Convergence analysis of approximation hierarchies for polynomial optimization

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Joint works with Etienne de Klerk and Lucas Slot

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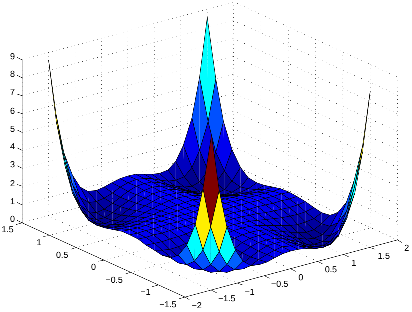
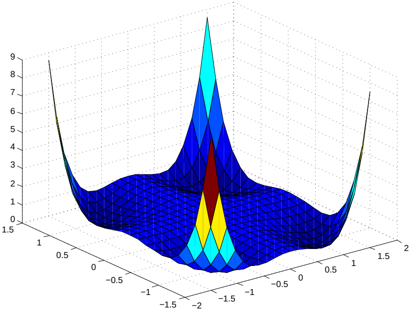


Minimize a **polynomial** f over a **compact** (semialgebraic) set K

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



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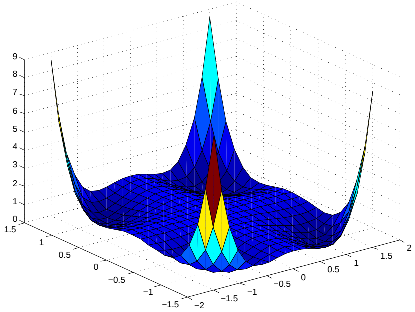
NP-hard problem: it captures, for instance, computing $\alpha(G)$
(the maximum cardinality of a stable set in graph G)
when K is a hypercube or a simplex and $\deg(f) = 2$,
or K is a sphere and $\deg(f) = 3$



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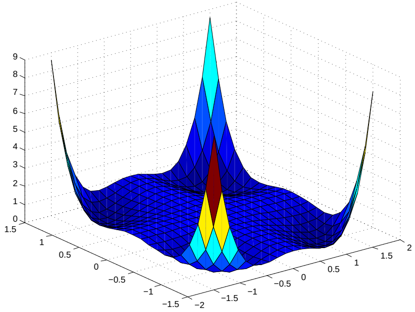
$$\alpha(G) = \max_{x \in [0,1]^n} \sum_{i=1}^{n} x_i - \sum_{ij \in E} x_i x_j \qquad \frac{1}{\alpha(G)} = \min_{x \in \Delta_n} \sum_{i=1}^{n} x_i^2 + 2 \sum_{ij \in E} x_i x_j$$



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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]

This lecture: hierarchies of **bounds** for polynomial optimization:

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

- Quick recap on the (usual) sums-of-squares based **lower bounds**
- Main focus on the measure-based **upper bounds**, in particular on the **analysis of their convergence rate**

Lasserre/Parrilo sums-of-squares based lower bounds

'Sums-of-squares' (SoS) lower bounds

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

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by the **easier** condition:

"$f(x) - \lambda$ is a 'weighted sum' of sums of squares of polynomials"

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

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

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  [Putinar 1993]: $p>0$ on K compact (*) $\Longrightarrow$ p has such SoS dec.

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- **Asymptotic convergence:** $f_{(r)} \nearrow f_{\min}$ as $r \to \infty$ [Lasserre 2001]
- Compute $f_{(r)}$ efficiently for **fixed** r, with **semidefinite programming**

Testing sums of squares of polynomials with SDP

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The SDP: $\left\{ \begin{array}{l} \displaystyle\sum_{\beta,\gamma | \beta+\gamma=\alpha} M_{\beta,\gamma} = f_\alpha \quad (|\alpha| \leq 2d) \\ M \succeq 0 \end{array} \right.$ **is feasible**

Gram-matrix method [Powers-Wörmann 1998]

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$$c = 0 \quad \rightsquigarrow \quad f = (x^2 + xy)^2 + \tfrac{3}{2}(xy + y^2)^2 + \tfrac{1}{2}(xy - y^2)^2$$

Convergence analysis in terms of relaxation order r

Theorem (Nie-Schweighofer 2007)

Under the conditions of Putinar's theorem: K compact (+ Archimedean), there exists a constant $c = c_K$ such that for any degree d polynomial f:

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

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Yes for the **unit sphere**

Theorem (Fang-Fawzi 2019)

Let $K = \mathbb{S}^{n-1}$ the unit sphere, f homogeneous polynomial of degree $2d$.

