Performance analysis of approximation hierarchies for polynomial optimization

CWI

Tilburg University

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Joint works with Lucas Slot and Etienne de Klerk

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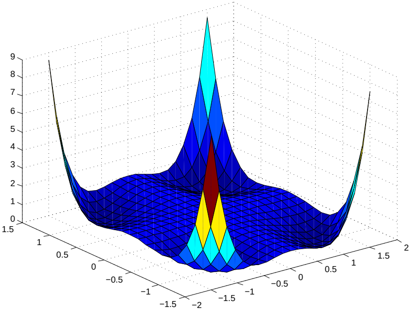
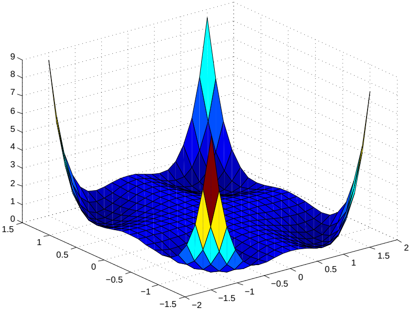


Minimize a **polynomial** f over a **compact** (semialgebraic) set K

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



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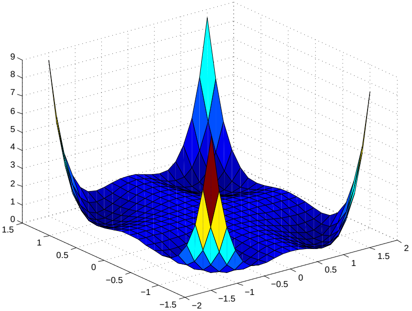
NP-hard problem: it captures hard combinatorial problems
(like computing $\alpha(G)$: the maximum size of a stable set in a graph G)
when K is a hypercube or a simplex and $\deg(f) = 2$,
or K is a sphere and $\deg(f) = 3$



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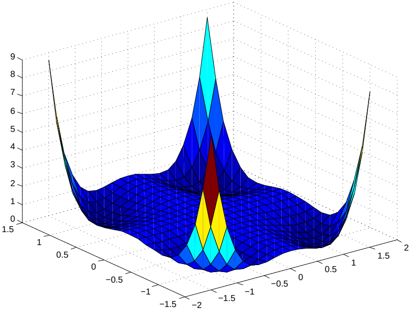
$$\alpha(G) = \max_{x \in [0,1]^n} \sum_{i=1}^{n} x_i - \sum_{ij \in E} x_i x_j \qquad \frac{1}{\alpha(G)} = \min_{x \in \Delta_n} \sum_{i=1}^{n} x_i^2 + 2 \sum_{ij \in E} x_i x_j$$



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$$\frac{2\sqrt{2}}{3\sqrt{3}} \sqrt{1 - \frac{1}{\alpha(G)}} = \max_{(x,y) \in \mathbb{S}^{n+|\overline{E}|-1}} 2 \sum_{ij \in \overline{E}} x_i x_j y_{ij}$$

[Motzkin-Straus'65, Nesterov'03]

Two hierarchies of **lower/upper bounds** for polynomial optimization:

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

(1) Lasserre/Parrilo *sums-of-squares based* **lower bounds:**

$$f_{(r)} \leq f_{\min}$$

(2) Lasserre *measure-based* **upper bounds:**

$$f_{\min} \leq f^{(r)}$$

Common feature:

- For fixed r the bounds can be computed via a semidefinite program (SDP) with matrix size $O(n^r)$

  (since *sum-of-squares polynomials can be modelled with SDP*)
- the bounds converge asymptotically to $f_{\min}$ as $r \to \infty$

This lecture: Main focus on the **error analysis** of these bounds

Lasserre/Parrilo sums-of-squares based lower bounds

‘Sums-of-squares’ (SoS) lower bounds

$$\textbf{(P)} \quad \boxed{f_{\min} = \min_{x \in K} f(x) = \sup_{\lambda \in \mathbb{R}} \lambda \ \text{ s.t. } \ f(x) - \lambda \geq 0 \ \text{ on } K}$$

