

# Semidefinite hierarchies for polynomial optimization



Monique Laurent

Journées SMAI-MODE 2016, Toulouse

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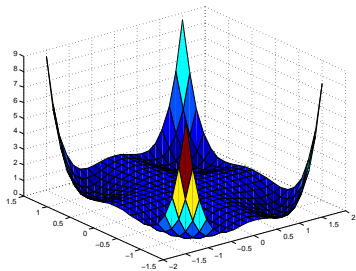


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Based on joint works with Etienne de Klerk (Tilburg), Zhao Sun (Montreal), Jean Lasserre, Roxana Hess (Toulouse), Pablo Parrilo (MIT)

# Polynomial optimization



Minimize a **polynomial** function  $f$  over a region

$$K = \{x \in \mathbb{R}^n : g_1(x) \geq 0, \dots, g_m(x) \geq 0\}$$

defined by **polynomial** inequalities

$$\text{Compute: } f_{\min} = \min_{x \in K} f(x)$$

This is a hard problem, even for simple sets  $K$  like

- ▶ the **standard simplex**

$$\Delta_n = \{x \in \mathbb{R}^n : x_1, \dots, x_n \geq 0, \sum_{i=1}^n x_i = 1\}$$

- ▶ the **hypercube**  $Q_n = [0, 1]^n$

- ▶ the **unit sphere**

$$S^{n-1} = \{x \in \mathbb{R}^n : \sum_{i=1}^n x_i^2 = 1\}$$

It captures **hard combinatorial optimization problems** like computing the **stability number**  $\alpha(G)$  and **Max-Cut**.

# Polynomial optimization formulations for $\alpha(G)$

- ▶ Optimization over the simplex: [Motzkin-Straus 1965]

$$\frac{1}{\alpha(G)} = \min x^T(I + A_G)x \quad \text{s.t.} \quad \sum_{v \in V} x_v = 1, \quad x_v \geq 0 \quad (v \in V)$$

- ▶ Optimization over the hypercube: [Park-Hong 2011]

$$\alpha(G) = \max \sum_{u \in V} x_u - \sum_{uv \in E} x_u x_v \quad \text{s.t.} \quad x \in [0, 1]^n$$

- ▶ Optimization over the unit sphere: [Nesterov 2003]

$$\frac{2\sqrt{2}}{3\sqrt{3}} \sqrt{1 - \frac{1}{\alpha(G)}} = \max 2 \sum_{ij \in \bar{G}} z_{ij} y_i y_j \quad \text{s.t.} \quad (y, z) \in S^{n+m-1}$$

# Lower bounds for polynomial optimization

To approximate:

$$f_{\min} = \min_{x \in K} f(x), \quad \text{where } K = \{x : g_1(x) \geq 0, \dots, g_m(x) \geq 0\}$$

use LP/SDP hierarchies

[Shor (1987), Nesterov (2000), Parrilo, Lasserre (2000–)]

- Express  $f_{\min} = \sup \lambda$  s.t.  $f(x) - \lambda \geq 0$  over  $K$
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Testing whether  $f$  is **nonnegative** is hard, but

testing whether  $f$  is a **sum-of-squares (SoS)**:  $f = \sum_j g_j^2$

can be done **efficiently** using semidefinite programming (SDP)

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 $\deg g^{\alpha}$ ,  $\deg(\sigma_J g^J)$ ,  $\deg(\sigma_j g_j) \leq r$ . Clearly:

$$\{ \underline{f}_{\text{lp}}^{(r)}, \underline{f}_{\text{sosP}}^{(r)} \} \leq \underline{f}_{\text{sosS}}^{(r)} \leq f_{\min}$$

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- ▶ What about the **rate of convergence**?

# Rate of convergence of SoS lower bounds

## Theorem

Assume  $K \subseteq (-1, 1)^n$ . For  $f = \sum_{\alpha} f_{\alpha} x^{\alpha}$ , set  $L_f = \max_{\alpha} |f_{\alpha}| \frac{\alpha!}{|\alpha|!}$ .

