the constraints’ statuses, building in psdness and making entrywise patterns appear “magically.”

III. Gramian Construction

High-Level Strategy: Surrogate Random Tensors

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To build in psdness, we will build $\boldsymbol{M}$ as a Gram matrix:

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Probabilistic interpretation: for $0 \leq d \leq D/2$, there are jointly Gaussian random symmetric tensors $\boldsymbol{G}^{(d)}$ such that

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Intuition: for a "random $\boldsymbol{x} \in \{\pm 1\}^n$ with $\sum_{i=1}^n x_i = 0$,"

$$\boldsymbol{G}^{(d)} = \boldsymbol{x}^{\otimes d}.$$

There is no such random $\boldsymbol{x}$, but we can build $\boldsymbol{G}$ to "fake it" as much as possible.

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Theorem: [K., Moore '22] For a particular choice of scaling of initial canonical Gaussian tensors, this sequence of $\boldsymbol{G}^{(d)}$ exactly recovers the Grigoriev-Laurent pseudomoments:

$$\widetilde{\mathbb{E}}[\boldsymbol{x}^S \boldsymbol{x}^T] = a_{|S \triangle T|} = \mathbb{E}[G_S^{(|S|)} G_T^{(|T|)}].$$

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3. A proof of Laurent’s empirical observations. In particular, the formerly mysterious recursive pattern in the eigenvalues may be seen to come from the conditional construction of $\boldsymbol{G}^{(d)}$ depending on the previous $\boldsymbol{G}^{(d')}$ over $d' < d$.

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Gaussian conditioning: $\boldsymbol{g} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$ conditional on $\langle \boldsymbol{a}_i, \boldsymbol{g} \rangle = b_i$ for $i \in [m]$ is:

- Constant on $\mathsf{span}(\boldsymbol{a}_1, \ldots, \boldsymbol{a}_m)$, plus...
- lower-dimensional $\mathcal{N}(\mathbf{0}, \boldsymbol{I})$ on $\mathsf{span}(\boldsymbol{a}_1, \ldots, \boldsymbol{a}_m)^\perp$.

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Interpret projection with **homogeneous polynomials**:

$$\boldsymbol{G} \leftrightarrow g(\boldsymbol{y}) := \langle \boldsymbol{G}, \boldsymbol{y}^{\otimes d} \rangle$$
$$\langle \boldsymbol{G}, \boldsymbol{H} \rangle = \langle g, h \rangle$$

under the **apolar inner product** of polynomials,

$$\langle g, h \rangle := \frac{1}{d!} g(\boldsymbol{\partial}) h(\boldsymbol{y}) \in \mathbb{R}.$$

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⇝ apolar orthogonal complement of ideal $\mathcal{I}$ generated by $p_1(\boldsymbol{y}), \dots, p_m(\boldsymbol{y})$ is the **multiharmonic polynomials**,

$$\mathcal{I}^\perp = \{f : p_i(\boldsymbol{\partial})f = 0 \text{ for } i = 1, \dots, m\}.$$

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Actually, treat our two families of conditions separately, and end up projecting to **simplex-harmonic** polynomials:

$$\mathcal{H}_{n,d} = \left\{ f \in \mathbb{R}[z_1, \dots, z_{n-1}]_d^{\mathsf{hom}} : \langle \boldsymbol{s}_i, \boldsymbol{\partial} \rangle^2 f = 0 \text{ for } i \in [n] \right\},$$

for $\boldsymbol{s}_1, \dots, \boldsymbol{s}_n \in \mathbb{R}^{n-1}$ vertices of an **equilateral simplex**.

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S_n acts on $\mathbb{R}^{n-1}$ by permuting the $\boldsymbol{s}_i$ ("standard" irrep)...

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Lemma: $\mathcal{H}_{n,d}$ is irreducible and isomorphic to the irrep of the $(n-d, d)$ partition. (New?)

$\rightsquigarrow$ project to $\mathcal{H}_{n,d}$ with standard character computations.

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$\rightsquigarrow$ multiharmonic polynomials from a random ideal

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$\rightsquigarrow$ only approximate Gramian factorization

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⇝ heuristic guess/estimate for multiharmonic projection

⇝ only approximate Gramian factorization

⇝ not yet much easier than “magical psdness” methods

Towards More Generic Settings

My original interest: SOS for random problems.

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Could simplify technical proofs of important evidence for **difficulty of average-case optimization**.

Thank you!