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When $$K = \{x \in \mathbb{R}^n : \ g_1(x) \geq 0, \ldots, g_m(x) \geq 0\}$$ with $g_j \in \mathbb{R}[x]$

one can replace the **hard** condition: “$f(x) - \lambda \geq 0$ on K”

by the **easier** condition:

“$f(x) - \lambda$ is a ‘weighted sum’ of sum-of-squares polynomials”

$\rightsquigarrow$ Get the SoS **bounds**:

$$f_{(r)} = \sup \ \lambda \ \text{ s.t. } \ f - \lambda = \underbrace{s_0}_{\deg \leq 2r} + \underbrace{s_1 g_1}_{\deg \leq 2r} + \ldots + \underbrace{s_m g_m}_{\deg \leq 2r}, \ s_j \ \text{ SoS}$$

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- $f_{(r)} \leq f_{(r+1)} \leq f_{\min}, \quad f_{(r)} \nearrow f_{\min}$ as $r \to \infty$
- Can compute $f_{(r)}$ with **semidefinite programming**

[Lasserre 2001]

Error analysis in terms of the relaxation order r

- [Nie-Schweighofer 2007] Let K semi-algebraic compact (+technical condition). There exists a constant $c = c_K$ such that for any degree d polynomial f:

$$f_{\min} - f_{(r)} \leq 6d^3 n^{2d} L_f \; \frac{1}{\sqrt[c]{\log \frac{r}{c}}} \qquad \text{for all } r \geq c \cdot e^{(2d^2 n^d)^c}$$

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- [Fang-Fawzi 2020] **Improved error analysis** in $O(1/r^2)$ for the **unit sphere** $K = \mathbb{S}^{n-1}$, for f homogeneous with degree $2d$:

$$f_{\min} - f_{(r)} \leq (f_{\max} - f_{\min}) \frac{C_d^2 n^2}{r^2} \quad \text{for } r \geq C_d \cdot n$$

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There is an intimate link with the **analysis of the upper bounds**

More later!

Lasserre measure-based upper bounds

Basic observation: identify **points** $x \in K$ with **Dirac measures on K**

$$f_{\min} = \min_{x \in K} f(x) = \min_{\nu \text{ probability measure on } K} \int_K f(x) d\nu(x)$$

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Theorem (Lasserre 2011)

For K compact, one may restrict to $d\nu(x) = h(x) d\mu(x)$, where μ is a **fixed** *measure with support K and σ is a sum-of-squares density:*

$$f_{min} = \inf_{\sigma} \int_K f(x)\sigma(x)\, d\mu \quad s.t. \quad \sigma \; SoS, \; \int_K \sigma(x)\, d\mu = 1$$

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Bound degree: $\deg(\sigma) \leq 2r \rightsquigarrow$ **upper bounds** $f^{(r)}$ converging to $f_{\min}$:

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- $f_{\min} \leq f^{(r+1)} \leq f^{(r)}$, $\quad f^{(r)} \searrow f_{\min}$, $\quad f^{(r)}$ can be computed via SDP
- **but** one needs to know the **moments** of μ: $\quad m_\alpha = \int_K x^\alpha d\mu(x)$
  to compute $\int_K f(x) d\mu = \int_K (\sum_\alpha f_\alpha x^\alpha) d\mu = \sum_\alpha f_\alpha m_\alpha$

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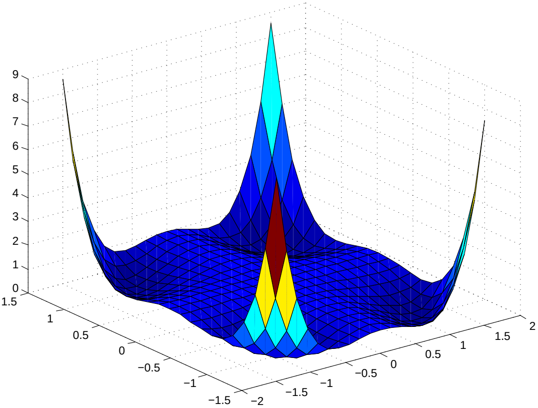
- m_α known if μ Lebesgue on cube, ball, simplex; Haar on sphere,...

