Semialgebraic Proofs and Efficient Algorithm Design

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Joint work with Pravesh Kothari and Toni Pitassi

Sum-of-Squares

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— Proofs correspond to a family of SDPs

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Powerful:
- Captures many famous approximation algorithms for NP hard problems such as the Goemans Williamson algorithm for MaxCut
- Gives optimal approximations of any CSP under the Unique Games Conjecture [Raghavendra08]

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Simple Algorithm Design Strategy:
- Sum-of-Squares proofs are automatizable.
- Proofs that a solution exist automatically give efficient algorithms for finding that solution. Main difficulty is rounding the solution.

Outline

1. Developing the Sum-of-Squares Relaxation
2. Phrasing the Relaxation as an SDP
3. The Dual Sum-of-Squares Proofs and Completeness
4. Convergence and Strong Duality
5. Upper Bounds
6. Lower Bounds

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Polynomial Optimization Problems

$\mathscr{P} \subseteq \mathbb{R}[x]$ a set of polynomials, $r \in \mathbb{R}[x]$ linear.

$$\begin{aligned} \max_x \quad & r(x) \\ \text{s.t.} \quad & p(x) \geq 0 \qquad \forall p \in \mathscr{P} \end{aligned}$$

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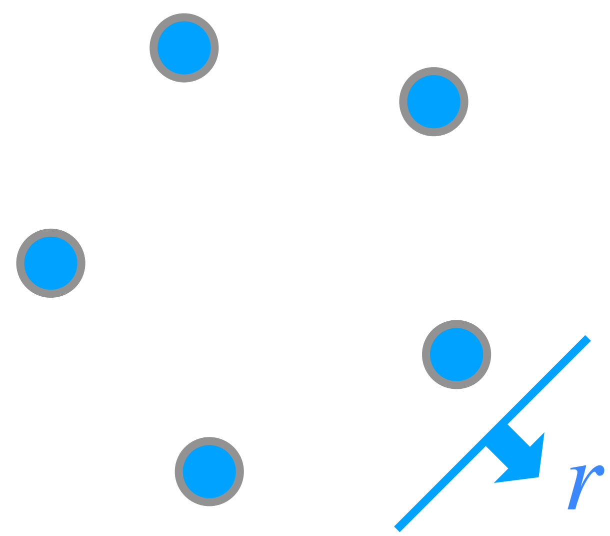

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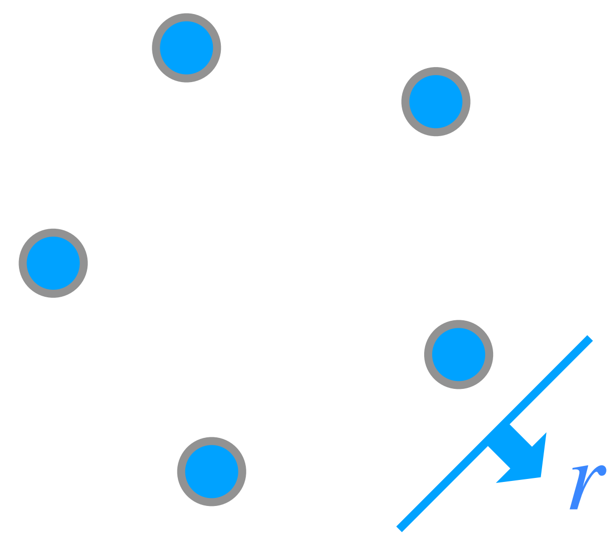

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Problem: Polynomial optimization problems are NP-hard to solve in general.

Goal: Develop a tractable relaxation that achieves good approximations to many problems we care about

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Take the convex relaxation of $K_{\mathscr{P}}$

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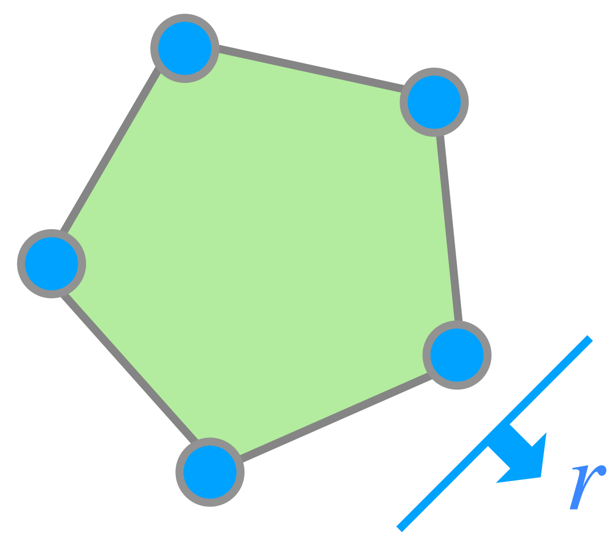

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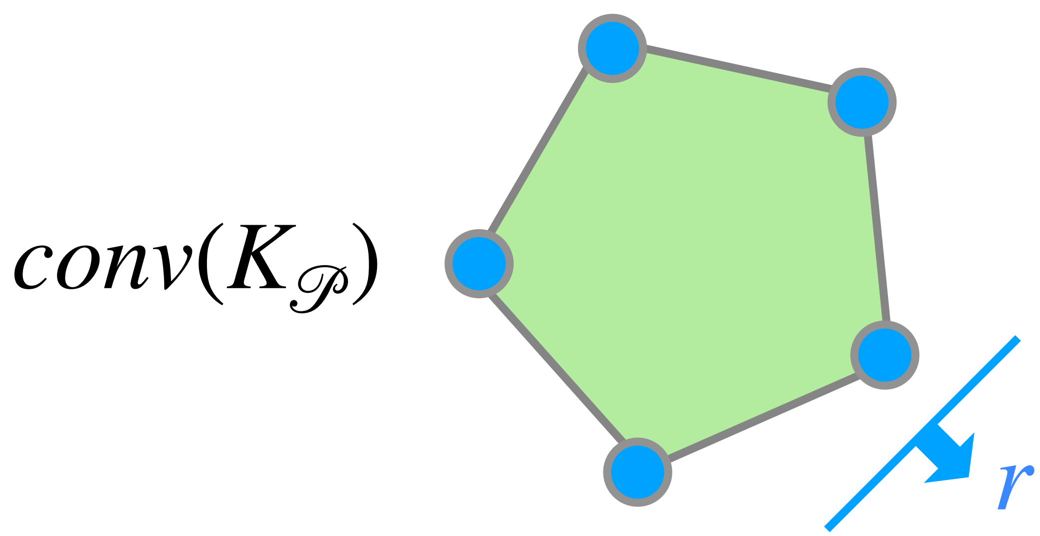

$$\max_{x \in K_{\mathscr{P}}} r(x) = \max_{x \in conv(K_{\mathscr{P}})} r(x)$$

By linearity of $r(x)$, any optimal solution $x \in conv(\mathscr{P})$ is a convex combination of optimal $x \in K_{\mathscr{P}}$