There exists a constant C_d such that

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

This improves the earlier $O(1/r)$ result of [Doherty-Wehner 2012]

Lasserre measure-based upper bounds

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

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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 h is a sum-of-squares density:*

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

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$$\boxed{f_{min} = \inf \int_K f(x)h(x)\, d\mu \quad s.t. \quad h \text{ SoS}, \ \int_K h(x)\, d\mu = 1}$$

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

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- $f_{\min} \le f^{(r)}$, $\quad f^{(r)} \searrow f_{\min}$, $\quad f^{(r)}$ 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 $\int_K f(x) d\mu = \int_K (\sum_\alpha f_\alpha x^\alpha) d\mu = \sum_\alpha f_\alpha m_\alpha$

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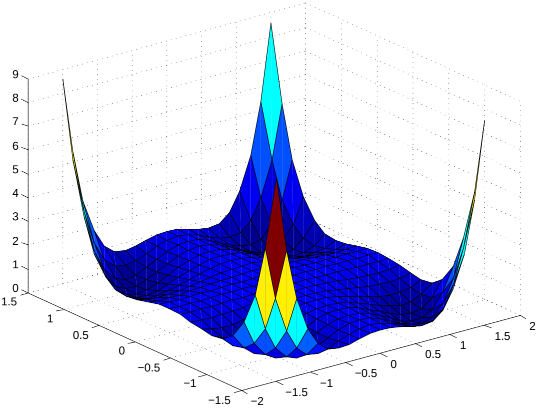
- m_α known if μ Lebesgue on cube, ball, simplex; Haar on sphere,...

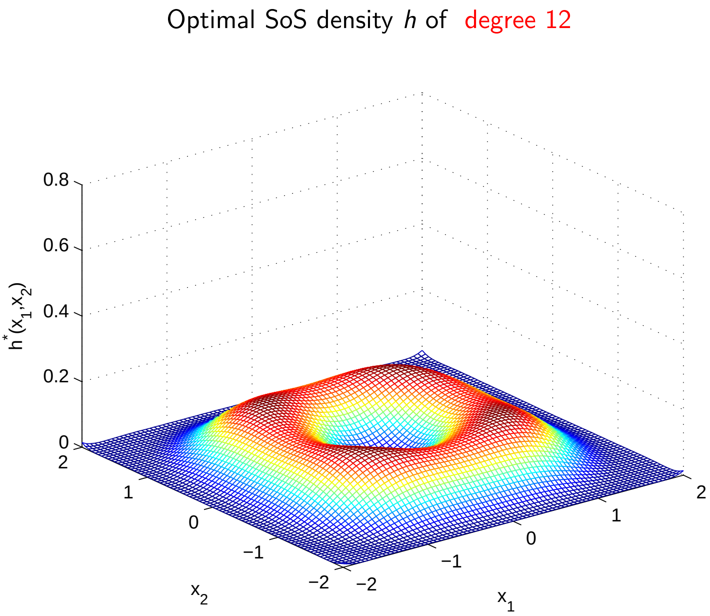
Example: Motzkin polynomial on $K = [-2, 2]^2$