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

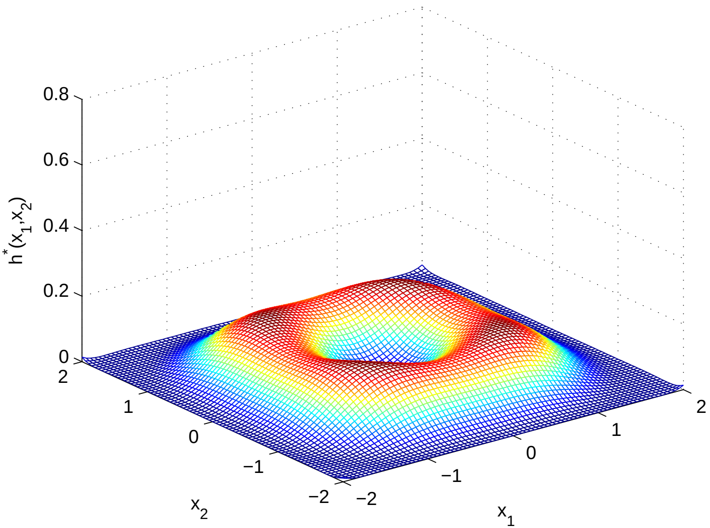
$$f(x_1, x_2) = x_1^4 x_2^2 + x_1^2 x_2^4 - 3x_1^2 x_2^2 + 1$$

Four global minimizers: $(-1, -1)$, $(-1, 1)$, $(1, -1)$, $(1, 1)$



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

Optimal SoS density σ of degree 12



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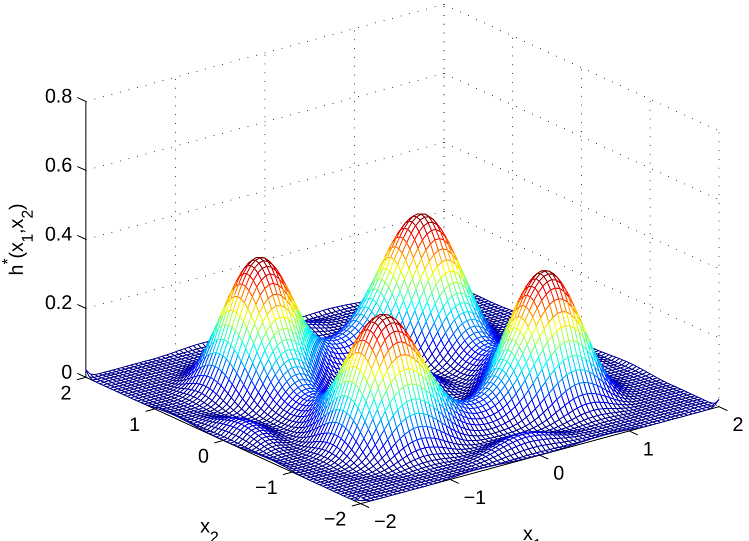
Optimal SoS density σ of degree 16