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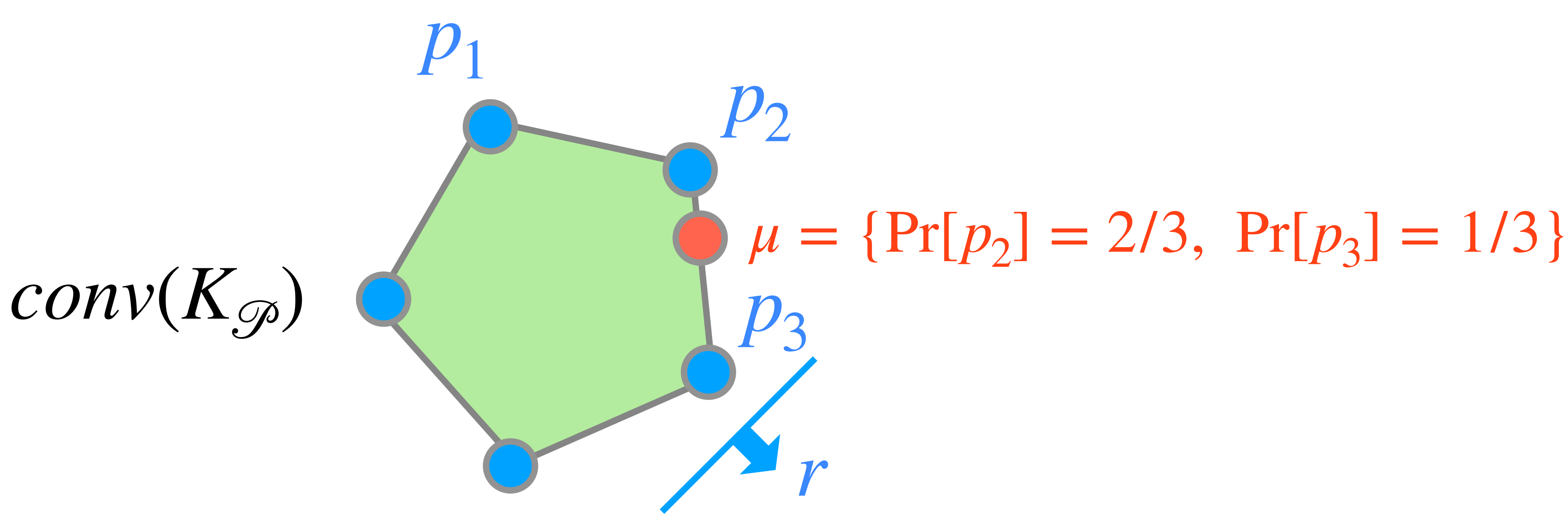
Distributional View: view the points in $conv(K_{\mathscr{P}})$ as distributions μ supported on the points $K_{\mathscr{P}}$



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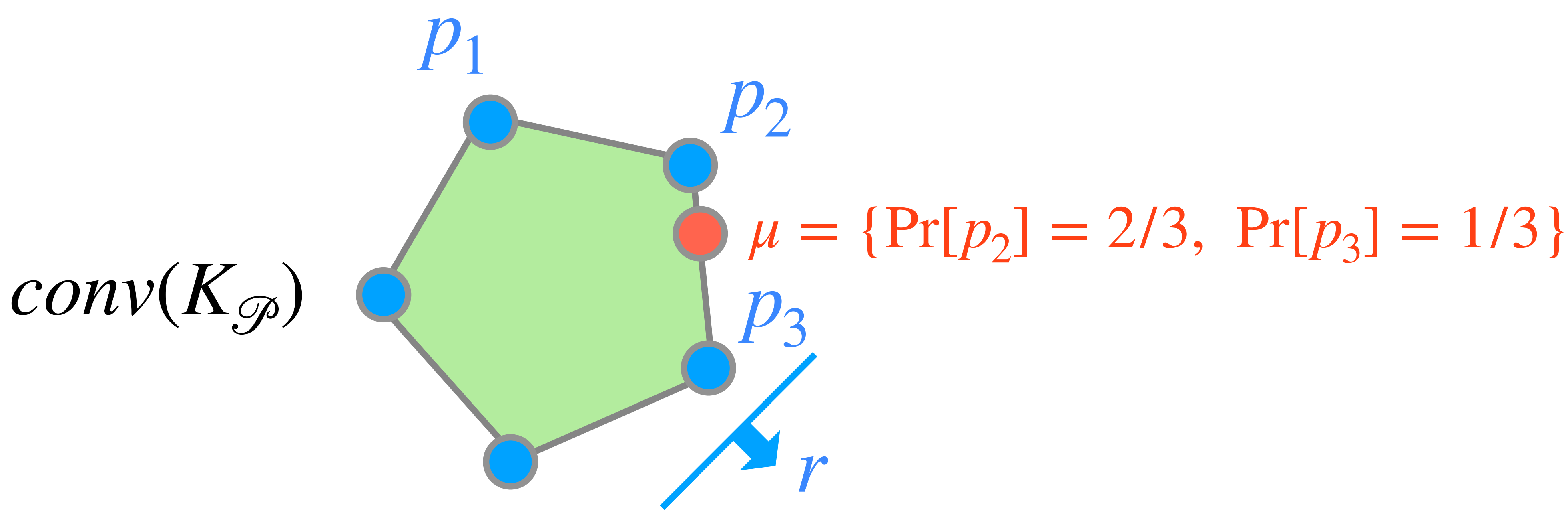

$$\max_{x \in K_{\mathscr{P}}} r(x) = \max_{x \in conv(K_{\mathscr{P}})} r(x) = \max \mathbb{E}_{\mu}[r(x)] : \mu \textbf{ is supported on } K_{\mathscr{P}}$$

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Distributions μ can be described by their moments $\mathbb{E}_\mu[x^I]$
where $x^I := \Pi_{i \in I} x_i$

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Relaxation: restrict attention to the degree $\leq d$ moments of these distributions, $\mathbb{E}[x^I]$ for $|I| \leq d$

– Only n^d such moments

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Therefore

Look for efficient tests which distinguish collections of moments which belong to distributions supported on K_P

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A set of efficient tests distinguishing $\tilde{\mathbb{E}}$ that agree with the moments of a true distribution on $K_{\mathscr{P}}$ from those that do not.

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Degree-d Pseudo-Expectation for $\mathscr{P}$: Any linear function $\tilde{\mathbb{E}} : \mathbb{R}[x]_{\le d} \to \mathbb{R}$ satisfying

1. $\tilde{\mathbb{E}}[1] = 1$
2. $\tilde{\mathbb{E}}[q^2(x)] \ge 0 \qquad \forall q \in \mathbb{R}[x]_{\le d/2}$
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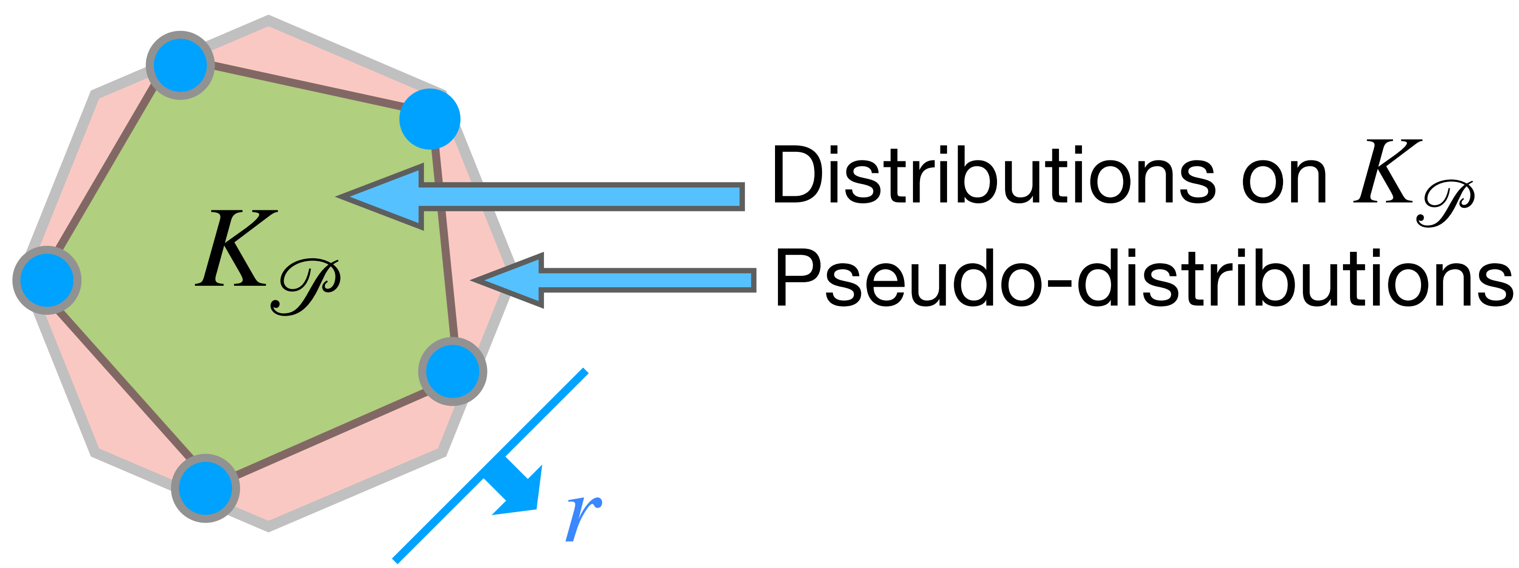

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$\tilde{\mathbb{E}}$ is linear

n^d variables, one for each monomial.