- ▶ [Schweighofer 2004] **Analysis of Schmüdgen type bounds:**

*There exists a constant  $c > 0$  such that for any polynomial  $f$  of degree  $d$ :*

$$f_{\min} - \underline{f}_{\text{-sos}}^{(r)} \leq cd^4 n^{2d} L_f \frac{1}{\sqrt[c]{r}} \quad \text{for } r \geq cd^c n^{cd}.$$

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**Can choose  $c = 1$  for Schmüdgen type bounds for simplex & cube.**



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For  $K$  compact one may use **sum-of-squares density functions**:

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... in  $O(1/\sqrt{r})$

# This talk

## Analysis of the rate of convergence:

- ▶ For the **simplex**  $\Delta_n$  and the **cube**  $Q_n$ : regular grid upper bounds and the LP lower bounds.
- ▶ For  $K$  **compact**: SoS-density upper bounds.
- ▶ For the **cube**  $Q_n$ : other upper bounds (using other density functions).



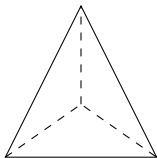
# POLYNOMIAL OPTIMIZATION OVER THE SIMPLEX

**Upper bounds:** For  $r \geq 1$

$$\Delta_n(r) = \{x \in \Delta_n : rx \in \mathbb{N}^n\}$$

$$f_{\min, \Delta_n(r)} = \min_{x \in \Delta_n(r)} f(x)$$

**Example:**  $n = 3$ :

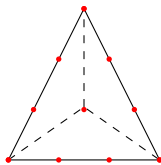


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$$r = 3$$

Let  $f = \sum_{|\beta|=d} f_{\beta} x^{\beta}$  homogeneous of degree  $d$ .

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**Lower bounds:**

$$f_{\min} \geq \underline{f}_{\text{lp}}^{(r)} = \sup \lambda \quad \text{s.t.} \quad f(x) - \lambda = \underbrace{h(x)}_{\mathbb{R}_+[x]_r} + \underbrace{u(x)(1 - \sum_{i=1}^n x_i)}_{\mathbb{R}[x]_r}$$

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where  $r^d = r(r-1) \cdots (r-d+1)$



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$$f_{\min} \leq f_{\min, \Delta_n(r)} = \min_{x \in \Delta_n(r)} f(x) = \min_{\alpha \in \mathbb{N}^n: |\alpha|=r} f(\alpha/r) \quad (= \sum_{|\beta|=d} f_\beta \frac{\alpha^\beta}{r^d})$$

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where  $r^d = r(r-1) \cdots (r-d+1)$

$$\underline{f}_{\text{lp}}^{(r)} \leq f_{\min} \leq f_{\min, \Delta_n(r)}$$

Error analysis:  $f_{\text{lp}}^{(r)} \leq f_{\text{min}} \leq f_{\text{min}, \Delta_n(r)}$

Theorem (De Klerk-L-Parrilo 2006)

- ▶ For any polynomial  $f$  of degree  $d$ :

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- ▶ [De Klerk-L-Sun 2015] May choose  $C_f = m C_d (f_{\max} - f_{\min})$ , if  $f$  has a **rational minimizer** with denominator  $m$ .

## Key idea for the $1/r$ convergence rate of $f_{\min, \Delta_n(r)}$

- ▶ Use the **Bernstein approximation** of  $f$  of order  $r$ :

$$B_r(f)(x) = \sum_{\alpha \in \mathbb{N}^n: |\alpha|=r} f\left(\frac{\alpha}{r}\right) \frac{r!}{\alpha!} x^\alpha.$$

- ▶ So  $B_r(f)(x)$  is the **average value** of  $f$  over the grid points in  $\Delta_n(r)$ .