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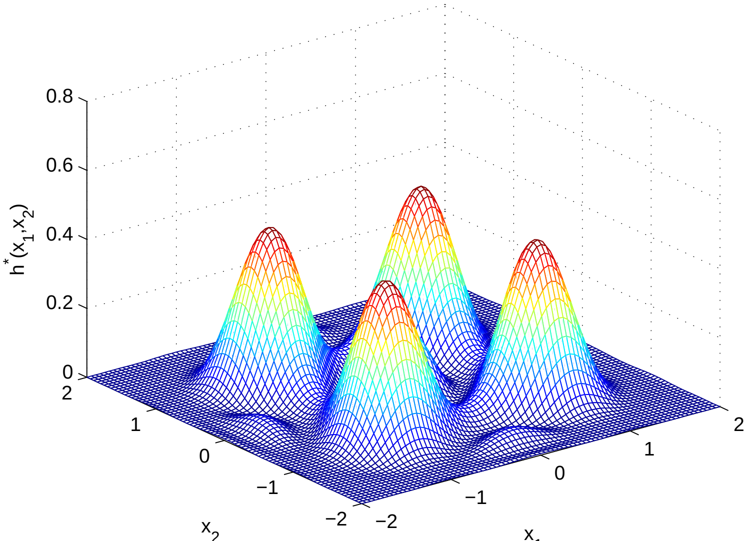
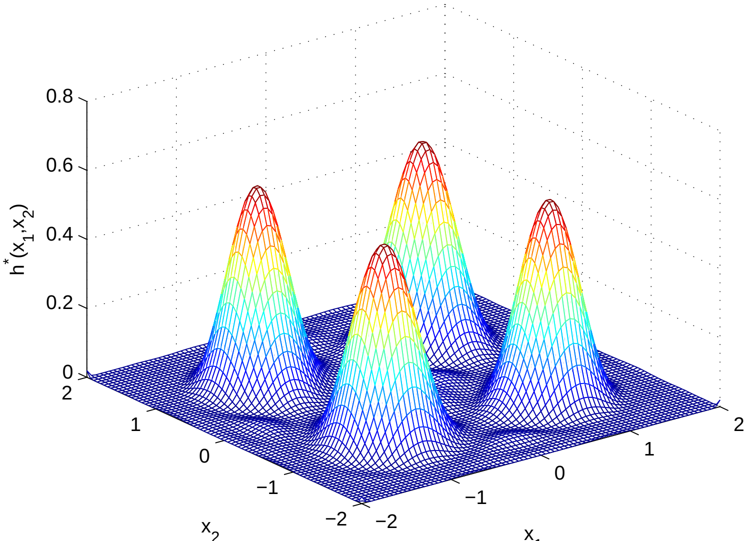
Optimal SoS density σ of degree 20



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

Optimal SoS density σ of degree 24



Goal: Analyze rate of convergence of error range:

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compact K	$E^{(r)}(f)$	μ	
Hypercube			
f linear	$\Theta(1/r^2)$	$(1-x^2)^\lambda$, $\lambda > -1$	de Klerk-L 2020
any f	$O(1/r^2)$	Chebyshev: $\lambda = -1/2$	" "
any f	$O(1/r^2)$	$\lambda \geq -1/2$	Slot-L 2020
Sphere			
f homogeneous	$O(1/r)$	Haar	Doherty-Wehner'12
any f	$O(1/r^2)$	Haar	de Klerk-L 2020
Ball			
any f	$O(1/r^2)$	$(1-\|x\|^2)^\lambda$, $\lambda \geq 0$	Slot-L 2020
Simplex, 'round' convex body	$O(1/r^2)$	Lebesgue	Slot-L 2020
Convex body, fat semialgebraic	$O((\log r)^2/r^2)$	Lebesgue	Slot-L 2020

Key proof strategies

(1) Design '*nice*' **SoS polynomial densities**
'*that look like the Dirac delta at a global minimizer*'
and reduce to the **univariate case**
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(2) Reformulate $f^{(r)}$ as an **eigenvalue problem** and
relate $f^{(r)}$ to **extremal roots of orthogonal polynomials**
$\leadsto$ $O(1/r^2)$ rate for the Chebyshev measure on $[-1,1]$,
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(3) Use more tricks (**Taylor approx.**, **integration**, **'local similarity'**) to
transport the $O(1/r^2)$ rate for $[-1, 1]$ to more sets (and measures):
hypercube, simplex, ball, sphere, 'round' convex bodies

Strategy 1: Use SoS approximations of Dirac measures

$\rightsquigarrow O(\frac{\log^2 r}{r^2})$ rate for general K

Step 1: Analyse cheaper (univariate) bounds

Instead of the **multivariate** upper bounds:

$$f^{(r)} = \inf_{\sigma} \int_K f(x)\sigma(x)\, d\mu \;\text{ s.t. }\; \sigma \text{ SoS},\; \int_K \sigma(x)\, d\mu = 1,\; \deg(\sigma) \leq 2r$$