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

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



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



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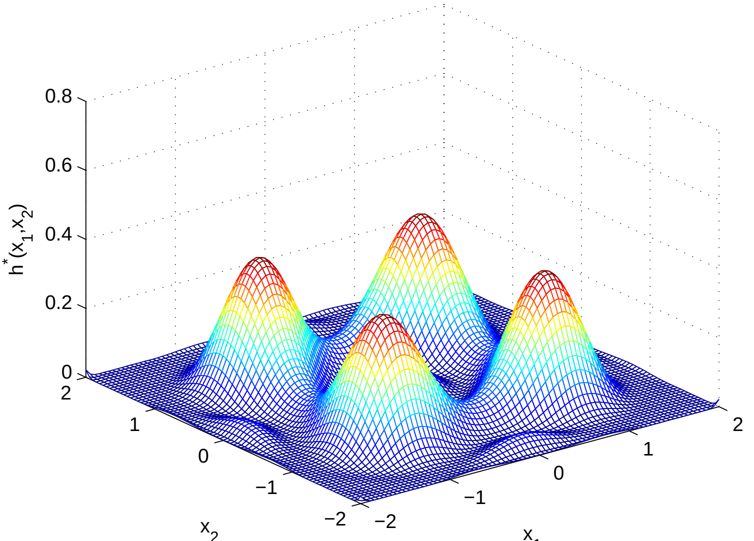
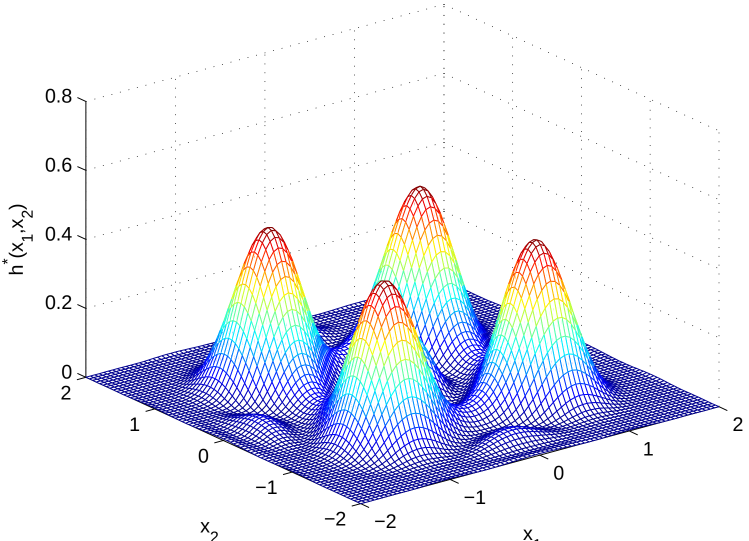
Optimal SoS density h of degree 16



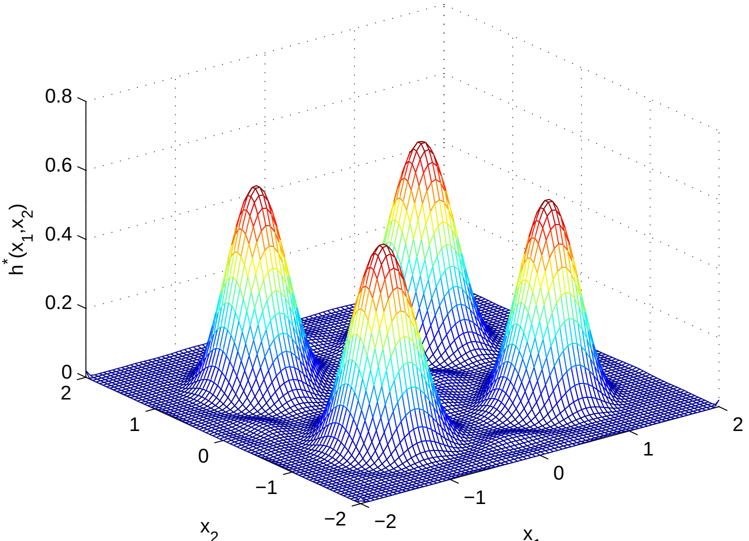
Example: Motzkin polynomial on $[-2,2]^2$ (ctd.)

Optimal SoS density h of degree 20



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

Optimal SoS density h of degree 24



Goal: Analyze rate of convergence of error range:

$$E^{(r)}(f) = E^{(r)}_{\mu,K}(f) := f^{(r)} - f_{\min}$$

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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'19
any f	$O(1/r^2)$	Chebyshev: $\lambda = -1/2$	de Klerk-L'19

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f homogeneous	$O(1/r)$	Haar	Doherty-Wehner'12
any f	$O(1/r^2)$	Haar	de Klerk-L'20
Ball			
any f	$O(1/r^2)$	$(1-\|x\|^2)^{\lambda}$, $\lambda \geq 0$	Slot-L'20
Simplex, 'round' convex body	$O(1/r^2)$	Lebesgue	Slot-L'20

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Convex body	$O((\log r)^2/r^2)$	Lebesgue	Slot-L'20