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- ▶ Using properties of Bernstein approximations, one can show:

$$\max_{x \in \Delta_n} B_r(f)(x) - f(x) \leq \frac{C_d}{r}.$$

# POLYNOMIAL OPTIMIZATION OVER THE HYPERCUBE

**Upper bounds:**

$$f_{\min} \leq f_{\min, Q_n(r)} = \min_{x \in Q_n(r)} f(x) = \min_{\alpha \in \mathbb{N}^n: \alpha_i \leq r} f(\alpha/r)$$

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- ▶ [De Klerk-L 2010] For  $r \geq dn$   $f_{\min} - \underline{f}_{\text{lp}}^{(r)} \leq \binom{d+1}{3} \frac{n^{d+1} L_f}{r}$ .



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**but**  $|Q_n(r)| = (r+1)^n \dots$

# MEASURE-BASED UPPER BOUNDS

## Upper bounds using SoS densities

Lasserre (2011) proved: For  $K$  compact

$$\begin{aligned} f_{\min} &= \min_{x \in K} f(x) = \min_{\mu \text{ probability measure on } K} \int_K f(x) d\mu \\ &= \inf \int_K f(x) h(x) dx \quad \text{s.t. } h \text{ SoS}, \int_K h(x) dx = 1. \end{aligned}$$

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## Theorem (De Klerk-L-Sun 2015)

Assume  $K$  is compact and 'nice' (e.g. convex body) and  $f$  has Lipschitz constant  $M_f$ . There exist constants  $C_K > 0$  and  $r_K \geq 1$  such that

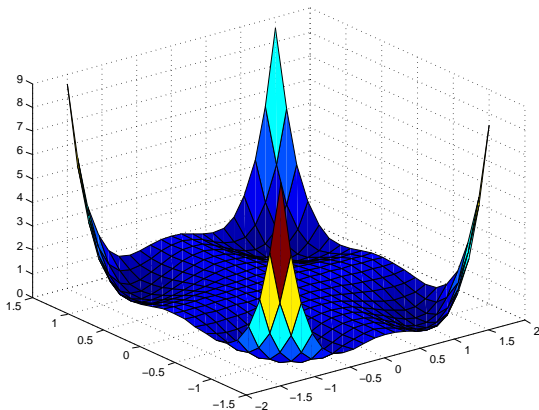
$$\bar{f}_{\text{SoS}}^{(r)} - f_{\min} \leq \frac{C_K M_f}{\sqrt{r}} \quad \forall r \geq r_K.$$



Example: Motzkin polynomial on  $K = [-2, 2]^2$

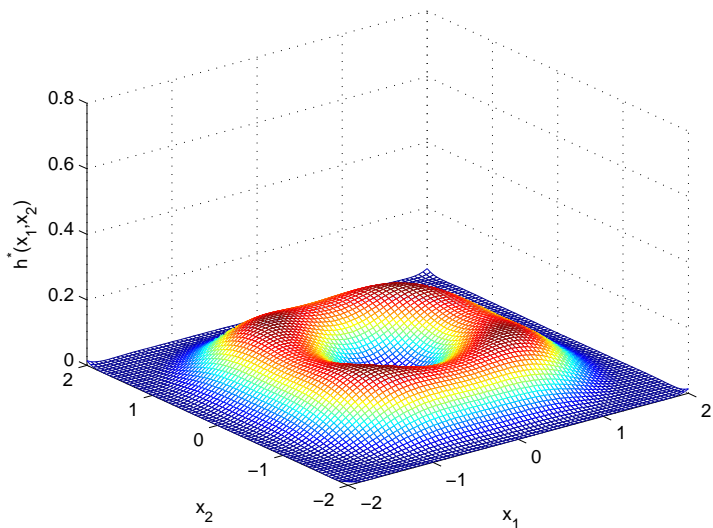
$$f(x_1, x_2) = x_1^4 x_2^2 + x_1^2 x_2^4 - 3x_1^2 x_2^2 + 1$$

Global minimizers:  $(-1, -1)$ ,  $(-1, 1)$ ,  $(1, -1)$ ,  $(1, 1)$ .