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Consider the **weaker univariate** upper bounds:

$$f_{pfm}^{(r)} \quad = \min_s \int_K f(x)s(f(x))d\mu(x) \ \text{ s.t. } \quad \int_K s(f(x))d\mu(x) = 1, \ \deg(s) \leq 2r$$

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Then: $f_{\min} \le f^{(rd)} \le f^{(r)}_{pfm}$ if $d = \deg(f)$

$f^{(r)}_{pfm} \searrow f_{\min}$ [Lasserre 2019]

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$f^{(r)}_{pfm} \searrow f_{\min}$ [Lasserre 2019]

Step 2: Use SoS approximations of the Dirac delta

Use the degree $4r$ (half-)**needle polynomials** $s_r^h(t)$ of [Kroó-Swetits'92] ($h > 0$, $r \in \mathbb{N}$, defined as squares of Chebyshev polynomials)

$$s_r^h(t) \begin{cases} = 1 & \text{at } t = 0 \\ \leq 1 & \text{at } t \in [0,1] \\ \leq 4e^{-\frac{1}{2}\sqrt{h}r} & \text{at } t \in [h,1] \end{cases}$$

as **univariate SoS density** (with $h = (\log r)^2/r^2$)

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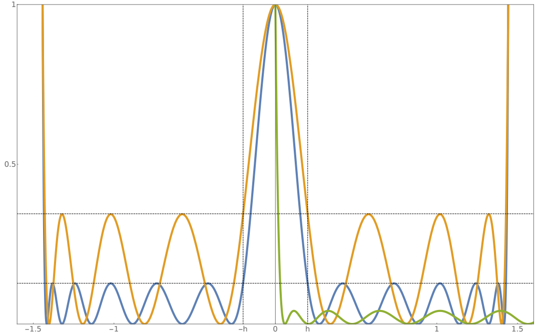

In green, the half-needle polynomial with $h = 1/5$

Theorem (Slot-L 2020)

Assume K is a **convex body**, *or K is a* **compact semialgebraic set** *with a* **dense interior** *(aka* **fat***). Then*

$$f_{pfm}^{(r)} - f_{min} = O\left(\frac{(\log r)^2}{r^2}\right)$$

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- The analysis is **almost tight**

  There can be a **separation** between the multivariate and univariate bounds:

  For $f(x) = x^{2d}$ and $K = [-1, 1]$:

$$f_{\min} = 0 \le f^{(2dr)} = O\Big(\frac{(\log r)^{2d}}{r^{2d}}\Big) \le f_{pfm}^{(r)} = \Omega\Big(\frac{1}{r^2}\Big)$$

Theorem (Slot-L 2020)

Assume K is a **convex body**, *or K is a* **compact semialgebraic set** *with a* **dense interior** *(aka* **fat***). Then*

$$f_{pfm}^{(r)} - f_{min} = O\left(\frac{(\log r)^2}{r^2}\right)$$

- The analysis is **almost tight**

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- Can one get rid of the factor $(\log r)^2$?

  Yes *for the* **multivariate bounds** $f^{(r)}$, *for some* **nice sets** K

First basic trick: Suffices to analyze quadratic polynomials

Analyze simpler upper estimators

Lemma

Let $\mathbf{a} \in K$ *be a global minimizer of* f *in* K*.*

Set $\gamma = \max_{x \in K} \|\nabla^2 f(x)\|$.

By Taylor's theorem, f *has a* **quadratic, separable** *upper estimator:*

$$f(x) \leq f(\mathbf{a}) + \langle \nabla f(\mathbf{a}), x - \mathbf{a} \rangle + \gamma \|x - \mathbf{a}\|^2 := g(x),$$

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$$E^{(r)}(f) \leq E^{(r)}(g)$$

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Hence, for all $r \in \mathbb{N}$,

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$\rightsquigarrow$ It suffices to analyze **quadratic** (separable) polynomials

and sometimes we may even obtain a **linear** upper estimator!
(e.g. for the sphere)