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Idea: rewrite polynomials as vector products
—Square polynomials become PSD constraints.

Solving the Relaxation

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Monomial vector: v_d where $(v_d)_I = x^I$ for $|I| \leq d$

Any $p \in \mathbb{R}[x]_{\leq d}$ can be written as

$$p(x) = \overrightarrow{p}^T v_d(x)$$

$\overrightarrow{p}$ is the coefficient vector of the monomials in $p(x)$

For $n = 2$:

$$x_1^2 + 3x_2 + 4 = \overset{\overrightarrow{p}}{\begin{bmatrix} 4 & 0 & 3 & 1 & 0 & 0 \end{bmatrix}} \overset{\overrightarrow{v_2}}{\begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_1 x_2 \\ x_2^2 \end{bmatrix}}$$

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$$\tilde{\mathbb{E}}[q^2(x)] = \tilde{\mathbb{E}}[\overrightarrow{q} v_d^T v_d \overrightarrow{q}^T] = \overrightarrow{q} \tilde{\mathbb{E}}[v_d^T v_d] \overrightarrow{q}^T \geq 0$$

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$$M_2 = \begin{bmatrix} \tilde{\mathbb{E}}[1], & \tilde{\mathbb{E}}[x_1], & \ldots, & \tilde{\mathbb{E}}[x_n] \\ \tilde{\mathbb{E}}[x_1], & \tilde{\mathbb{E}}[x_1 x_1], & \ldots, & \tilde{\mathbb{E}}[x_1 x_n] \\ \vdots & \vdots & \cdots & \vdots \\ \tilde{\mathbb{E}}[x_n], & \tilde{\mathbb{E}}[x_n x_1], & \ldots, & \tilde{\mathbb{E}}[x_n x_n] \end{bmatrix}$$

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SoS SDP Relaxation

$$SOS_d(\mathscr{P}) \left\{ \begin{array}{lll} \max & \tilde{\mathbb{E}}[r(x)] & \\ \text{s.t.} & M_d \succeq 0 & \\ & M_d^p \succeq 0 & \forall p \in \mathscr{P} \\ & \tilde{\mathbb{E}}[1] = 1 & \end{array} \right\}$$

$|\mathscr{P}| \cdot n^{O(d)}$ size SDP

Solving the Relaxation

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Solvable by the Ellipsoid Method in time $|\mathscr{P}|\, n^{O(d)} \log(1/\varepsilon)$ to within an additive error ε

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A solution to $SOS_d(\mathscr{P})$ is on n^d variables.

Obtain an approximate solution to $\mathscr{P}$ by projecting to $[n]$

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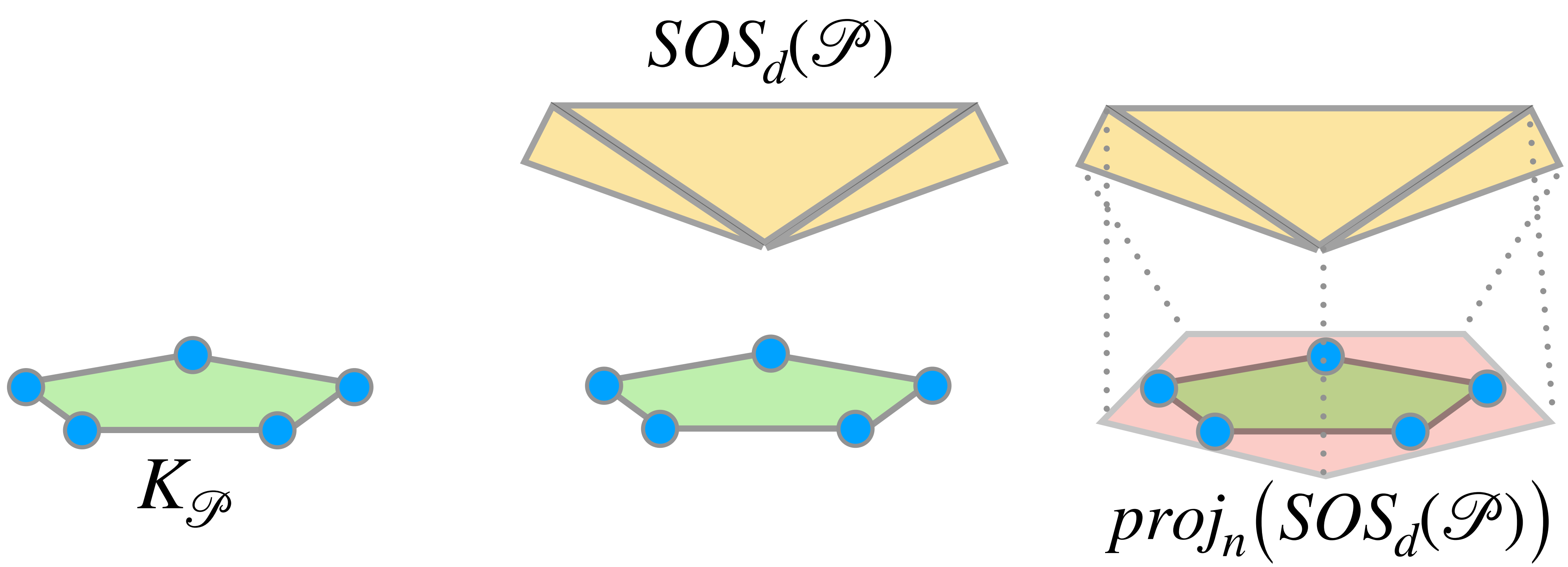

Max Cut

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$$\max \sum_{i<j} w_{i,j}(x_i - x_j)^2$$

$$\text{s.t. } x_i^2 - x_i \geq 0$$

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Degree-2 SOS Relaxation

SDP Formulation

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Degree-2 SOS Relaxation

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$$\text{s.t. } \tilde{\mathbb{E}}[q^2(x)] \geq 0 \quad \forall q \in \mathbb{R}[x]_{\leq 1}$$

$$\tilde{\mathbb{E}}[x_i^2 - x_i] \geq 0$$

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Degree-2 SOS Relaxation

$$\max \sum_{i<j} w_{i,j}\tilde{\mathbb{E}}[(x_i - x_j)^2]$$
$$\text{s.t. } \tilde{\mathbb{E}}[q^2(x)] \geq 0 \quad \forall q \in \mathbb{R}[x]_{\leq 1}$$
$$\tilde{\mathbb{E}}[x_i^2 - x_i] \geq 0$$
$$\tilde{\mathbb{E}}[x_i - x_i^2] \geq 0$$
$$\tilde{\mathbb{E}}[1] = 1$$