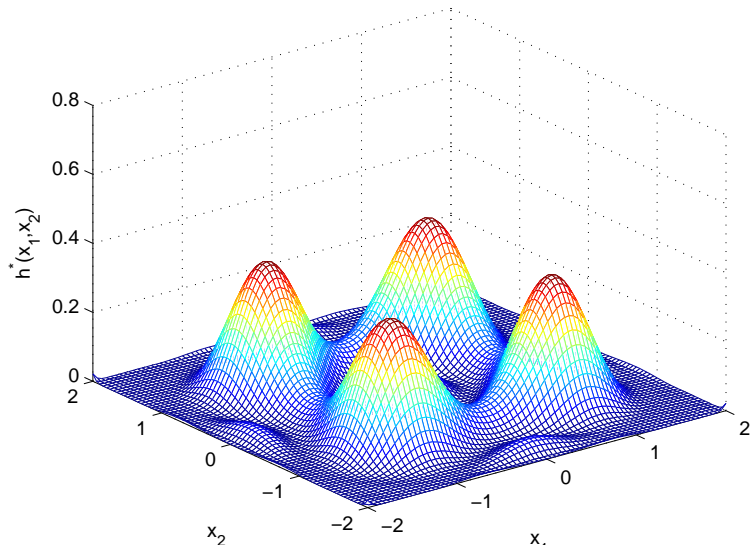
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Optimal SoS density  $h$  of **degree 12**



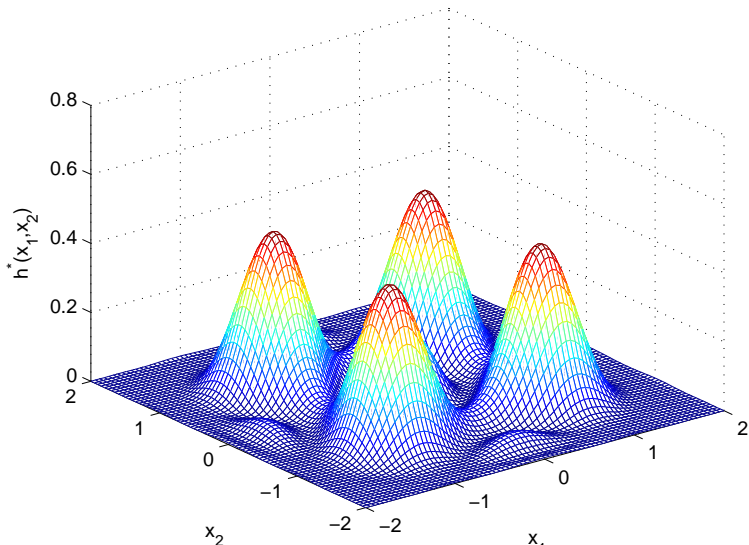
# Example: Motzkin polynomial on $[-2, 2]^2$ (ctd.)

Optimal SoS density  $h$  of **degree 16**



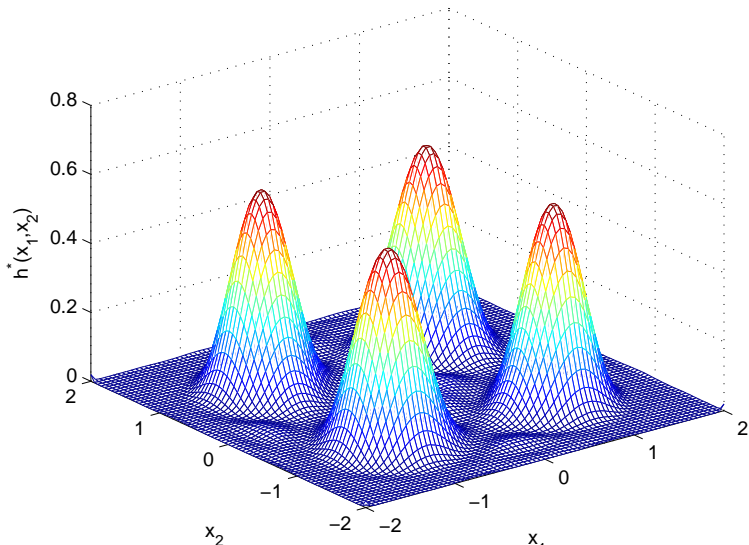
# Example: Motzkin polynomial on $[-2, 2]^2$ (ctd.)