Eigenvalue reformulation

μ given measure with support K

$$f^{(r)} = \min \int_K f\sigma \, d\mu \quad \text{s.t.} \quad \sigma \text{ SoS}, \int_K \sigma \, d\mu = 1, \; \deg(\sigma) \le 2r$$

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Then: σ SoS $\iff$ $\sigma = ((p_\alpha)_{|\alpha|\leq r})^\mathsf{T} X (p_\alpha)_{|\alpha|\leq r}$ for some $(X_{\alpha,\beta}) \succeq 0$

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$$f^{(r)} = \min \left\{ \langle M_r(f), X\rangle : \; \mathrm{Tr}(X) = 1, \; X \succeq 0 \right\} = \lambda_{\min}(M_r(f))$$

[Lasserre 2011]

Analysis in the univariate case: $K = [-1, 1]$

suffices to consider:

f linear, or quadratic

$K = [-1, 1]$, linear case: $f(x) = x$

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Theorem (classical theory of orthogonal polynomials)

Let $\{p_0, p_1, p_2, \ldots\}$ be a (graded) orthonormal basis of $\mathbb{R}[x]$ w.r.t. μ. Then the polynomials p_k satisfy a **3-term recurrence***:*

$$xp_k = a_k p_{k+1} + b_k p_k + a_{k-1} p_{k-1} \quad \text{for } k \geq 0, \quad p_0 \text{ constant}$$

$\rightsquigarrow$ *the (Jacobi) matrix* $M_r(x) = \left(\int_{-1}^{1} x p_i p_j \, d\mu\right)_{i,j=0}^{r}$ *is tri-diagonal and its eigenvalues are the roots of* p_{r+1}

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For $f(x) = x$:

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$M_r(f) = \left(\int_{-1}^{1} (x^2 + kx) p_i p_j d\mu \right)_{i,j=0}^{r}$ is 5-diagonal **'almost' Toeplitz**:

$$M_r(f) = \left(\begin{array}{cc|ccccccc}
1/2 & \frac{k}{\sqrt{2}} & \frac{4}{\sqrt{2}} & & & & & & \\
\frac{k}{\sqrt{2}} & 3/4 & \frac{k}{2} & \frac{1}{4} & & & & & \\
\hline
\frac{4}{\sqrt{2}} & \frac{k}{2} & a & b & c & & & & \\
 & \frac{1}{4} & b & a & b & c & & & \\
 & & c & b & \ddots & \ddots & \ddots & & \\
 & & & c & \ddots & \ddots & \ddots & \ddots & \\
 & & & & \ddots & \ddots & \ddots & \ddots & c \\
 & & & & & \ddots & \ddots & \ddots & b \\
 & & & & & & c & b & a
\end{array}\right), \qquad a = \frac{1}{2},\; b = \frac{k}{2},\; c = \frac{1}{4}$$

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For the **Chebyshev measure** $\prod_i (1-x_i^2)^{-1/2}$ *on* $[-1,1]^n$ *and for any polynomial* f*:*

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Next: extend to the Jacobi measure $(1-x^2)^{\lambda}$ on $[-1,1]$ with $\lambda \ge -1/2$ and to other sets

Extension:
$O(\frac{1}{r^2})$ convergence rate for the sphere

using an integration trick

Key steps

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By Taylor, f has a **quadratic** upper estimator:

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This is based on the **integration trick**:

$$\int_{-1}^{1} \sigma(x_1)(1 - x_1^2)^{\frac{n-3}{2}} dx_1 = C \int_{S^{n-1}} \sigma(x_1) d\mu$$

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[de Klerk-L 2020]

Extension:

$O(\frac{1}{r^2})$ convergence rate for

box, ball, simplex, round convex body

using ‘local similarity’ trick

‘Local similarity’: lift results from $(\widehat{K}, \widehat{w})$ to (K, w)

Lemma (Slot-L 2020)

Let $\mathbf{a} \in K$ be a global minimizer of f in K. Assume:

$K \subseteq \widehat{K}$*,* w *a weight function on* K*,* $\widehat{w}$ *weight function on* $\widehat{K}$ *satisfy:*