SDP Formulation

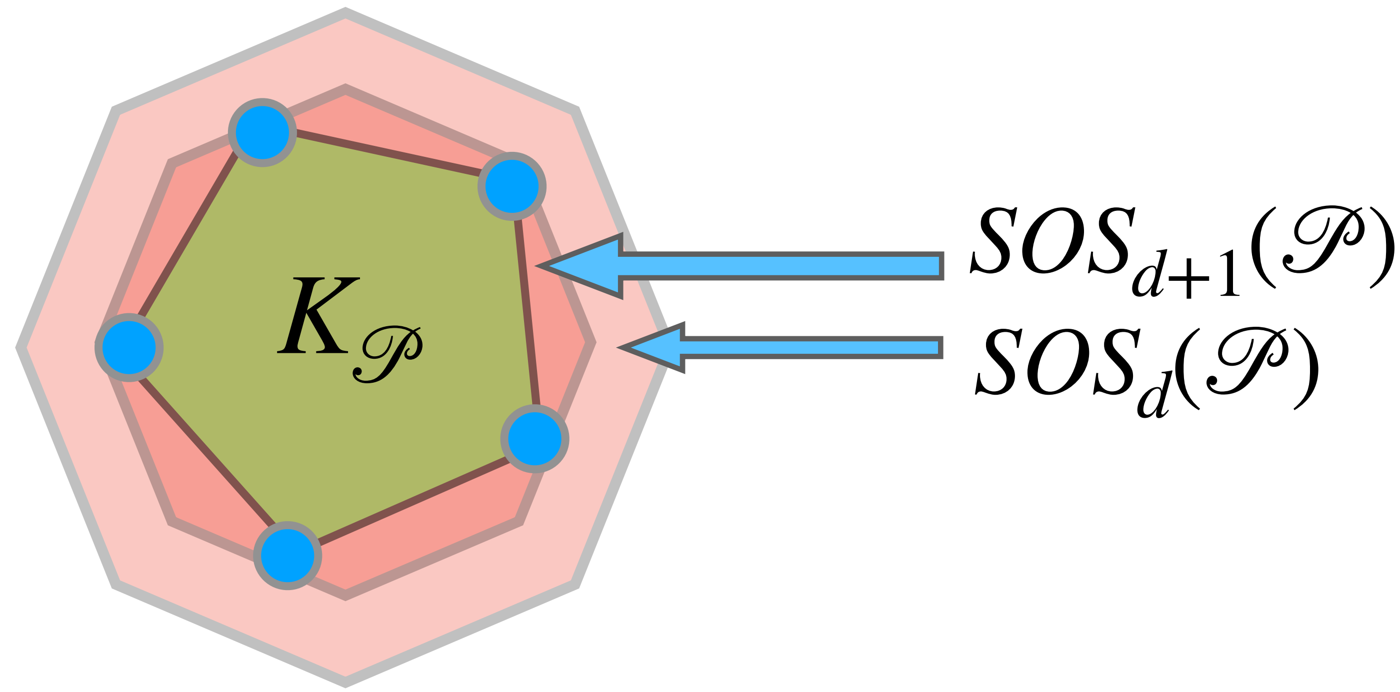
$$\max \sum_{i<j} w_{i,j}\tilde{\mathbb{E}}[(x_i - x_j)^2]$$
$$\text{s.t. } M_2 \succeq 0$$
$$M_2^{x_i - x_i^2 \geq 0} \succeq 0$$
$$M_2^{x_i^2 - x_i \geq 0} \succeq 0$$
$$\tilde{\mathbb{E}}[1] = 1$$

Moment Matrices

$$M_2 = \begin{bmatrix} \tilde{\mathbb{E}}[1], & \tilde{\mathbb{E}}[x_1], & \ldots, & \tilde{\mathbb{E}}[x_n] \\ \tilde{\mathbb{E}}[x_1], & \tilde{\mathbb{E}}[x_1x_1], & \ldots, & \tilde{\mathbb{E}}[x_1x_n] \\ \vdots & \vdots & \ldots & \vdots \\ \tilde{\mathbb{E}}[x_n], & \tilde{\mathbb{E}}[x_nx_1], & \ldots, & \tilde{\mathbb{E}}[x_nx_n] \end{bmatrix}$$
$$M_2^{x_i^2 - x_i} = \tilde{\mathbb{E}}[x_i^2 - x_i]$$
$$M_2^{x_i - x_i^2} = \tilde{\mathbb{E}}[x_i - x_i^2]$$

Hierarchy of Relaxations

The Sum-of-Squares relaxations form a hierarchy of ever-tightening spectahedrons parameterized by the degree d of the relaxation



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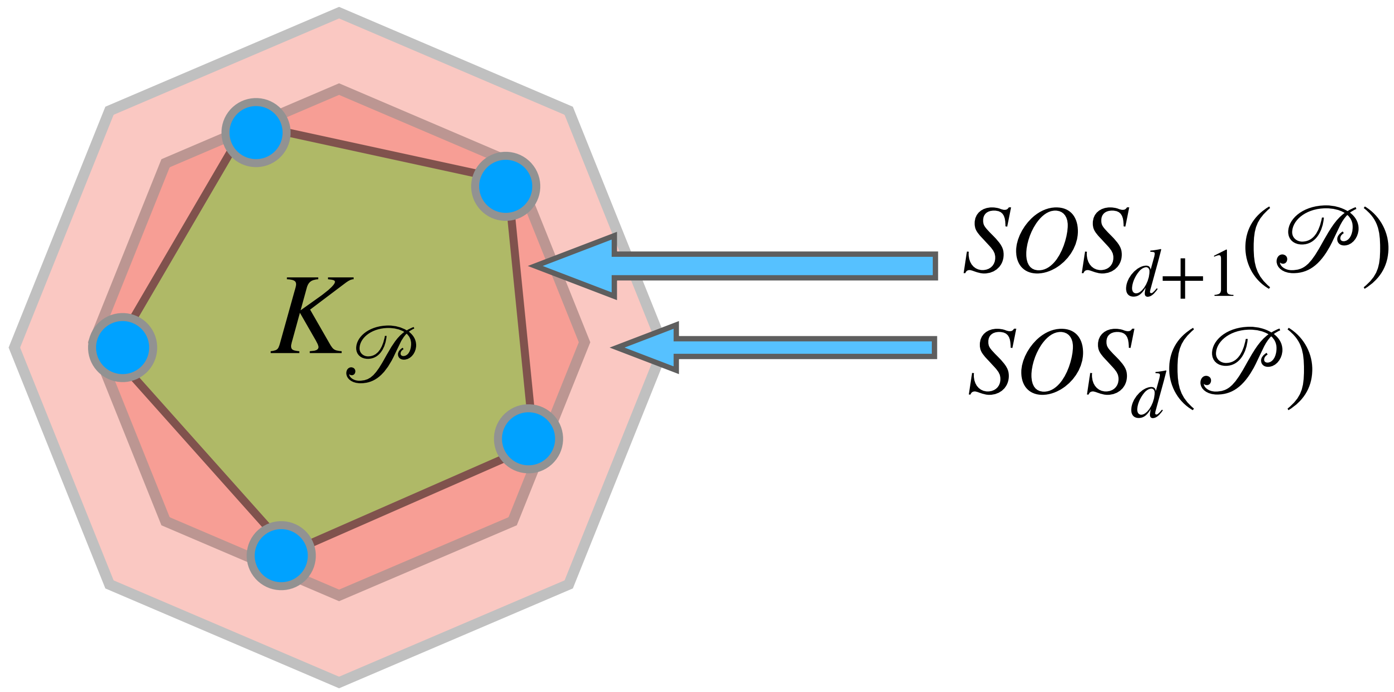

Can we guarantee convergence to $K_{\mathscr{P}}$?

—Not known to be true in General.