Key proof strategies

(1) Reformulate $f^{(r)}$ as an **eigenvalue problem** and relate $f^{(r)}$ to **roots of orthogonal polynomials**

$\rightsquigarrow$ $O(1/r^2)$ rate for the Chebyshev measure on $[-1, 1]$ and other measures (with Jacobi weight) for **linear** polynomials

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(2) Design '*nice*' **SoS polynomial densities** '*that look like the Dirac delta at a global minimizer*', (combined with using **push-up measures**) to get the $O((\log r)^2/r^2)$ rate for general K by reducing to the **univariate case** of $[0,1]$

First basic trick: reduction to the analysis of quadratic and separable polynomials

Analyze simpler upper estimators

Lemma

Let $a \in K$ 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:*

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

where $f(a) = g(a) \quad \rightsquigarrow \quad f_{min} = g_{\min}.$

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

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

$\rightsquigarrow$ It suffices to analyze **quadratic** polynomials

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

Eigenvalue reformulation & application to the univariate case: $K = [-1, 1]$

μ given measure with support K

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

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Choose an **orthonormal basis** $\{p_\alpha : |\alpha| \leq 2r\}$ of $\mathbb{R}[x]_{2r}$ w.r.t. μ and set

$$\boxed{M_r(f) := \left(\int_K f \ p_\alpha p_\beta \ d\mu\right)_{|\alpha|,|\beta| \leq r}}$$

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Note: $\quad h \text{ SoS} \iff h = ((p_\alpha)_{|\alpha| \le r})^{\mathsf{T}} X (p_\alpha)_{|\alpha| \le r} \quad$ for some $X \succeq 0$

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$$\rightsquigarrow \quad \int_K f h \, d\mu \ = \ \langle M_r(f), X \rangle, \quad \int_K h \, d\mu = Tr(X)$$

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For $K = [-1, 1]$, can analyze $f^{(r)}$ for Chebyshev measure $d\mu = (1 - x^2)^{-1/2} dx$ and any Jacobi measure $d\mu = (1 - x^2)^\lambda dx$ $(\lambda > -1)$ when f is linear

Recall it is enough to deal with f **quadratic**: $f(x) = x$, $f(x) = x^2 + kx$

$K = [-1, 1]$, 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***:*

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

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$$M_r(x) = \begin{pmatrix} b_0 & a_0 & & & & & \\ a_0 & b_1 & a_1 & & & & \\ & a_1 & b_2 & a_2 & & & \\ & & a_2 & b_3 & a_3 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & a_{r-2} & b_{r-1} & a_{r-1} \\ & & & & & a_{r-1} & b_r \end{pmatrix}$$

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Theorem (de Klerk-L'19)

For the Jacobi measure $d\mu = (1-x^2)^\lambda dx$ with $\lambda > -1$, and $f(x) = x$:

$$\boxed{f^{(r)} = \lambda_{\min}(M_r(x)) = \text{smallest root of } p_{r+1} = -1 + \Theta(1/r^2) = f_{\min} + \Theta(1/r^2)}$$

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(2) Minimizer in **interior**: Then, $\; f^{(r)} = \lambda_{\min}(M_r(f)) \quad$ where

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

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

Write $M_r(f) = \begin{pmatrix} * & * & \cdots \\ * & * & \cdots \\ \vdots & \vdots & B \end{pmatrix}$, with B 5-diagonal **Toeplitz** of size $r-1$

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Theorem (de Klerk-L'19)

For the **Chebyshev measure** *on* $[-1,1]^n$ *and any polynomial* f*:*

$$f^{(r)} - f_{min} = O(1/r^2)$$

$O\left(\frac{1}{r^2}\right)$ CONVERGENCE RATE FOR THE SPHERE

Key steps

(1) Reduce to the case when f is **linear**:

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

$f(x) \leq f(a) + \nabla f(a)^T (x - a) + \gamma \|x - a\|^2$

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[de Klerk-L'20]

The bound $1/r^2$ is tight for linear polynomials

Theorem (de Klerk-L'20)

For any linear polynomial $f(x) = (-1)^d (c^T x)^d$, *the analysis is* **tight***:*

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Fact (Martinez et al.'19)

Let $\{(x^{(i)}, w_i) : i \in [N]\}$ *be a* **positive cubature rule** *on* K *that is* **exact for integrating polynomials of degree** $d + 2r$*. If* f *has degree* d

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For $K = \mathbb{S}^{n-1}$, use cubature rule from the roots of Gegenbauer polys.