Optimal SoS density  $h$  of degree 20



# Example: Motzkin polynomial on $[-2, 2]^2$ (ctd.)

Optimal SoS density  $h$  of **degree 24**



## Convergence analysis: sketch of proof

- ▶ Let  $\mathbf{a}$  be a global minimizer of  $f$  in  $K$ .
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$$\text{Vol}(B_\epsilon(\mathbf{a}) \cap K) \geq \eta_K \text{Vol}(B_\epsilon(\mathbf{a})) \quad \forall 0 < \epsilon \leq \epsilon_K.$$

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- ▶ The analysis will work when selecting:

$$\sigma \sim \frac{1}{\sqrt{2r+1}}$$

# Convergence analysis

- ▶ Define the **normalizing constant**:  $c_a^r \int_K H_{r,a}(x) dx = 1$ .
- ▶  $K$  is **nice at  $a$**  if there exist constants  $\eta_K$  and  $\epsilon_K$  such that

$$\text{Vol}(B_\epsilon(a) \cap K) \geq \eta_K \text{Vol}(B_\epsilon(a)) \quad \forall 0 < \epsilon \leq \epsilon_K.$$

Will be used to control the constant  $c_a^r$ .

- ▶ The analysis will work when selecting:

$$\sigma \sim \frac{1}{\sqrt{2r+1}}$$

▶

**Main result:** If  $f$  has Lipschitz constant  $M_f$  and  $K$  is **nice at  $a$**  then

$$\int_K f(x) c_a^r H_{r,a}(x) dx - f_{\min} \leq \frac{C_K M_f}{\sqrt{r}}.$$

# OTHER MEASURE-BASED UPPER BOUNDS FOR THE HYPERCUBE:

- HANDELMAN TYPE DENSITIES
- SCHMÜDGEN TYPE DENSITIES



## Using Handelman type densities for $K = [0, 1]^n$

For  $K = [0, 1]^n$ , consider the upper bound:

$$\bar{f}_{\text{lp}}^{(r)} = \min \int_K f(x) h(x) dx \quad \text{s.t.} \quad h(x) = \sum_{\alpha, \beta \in \mathbb{N}^n} \underbrace{\lambda_{\alpha, \beta}}_{\geq 0} x^\alpha (1-x)^\beta, \quad \int_K h(x) dx = 1.$$

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Theorem (De Klerk-Lasserre-L-Sun 2015)

- ▶  $\bar{f}_{\text{lp}}^{(r)}$  needs  $O(n^r)$  elementary computations:

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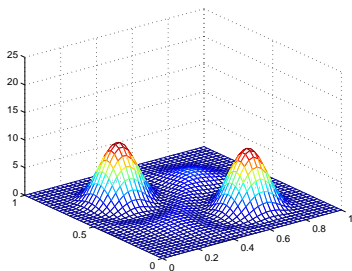
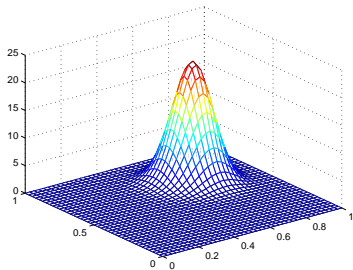
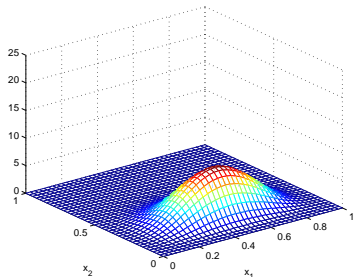
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$$\bar{f}_{\text{lp}}^{(r)} - f_{\min} \leq \frac{C_f}{\sqrt{r}}, \quad \leq \frac{C'_f}{r} \quad \text{if } f \text{ has a rational minimizer.}$$