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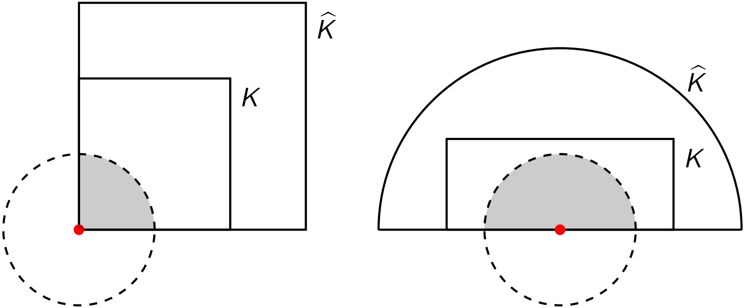

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(2) $w, \widehat{w}$ *are* **‘locally similar’ at** *a:*

$$m \cdot \widehat{w}(x) \leq w(x) \text{ on } \mathrm{int}(K) \cap B_\epsilon(\mathbf{a}) \quad \text{for some } \epsilon, m > 0.$$

(3) $w(x) \leq \widehat{w}(x)$ *for all* $x \in \mathrm{int}(K)$.

‘Local similarity’: lift results from $(\widehat{K}, \widehat{w})$ to (K, w)

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Let $\mathbf{a} \in K$ *be a global minimizer of* f *in* K*. Assume:*

$K \subseteq \widehat{K}$, w *a weight function on* K, $\widehat{w}$ *weight function on* $\widehat{K}$ *satisfy:*

(1) $K, \widehat{K}$ *are* **‘locally similar’ at a***:*

$$K \cap B_\epsilon(\mathbf{a}) = \widehat{K} \cap B_\epsilon(\mathbf{a}) \quad \text{for some } \epsilon > 0.$$

(2) $w, \widehat{w}$ *are* **‘locally similar’ at** *a:*

$$m \cdot \widehat{w}(x) \le w(x) \ \text{ on } \ \mathrm{int}(K) \cap B_\epsilon(\mathbf{a}) \quad \text{for some } \epsilon, m > 0.$$

(3) $w(x) \le \widehat{w}(x)$ *for all* $x \in \mathrm{int}(K)$.

Then, f *has an upper estimator* g *on* $\widehat{K}$*, exact at* $\mathbf{a}$*, satisfying*

$$E^{(r)}_{K,w}(f) \le E^{(r)}_{\widehat{K},\widehat{w}}(g).$$

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Note: (1),(2) clearly hold if $\mathbf{a} \in \mathrm{int}(K)$

Lift known $O(1/r^2)$ rate for $\widehat{K} = [-1,1], \lambda = -\frac{1}{2}$

(1) to $K = [-1,1]$, with $w(x) = (1-x^2)^\lambda$, $\lambda \geq -1/2$, any f

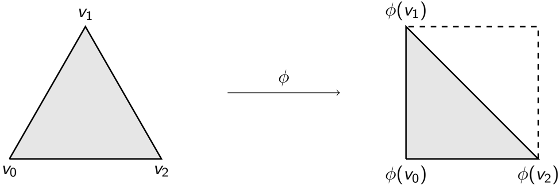
[using Chebyshev weight $\widehat{w}(x) = (1-x^2)^{-1/2}$], to $K = [-1,1]^n$

(2) to any K, with $w = 1$, when minimizer a lies in the **interior** of K

[using $K \subseteq \widehat{K} = [-1,1]^n$ with $\widehat{w} = 1$]

(3) to K simplex, with $w = 1$, when minimizer lies on the **boundary**

[after applying affine mapping and using $\widehat{K} = [-1,1]^n$ with $\widehat{w} = 1$]



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(4) to K ball, with $w(x) = (1-\|x\|^2)^\lambda$, $\lambda \geq 0$

[using a linear upper estimator and an integration trick, when the minimizer lies on the **boundary**]

(5) to K 'round' convex body, with $w = 1$ (i.e., K has inscribed and circumscribed tangent balls at any boundary point)

[using the result for the ball $\widehat{K}$ with $\widehat{w} = 1$]