—We will see later that convergence can be guaranteed under certain assumptions on $\mathscr{P}$. This follows from duality.

Outline

1. Developing the Sum-of-Squares Relaxation
2. Phrasing the Relaxation as an SDP
3. The Dual Sum-of-Squares Proofs and Completeness
4. Convergence and Strong Duality
5. Upper Bounds
6. Lower Bounds

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—Find the minimum $\lambda \in \mathbb{R}$ such that $\lambda - r(x)$ is non-negative over $SOS_d(\mathscr{P})$

Dual program corresponds to finding a good sum-of-squares decomposition of $\lambda - r(x)$

Dual:

$$\begin{aligned} &\min \lambda \\ &\text{s.t.} \quad \lambda - r(x) = \sum_{p \in \mathscr{P} \cup \{1\}} p(x) q_p^2(x) \\ &\qquad\quad q_p \in \mathbb{R}[x]_{\leq (d - deg(p))/2} \\ &\qquad\quad \lambda \in \mathbb{R} \end{aligned}$$

Weak Duality

$$\max \tilde{\mathbb{E}}[r(x)]$$

s.t. $\tilde{\mathbb{E}}[1] = 1$

$\tilde{\mathbb{E}}[q^2(x)] \geq 0$

$\tilde{\mathbb{E}}[p(x)q^2(x)] \geq 0$

$\tilde{\mathbb{E}}$ is linear

Primal

$$\min \lambda$$

s.t. $\lambda - r(x) = \sum_{p \in \mathscr{P} \cup \{1\}} p(x) q_p^2(x)$

$q_p \in \mathbb{R}[x]_{\leq (d - deg(p))/2}$

$\lambda \in \mathbb{R}$

Dual

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Weak Duality: Let $\tilde{\mathbb{E}} \in SOS_d(\mathscr{P})$ and $r(x) = \lambda - \Sigma_{p \in \mathscr{P} \cup \{1\}} p(x) q_p^2(x)$ then $\tilde{\mathbb{E}}[r(x)] \leq \lambda$.

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Proof: $\tilde{\mathbb{E}}[r(x)] = \tilde{\mathbb{E}}[\lambda] - \sum_{p \in \mathscr{P} \cup \{1\}} \tilde{\mathbb{E}}[p(x)q_p^2(x)]$ (Linearity)

$= \lambda - \sum_{p \in \mathscr{P} \cup \{1\}} \tilde{\mathbb{E}}[p(x)q_p^2(x)]$ ($\tilde{\mathbb{E}}[1] = 1$)

$\leq \lambda$ ($\tilde{\mathbb{E}}[p(x)q_p^2(x)] \geq 0$)

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$$= \lambda - \sum_{p \in \mathscr{P} \cup \{1\}} \tilde{\mathbb{E}}[p(x)q_p^2(x)] \qquad (\tilde{\mathbb{E}}[1] = 1)$$

$$\leq \lambda \qquad (\tilde{\mathbb{E}}[p(x)q_p^2(x)] \geq 0)$$

Writing $\lambda - r(x)$ as a degree-d sum of squares is a Sum-of-Squares proof that the maximum over $SOS_d(\mathscr{P})$ is at most λ

Sum-of-Squares Proofs

Sum-of-Squares Proof: A degree-d SoS proof of $r \in \mathbb{R}[x]$ from $\mathscr{P} \subseteq \mathbb{R}[x]$ is a set of polynomials $q_p \in \mathbb{R}[x]_{(d-deg(p))/2}$ such that

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Proof: Let $-1 = \Sigma_{\mathscr{P} \cup \{1\}} p(x) q_p^2(x)$ be a degree-d refutation and $\tilde{\mathbb{E}}$ be a degree-d pseudo-expectation for $\mathscr{P}$ then

$$-1 = -\tilde{\mathbb{E}}[1] = \tilde{\mathbb{E}}[-1] = \Sigma_{p \in \mathscr{P} \cup \{1\}} \tilde{\mathbb{E}}[p(x) q_p^2(x)] \geq 0$$

Sum-of-Squares Proofs

Proofs of CNF formulas: $x_1 \vee x_2 \vee \neg x_3$ becomes $x_1 + x_2 + (1 - x_3) - 1 \geq 0$.

Also include boolean axioms $x_i^2 - x_i = 0$.

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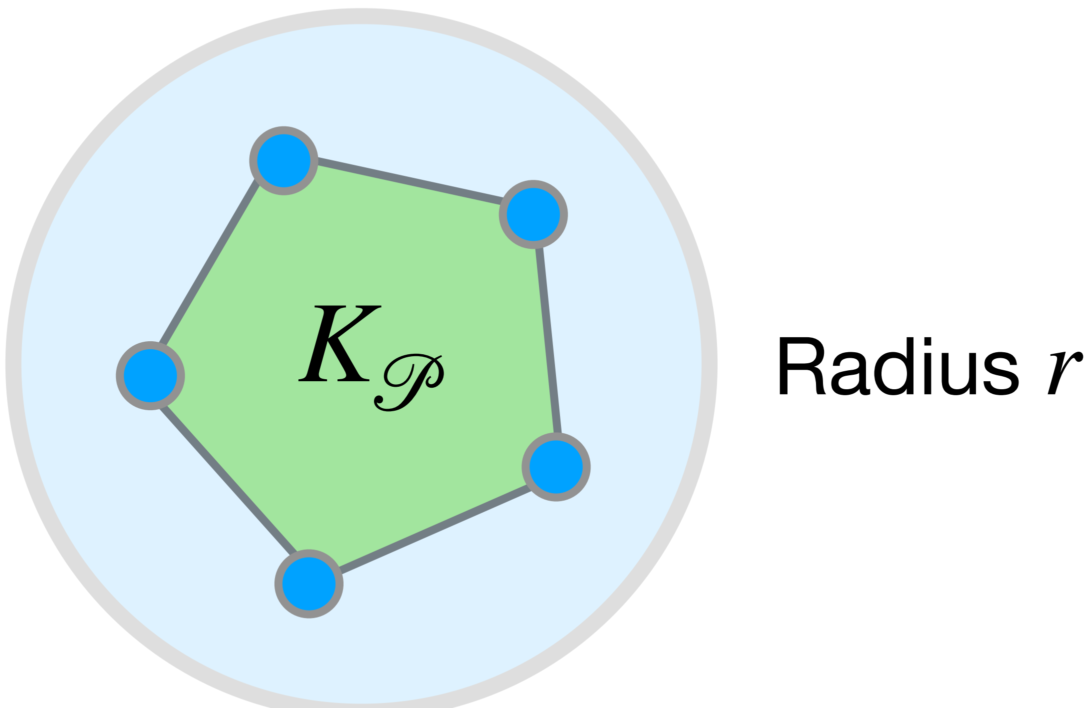
Archimedean Assumption: $\mathscr{P}$ contains a constraint of the form $r^2 - \Sigma_{i\in[n]} x_i^2 \geq 0$ for some r.