↪ Link to the **beta distribution**

Motzkin polynomial:

$f(x, y) = (4x - 2)^4(4y - 2)^2 + (4x - 2)^2(4y - 2)^4 - 3(4x - 2)^2(4y - 2)^2 + 1$   
over  $K = [0, 1]^2$ : Handelman-type densities (deg 24, 50) & SOS (deg 24)



# Using Schmüdgen type densities for $K = [-1, 1]^n$

For  $K = [-1, 1]^n$  consider the upper bound:

$$\bar{f}_{\text{SoS}}^{(r)} = \min \int_K f(x) h(x) d\mu_n \quad \text{s.t.} \quad h(x) = \sum_{I \subseteq [n]} \underbrace{\sigma_I}_{\text{SoS}} (1 - x^2)^I, \quad \int_K h(x) d\mu_n = 1$$

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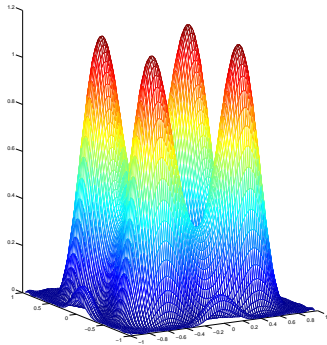
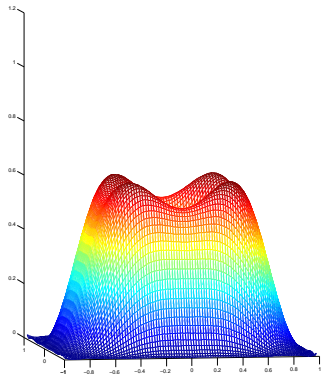
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Motzkin polynomial:  $f(x, y) = 64(x^4y^2 + x^2y^4) - 48x^2y^2 + 1$   
over  $K = [-1, 1]^2$

Optimal Schmüdgen type densities of **degree 12, 16**:



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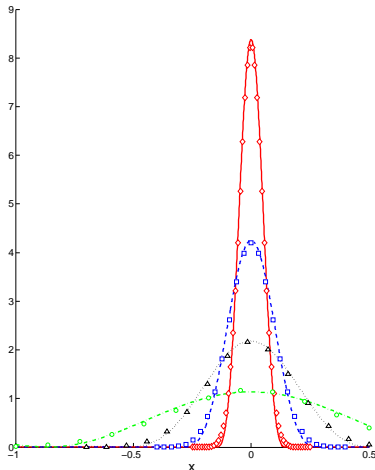
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$\rightsquigarrow$  rate of convergence in  $1/r^2$  for  $\bar{f}_{\text{SoS}}^{(r)}$ .

Kernel approximations  $\delta_0^{(r)}(x)$  of the Dirac at degree  $r = 8, 16, 32, 64$ :



$$\frac{\delta_0^{(r)}(x)}{\pi\sqrt{1-x^2}} \sim \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right), \quad \text{with } \sigma \sim \frac{\pi}{r+2}.$$

## Concluding remarks

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r	Matyas		Three-Hump Camel		Motzkin	
	Value	Time (sec.)	Value	Time (sec.)	Value	Time (sec.)
2	8.26667	0.000739	265.774	0.000742	4.2	0.000719
6	4.28172	0.000072	29.0005	0.000066	1.06147	0.000080
12	2.99563	0.000263	4.43983	0.000263	0.801069	0.000208
18	1.83356	0.000655	2.55032	0.000586	0.565553	0.000766
24	1.11785	0.001753	1.2775	0.001693	0.406076	0.001712
30	0.8524	0.002270	1.0185	0.002936	0.3004	0.002351
36	0.5760	0.005510	0.7113	0.004882	0.2300	0.006060
40	0.4815	0.006975	0.6064	0.007031	0.1817	0.007686

Matyas:  $f = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2$ ,  $K = [-10, 10]^2$ .