Back to analyzing the lower bounds

for the unit sphere

Polynomial kernel approach for the unit sphere

Goal: Let $f \in \mathcal{P}_d$: polynomial of degree d on $\mathbb{S}^{n-1}$

$$f_{(r)} = \sup\ \lambda\ \text{ s.t. } f(x) - \lambda = \sigma(x)\ \text{ on } \mathbb{S}^{n-1}, \text{ where } \sigma \text{ SoS}, \deg(\sigma) \leq 2r$$

Theorem: [Fang-Fawzi 2020] $f_{\min} - f_{(r)} = O(\frac{1}{r^2})$

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$\rightsquigarrow$ **kernel operator K** : $p \in \mathcal{P} \mapsto \mathbf{K}p(x) = \int_{\mathbb{S}^{n-1}} p(y) K(x, y) d\mu(y) \ \in \mathcal{P}$

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Deriving the analysis of $f_{(r)}$

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By (A1), (A4): $f + 3\epsilon = \mathbf{K}(\mathbf{K}^{-1}f + 3\epsilon)$ is SoS with degree $2r$ on $\mathbb{S}^{n-1}$

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Next: Construct such kernel $K(x, y)$ with $\epsilon = O(1/r^2)$ using *Fourier analysis* and reducing to the *upper bound approach* (in univariate case)

- Select $K(x, y)$ invariant under action of $O(n) \times O(n)$ on $\mathbb{S}^{n-1} \times \mathbb{S}^{n-1}$

- Select $K(x, y)$ invariant under action of $O(n) \times O(n)$ on $\mathbb{S}^{n-1} \times \mathbb{S}^{n-1}$
- Harmonic decomposition: $\mathcal{P} = \oplus_{k \geq 0} \mathrm{Harm}_k = \mathrm{span}(e_{k,i}) : i \in [h_k]\}$

Select: $K(x, y) = \sum_{k=0}^{2r} \lambda_k \left(\sum_{i=1}^{h_k} e_{ki}(x) e_{ki}(y)\right)$

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Write: $q(t)^2 = \sum_{k=0}^{2r} \lambda_k C_k^n(t)$, where $C_k^n(t)$ are the Gegenbauer orthogonal polynomials on $[-1,1]$ w.r.t. $d\nu(t) = (1-t^2)^{(n-3)/2} dt$

Final step: select λ_k via the 'upper bound' approach

Want: $q(t)^2 = \sum_{k=0}^{2r} \lambda_k C_k^n(t)$, where $\lambda_0 = 1$ and $\sum_{k=1}^{d}(1-\lambda_k)$ is small
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Note: $\lambda_k = \int_{-1}^{1} q(t)^2 C_k^n(t) d\nu(t), \quad 1 = \lambda_0 = \int_{-1}^{1} q(t)^2 d\nu(t)$

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So we arrive at the problem:

$$F^{(r)} = \min_{q \in \mathbb{R}[t]_r} \int_{-1}^{1} q(t)^2 \; F(t) \; d\nu(t) \text{ s.t. } \int_{-1}^{1} q(t)^2 d\nu(t) = 1$$

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$\rightsquigarrow$ optimal q gives desired λ_k $\rightsquigarrow$ desired kernel $K(x,y)$

$\rightsquigarrow$ desired rate $O(1/r^2)$ for SoS lower bounds $f_{(r)}$

Concluding remarks

- Interesting interplay between the **lower** and **upper** bounds
- An analogous technique can be applied to analyse the **lower bounds** $f_{(r)}$ when minimizing f on the Boolean cube $\{0,1\}^n$

  [Slot-L 2021]
- For the box $[-1,1]^n$, one can derive an analysis in $O(1/r^2)$ for the **lower bounds** based on the *preordering* (instead of the *quadratic module*)
- Open question: Can one get an improved analysis for the **lower bounds** based on the quadratic module for the box, the ball, etc. ?
- The error analysis for the **upper bounds** $f^{(r)}$ extends to **rational** functions f [dK-L'19]

  and can be adapted to the **general problem of moments**

  [de Klerk-Postek-Kuhn'19]

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