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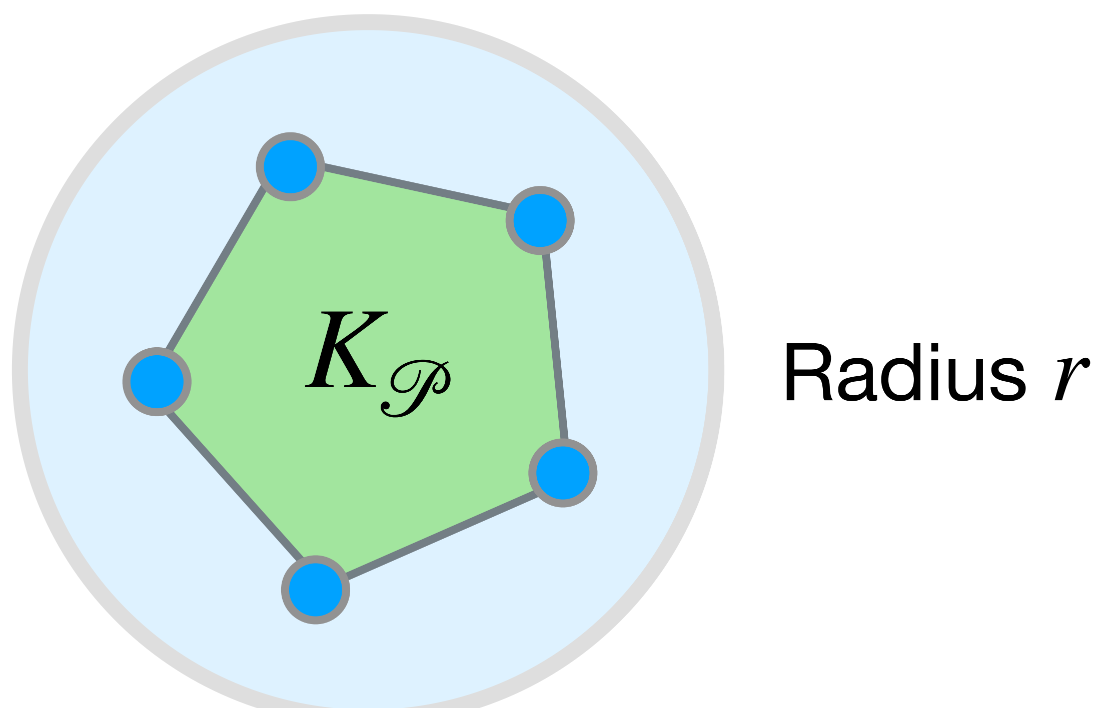

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Putinar's Positivstellensatz: Let $\mathscr{P} \subseteq \mathbb{R}[x]$ satisfy the Archimedean assumption. Then $r(x) > 0$ for all $x \in K_{\mathscr{P}}$ iff

$$r(x) = \sum_{p \in \mathscr{P} \cup \{1\}} p(x) q_p^2(x)$$

for some $q_p \in \mathbb{R}[x]$.

Sum-of-Squares Proof of PHP

Pigeonhole Principle:

a. $\Sigma_{j\in[n]} p_{i,j} - 1 \geq 0 \qquad \forall i \in [n+1]$

b. $1 - p_{i,j} - p_{i',j} \geq 0 \qquad \forall i \neq i' \in [n+1], \forall j \in [n]$

c. $p_{i,j}^2 - p_{i,j} = 0 \qquad \forall i \in [n+1], j \in [n]$

SoS Refutation of PhP:

1. Derive $1 - \Sigma_{i\in[n+1]} p_{i,j} \quad \forall j$ "Each hole has one pigeon"
2. Sum the constraints in 1 over $j \in [n]$
$$\Sigma_{j\in[n]}(1 - \Sigma_{i\in[n+1]} p_{i,j}) = n - \Sigma_{i,j} p_{i,j}$$
3. Sum the constraints in a. over $i \in [n+1]$ to get.
$$\Sigma_{i\in[n+1]}\left(\Sigma_{j\in[n]} p_{i,j} - 1\right) = \Sigma_{i,j} p_{i,j} - (n+1)$$
4. Add 2 and 3 to derive -1.

Proof of 1 as an SoS polynomial:

$$\Sigma_{i\neq i'\in[n]}(1 - p_{i,j} - p_{i',j})p_{i,j} + (1 - \Sigma_{i\in[n]} p_{i,j})^2 = 1 - \Sigma_{i\in[n]} p_{i,j}$$

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Convergence of the SoS hierarchy

Can we guarantee that our hierarchy of SDP relaxations converges to $K_{\mathscr{P}}$?

– Does $\lim_{d\to\infty} \max_{\tilde{E}\in SOS_d(\mathscr{P})} \tilde{\mathbb{E}}[r(x)] = \max_{x\in K_{\mathscr{P}}} r(x)$?

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Strong Duality: For all $\mathscr{P} \subseteq \mathbb{R}[x]$ satisfying the Archimedean Assumption

$$\min_{\lambda - r(x) = \Sigma p(x) q_p^2(x)} \lambda = \max_{\tilde{\mathbb{E}} \in SOS_d(\mathscr{P})} \tilde{\mathbb{E}}[p]$$

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When can we guarantee faster convergence?

— Inclusion of axioms such as

- $x_i^2 - x_i = 0 \ \forall i \in [n]$ (hypercube), or
- $1 - x_i^2 = 0 \ \forall i \in [n]$ (hypersphere)

guarantee convergence in degree $2n + deg(\mathscr{P})$

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PSD Matrices $Z \in \mathbb{R}^{n^d \times n^d}$ define square polynomials:

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Rephrase $\lambda - r(x) = \Sigma_{p \in \mathscr{P} \cup \{1\}} p(x) q_p^2(x)$ as

$$\begin{aligned} \min \quad & \lambda \\ \text{s.t.} \quad & \lambda - r(x) = \sum_{p \in \mathscr{P} \cup \{1\}} p(x) v_{d_p}^T Z_p v_{d_p} & & d_p := (d - deg(p))/2 \\ & Z_p \succeq 0 & & \forall p \in \mathscr{P} \end{aligned}$$

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Removing x variables, this becomes

$$\begin{aligned} \min \quad & \lambda \\ \text{s.t.} \quad & \lambda 1_{[I = \varnothing]} - \vec{r}_I = \sum_{p \in \mathscr{P} \cup \{1\}} \sum_{S+T+K=I} \vec{p}_K (Z_p)_{S,T} && \forall |I| \leq deg(r) \\ & Z_p \succeq 0 && \forall p \in \mathscr{P} \end{aligned}$$

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Dual:

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Primal:

$$\begin{aligned} \max \quad & \tilde{\mathbb{E}}[p(x)] \\ \text{s.t.} \quad & M_d \succeq 0 \\ & M_d^p \succeq 0 \quad \forall p \in \mathscr{P} \\ & \tilde{\mathbb{E}}[1] = 1 \end{aligned}$$

Strong duality follows by the SDP strong duality theorem

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Claimed: One can find a degree-d Sum-of-Squares proof in time $|\mathscr{P}| \cdot n^{O(d)}$ if it exists.

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Reasoning: SoS dual is an $|\mathscr{P}| \cdot n^{O(d)}$-size SDP. Can be solved in time $|\mathscr{P}| \cdot n^{O(d)}$ by the Ellipsoid Method (up to additive error ε).

Automatizability

Can we find a Sum-of-Squares proof efficiently if it exists?

Claimed: One can find a degree-d Sum-of-Squares proof in time $|\mathscr{P}| \cdot n^{O(d)}$ if it exists.

Reasoning: SoS dual is an $|\mathscr{P}| \cdot n^{O(d)}$-size SDP. Can be solved in time $|\mathscr{P}| \cdot n^{O(d)}$ by the Ellipsoid Method (up to additive error ε).

This claim is not known to be true in general

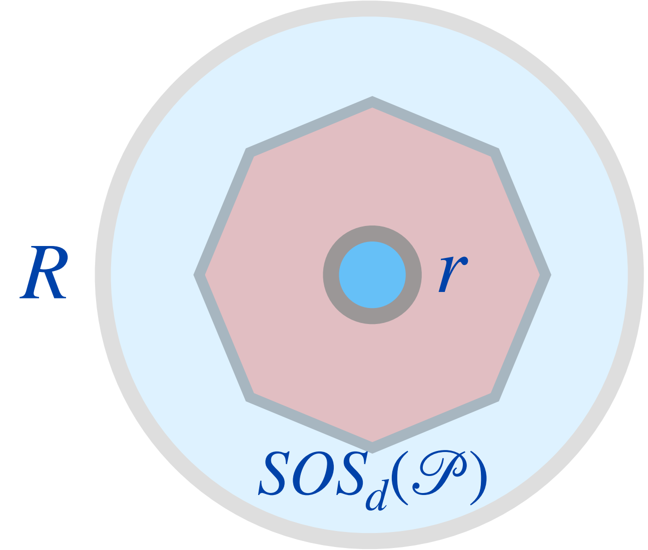
—Even for $\mathscr{P}$ satisfying the Archimedean assumption.