Three-Hump Camel:  $f = 2x_1^2 - 1.05x_1^4 + \frac{1}{6}x_1^6 + x_1x_2 + x_2^2$ ,  $K = [-5, 5]^2$ .

Motzkin:  $f = x_1^4x_2^2 + x_1^2x_2^4 - 3x_1^2x_2^2 + 1$ ,  $K = [-2, 2]^2$ .

$f_{\min} = 0$ , bounds  $\bar{f}_{\text{SOS}}^{(r)}$  with SoS density.

## Concluding remarks

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Better theoretical convergence results for the upper bounds, but slower in practice...

- ▶ **Problem:** Show **better convergence rates** for the lower bounds.

New techniques needed ...



## Concluding remarks

- ▶ One can use the upper bounds to generate good feasible solutions using sampling.

r	$\bar{f}_{\text{SoS}}^{(r)}$	Mean	Variance	Minimum	Sample Size
2	265.774	216.773	177142.0	0.106854	20
		261.23	193466.0	0.11705	1000
4	29.0005	28.0344	2964.85	1.1718	20
		27.712	6712.8	0.014255	1000
14	4.43983	3.96711	20.3193	0.260331	20
		3.7911	57.847	0.0076111	1000
22	1.71275	1.30757	1.90985	0.0320489	20
		1.6379	7.2518	0.0021144	1000
24	1.27749	0.841194	0.914514	0.0369565	20
		1.2105	2.3	0.0005154	1000
Uniform Sample		304.032	163021.0	1.65885	20
		243.216	183724.0	0.00975034	1000

SoS upper bounds for the Three-Hump Camel function:

$$f = 2x_1^2 - 1.05x_1^4 + \frac{1}{6}x_1^6 + x_1x_2 + x_2^2 \text{ over } K = [-5, 5]^2.$$

THANK YOU

## Based on the papers

- ▶ *Improved convergence rates for Lasserre-type hierarchies of upper bounds for box-constrained polynomial optimization.* With E. de Klerk, R. Hess, arXiv:1603.03329.
- ▶ *Bound-constrained polynomial optimization using only elementary calculations.* With E. de Klerk, J. Lasserre and Z. Sun, arXiv:1507.04404.
- ▶ *Convergence analysis for Lasserre's measure-based hierarchy of upper bounds for polynomial optimization.* With E. de Klerk and Z. Sun, arXiv:1411.6867
- ▶ *On the convergence rate of grid search for polynomial optimization over the simplex.* With E. de Klerk, Z. Sun, J. Vera, Opt. Letters, 2016.
- ▶ *An alternative proof of a PTAS for fixed-degree polynomial optimization over the simplex.* With E. de Klerk and Z. Sun. Math.Prog. 2014.
- ▶ *A PTAS for the minimization of polynomials of fixed degree over the simplex.* With E. De Klerk and P. Parrilo. TCS, 2006.

# Optimization over the unit sphere

SOS lower bounds:

$$\underline{f}_{\text{SOS}}^{(r)} = \sup \lambda \quad \text{s.t.} \quad f(x) - \lambda = \underbrace{\sigma_0}_{\text{SOS of degree } 2r} + u(1 - \sum_{i=1}^n x_i^2).$$

## Theorem

Let  $f$  be a homogeneous polynomial of even degree.

- ▶ [Faybusovich 2003]  $f_{\min} - \underline{f}_{\text{SOS}}^{(r)} = O(\frac{1}{r})$  for  $r = O(n)$ .
- ▶ In addition, Doherty-Wehner (2013) construct measure-based upper bounds with the same performance guarantee.
- ▶ Parrilo-Wehner announced convergence in  $O(\frac{1}{r^2})$  for both upper and lower bounds.