‘Local similarity’ trick

&

Application to box, ball, simplex, round convex body

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

Lemma (Slot-L'20)

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

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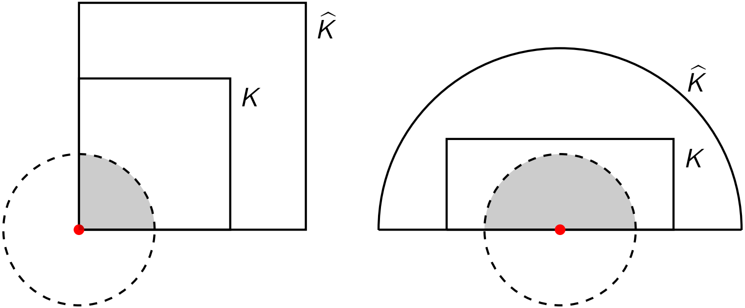

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Note: (1),(2) clearly hold if $a \in \mathrm{int}(K)$

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

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

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

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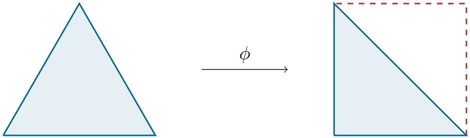

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(5) to K ‘round’ convex body, with $w = 1$ (i.e., K has inscribed and circumscribed tangent balls at any boundary point)

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

SoS approximations of Dirac measures & application to general convex bodies

Cheaper bounds using the ‘push-forward measure’

- μ measure supported by K (e.g., Lebesgue measure)

$\rightsquigarrow$ μ_f **push-forward** of μ by f, supported by $f(K) = [f_{\min}, f_{\max}] \subseteq \mathbb{R}$:

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s **univariate** sum-of-squares

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Hence: $\quad f_{\min} \le f^{(rd)} \le \tau_r(f) \quad$ if $d = \deg(f)$

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$\tau_r(f)$ = smallest root of orthogonal polynomial p_{r+1} w.r.t. measure μ_f, but these are **not known** in general! $\rightsquigarrow$ needs another approach

- May assume $f(K) = [0,1]$ (up to affine transformation)

- Use the (half-)**needle polynomials** $s_r^h(t)$ of [Kroó-Swetits 1992]
($h > 0$, $r \in \mathbb{N}$, defined as squares of Chebyshev polynomials)
with degree $4r$ and satisfying

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

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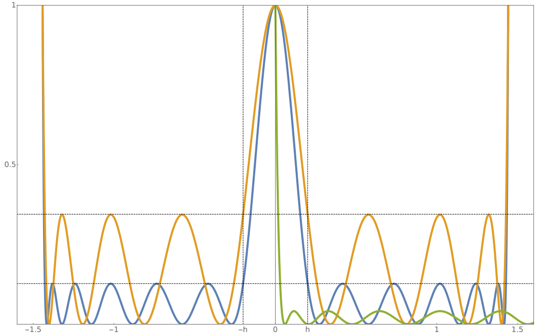

In green, the half-needle polynomial with $h = 1/5$

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Theorem (L-Slot 2020)

Assume K is a convex body. Then

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- May assume $f(K) = [0,1]$ (up to affine transformation)

- Use the (half-)**needle polynomials** $s_r^h(t)$ of [Kroó-Swetits 1992] ($h > 0$, $r \in \mathbb{N}$, defined as squares of Chebyshev polynomials) with degree $4r$ and satisfying

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

Theorem (L-Slot 2020)

Assume K is a convex body. Then

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

Key: Can analyze the error when using the needle polynomials s_r^h (with $h = (\log r)^2/r^2$) as univariate SoS density

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

Concluding remarks

- Can compute $f^{(r)}$ as smallest eigenvalue of a matrix with size $O(n^r)$, and the bounds $\tau_r(f)$ as smallest eigenvalue of a matrix of size $r+1$
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If $\epsilon(r)$ is convergence rate for polynomial minimization on K, then

$$\Delta(r) = O(\sqrt{\epsilon(r)})$$

[De Klerk,Postek,Kuhn'19]

Thank you!