—Even for $\mathscr{P}$ containing $x_i^2 - x_i = 0$ for all $i \in [n]$

Automatizability

Issue:

- Ellipsoid Method requires the feasible set of the SDP to be contained within a ball of radius $R = |\mathscr{P}| \cdot n^{O(d)}$
- i.e. there must exist a proof with bit size $|\mathscr{P}| \cdot n^{O(d)}$



Ellipsoid Method: Let C be a convex set with a polynomial-time separation oracle. For $r, R > 0$ and $c \in \mathbb{R}^n$ such that $Ball(c, r) \subseteq C \subseteq Ball(0,R)$, maximizing over C to an additive error $\varepsilon > 0$ can be done in time $poly(|C|) \cdot \log(R/r\varepsilon)$.

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[RW17] Extending [O'Do17]: There exists small, degree 2 polynomials $\mathscr{P}$, $r(x)$ such that
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Good News: [RW17] provide a set of sufficient conditions under which SoS derivations can be found in time $|\mathscr{P}| \cdot n^{O(d)}$.
—MaxCSP, MaxClique, Balanced Separator, MaxBisection

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Any SoS derivation of monomial size s_m from a set $\mathscr{P}$ satisfying the conditions of [RW17] can be found in time $n^{O\left(\sqrt{n \log s_m} + deg(\mathscr{P})\right)}$.

Upper Bounds via Sum-of-Squares

Upper bounds leverage strong duality and the $n^{O(d)}$-time SoS algorithm to transform certificates that a solution exists into algorithms for finding that solution.
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[Rag08]: Assuming the Unique Games Conjecture, degree-2 SoS gives the optimal approximation ratio for every CSP.
— Does not tell us what this approximation ratio is.

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[ABS10,BRS11,GS11]: Subexponential-time algorithm for Unique Games based on SoS.

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Global Correlation Rounding:

- Given a pseudo-expectation $\tilde{\mathbb{E}}$, one way to round it is to assign each variable $x_i = 1$ with probability $\tilde{\mathbb{E}}[x_i]$. This can result in poor solutions due to correlations.
- Global Correlation Rounding: for 2CSPs, in expectation, global correlation drops under conditioning on the outcome of a set of random variables, while the objective value remains the same.

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[BKS13, BKS17]: Developed new rounding techniques for high-dimensional SoS
— Obtained algorithms for problems in quantum information theory, such as Best Separable State.

Average-Case Upper Bounds

Recently, lots of work on average-case algorithms using SoS
—Partly due to an average-case rounding framework introduced in [BKS14]

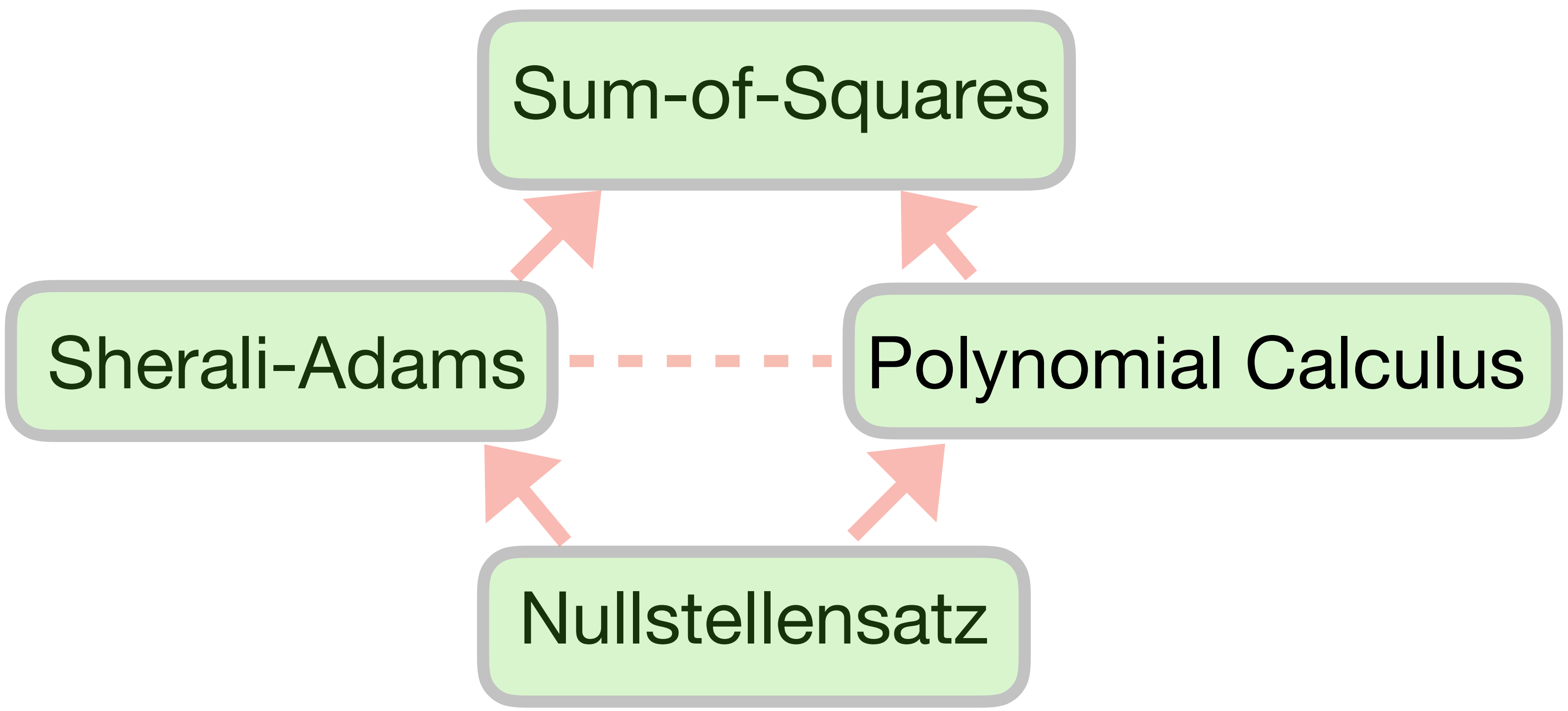
Led to SoS-based algorithms for average-case problems including:
—Dictionary Learning [BKS14],
—Tensor Completion [BM16, PS16],
—Clustering Mixture Models [HL18, KS17],
—Outlier Robust Moment Estimation [KS17],
—Robust Linear Regression [KKM18],
—Attacking cryptographic PRGs [BBKK18, BHKS19].

Outline

1. Developing the Sum-of-Squares Relaxation
2. Phrasing the Relaxation as an SDP
3. The Dual Sum-of-Squares Proofs and Completeness
4. Convergence and Strong Duality
5. Upper Bounds
6. Lower Bounds

Comparison with other Proof Systems

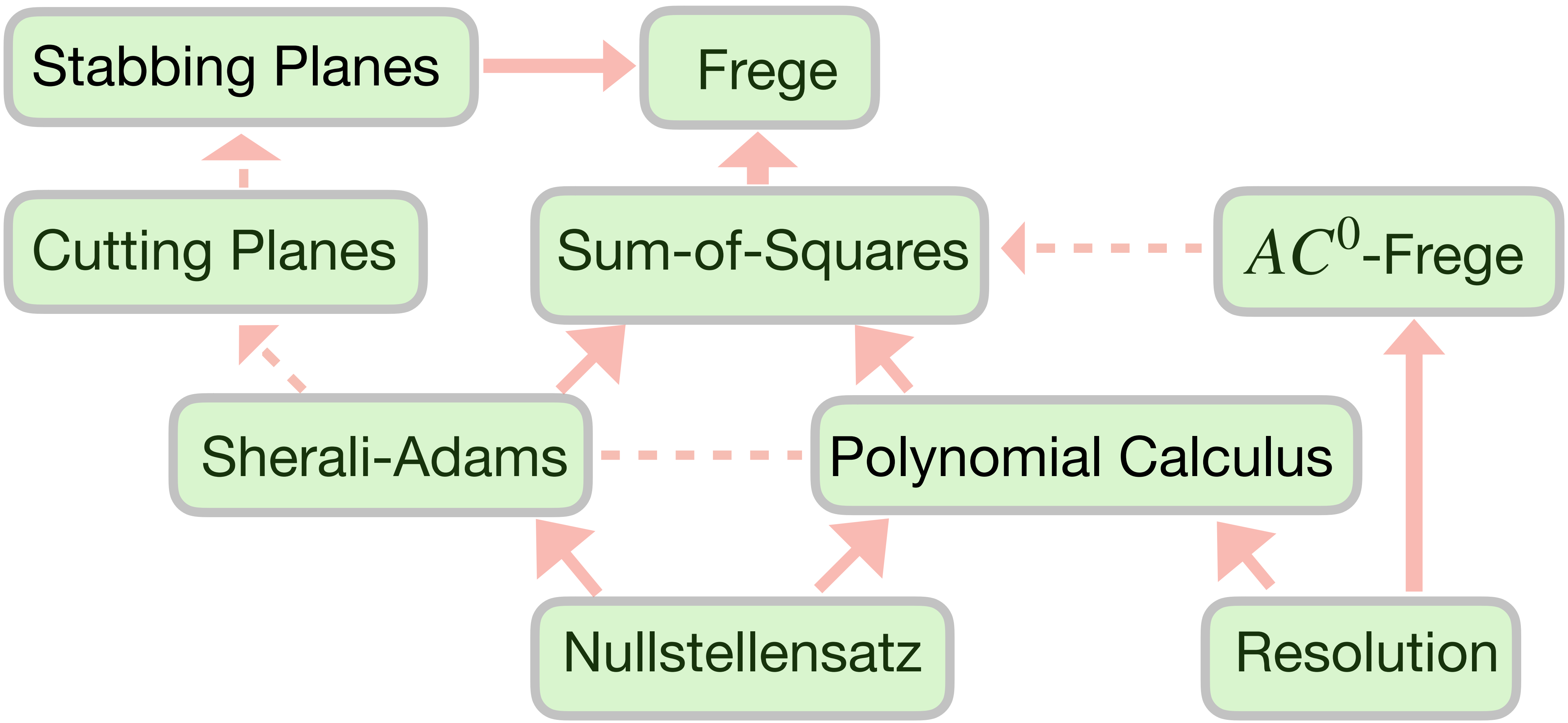
Simulations in terms of degree



Many of these separations as well as the simulation of PC by SoS are due to [Ber18]

Comparison with other Proof Systems

Simulation in terms of size



Open Questions:

— Does SoS simulate AC^0-Frege?

— How does SoS compare to Cutting Planes?

— How does SoS compare to Stabbing Planes / R(CP)?

Lower Bounds on SoS

If degree-d SoS cannot refute $\mathscr{P} \cup \{r(x) - \lambda\}$ then maximizing $r(x)$ over the degree-d SoS relaxation of $\mathscr{P}$ attains a value of at least λ.

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Random 3XOR: [Gri01, Sch08] systems of random 3XOR equations require degree $\Omega(n)$.

- Reduction to Resolution width lower bounds.
- Builds on earlier ideas [BGIP01, Gri98] for NS and PC.
- [Sch08] Implies lower bounds on Max3SAT, Max Ind Set.

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- Pairwise Independent: $P^{-1}(1)$ supports a distribution μ such that the pairwise marginals $\mu_i \mu_j$ for $i \neq j$ is uniform over $\{0,1\}^2$.
- Algebraically Linear: μ is also the uniform distribution over a subspace $V \subseteq GF(2)$.

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[AM09]: Assuming the UGC, any predicate $P : \{0,1\}^k \to \{0,1\}$ that is pairwise uniform is approximation resistant

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- A random assignment is essentially optimal
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- Method for doing reductions in SoS
- Lower bounds for problems such as Vertex Cover, IndSet

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[BCK15]: Any CSP defined on pairwise uniform predicates is approximation resistant for degree $\Omega(n)$ SoS

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Average-Case Lower Bounds

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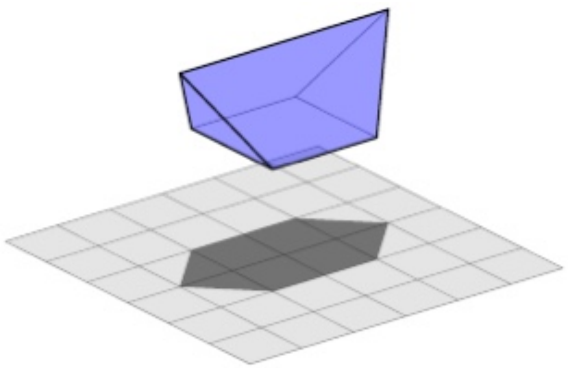
Planted Clique: [MPW15, HKPRS18], culminating in [BHKKMP18] proved nearly tight lower bounds on the degree of SoS proofs of the Planted Clique problem.
— Introduced the pseudo-calibration framework; a computational bayesian approach to constructing pseudo-expectations.

Applications of Lower Bounds

(SDP) Extended Formulation: Of a polytope P is any polytope (spectahedron) Q such that there exists a linear projection such that $proj(Q) = P$.

— Restriction: Polytope is instance independent



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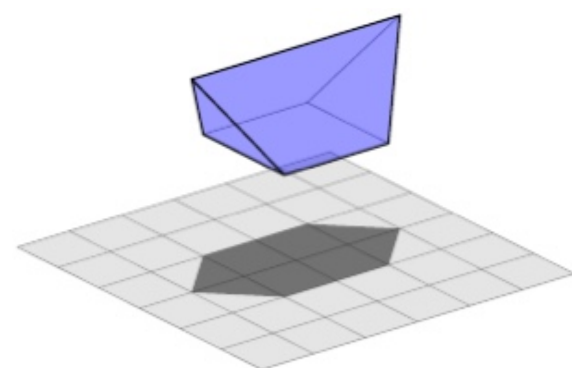

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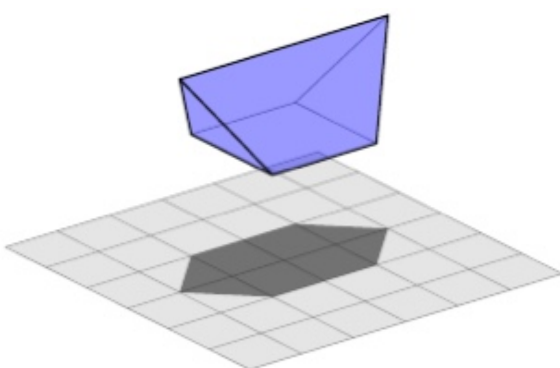

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[LRS14] For any CSP, there exists a constant c such that no size $c(n/\log n)^{d/4}$ SDP extended formulation can achieve a better approximation on any instance of $N = n^{4d}$ variables than degree-d Sum-of-Squares can on n variables.

Thank You!