

Sums of squares, moments and optimization

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A system of inequalities

might get easier to solve then you add a few other inequalities

to it.

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$$-X^{12} + 938X^9 - 56629X^6 - 54758X^{10} + 109984X^7 - 55694X^4 - 110449X^8 + 219494X^5 - 109513X^2 + 468X^{11} + 110448X^3 + 468X - 54756 \geq 0$$

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- . . . and the preorder $T := \sum \mathbb{R}[X]^2 + \sum \mathbb{R}[X]^2 g$

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$$\mathbb{R}[X]^2 := \{p^2 \mid p \in \mathbb{R}[X]\}$$

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is a set of polynomials which are

for obvious reasons ≥ 0 on $S = \{x \in \mathbb{R}^n \mid g(x) \geq 0\}$.

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is the preorder generated by g .

We call $P \subseteq \mathbb{R}[X]$ a preorder if $\mathbb{R}[X]^2 \subseteq P$, $P + P \subseteq P$ and $PP \subseteq P$.

Everything works for **basic closed semialgebraic sets**

$$S = \{x \in \mathbb{R}^n \mid g_1(x) \geq 0, \dots, g_m(x) \geq 0\}.$$

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Thomas Jacobi, Alexander Prestel and Mihai Putinar.

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- The converse is trivial.
- Rediscovered by Stengle. Usually attributed to him.

Gilbert Stengle: A Nullstellensatz and a Positivstellensatz in semialgebraic geometry

Math. Ann. **207**, 87–97 (1974)

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Positivstellensatz. $f > 0$ on $S \implies \exists q \in T : qf \in 1 + T$

Tentative proof.

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Tentative proof. **Suppose** $\forall q \in T : qf \notin 1 + T$, i.e., $-1 \notin T - Tf$.

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(Like in the proof of the intermediate value theorem.)

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Hope:

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Then, for any $p \in P$, $p(x) \in p(X) + I = p + I \subseteq P + P \subseteq P$.

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Hence $p(x) \in P \cap \mathbb{R}$

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Then, for any $p \in P$, $p(x) \in p(X) + I = p + I \subseteq P + P \subseteq P$.
Hence $p(x) \in P \cap \mathbb{R} = [0, \infty)$, i.e., $p(x) \geq 0$.

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Hence $p(x) \in P \cap \mathbb{R} = [0, \infty)$, i.e., $p(x) \geq 0$.

In particular, $g(x) \geq 0$ and $-f(x) \geq 0$.

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$$\forall p, q \in \mathbb{R}[X] : (-pq \in P \implies p \in P \text{ or } q \in P)$$

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If $-pq \in P, p \notin P$ and $q \notin P$, then $-1 \in P + Pp$ and $-1 \in P + Pq$, i.e., there are $a, b, c, d \in P$ such that

$$-1 = a + bp$$

$$-1 = c + dq$$

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If $-pq \in P, p \notin P$ and $q \notin P$, then $-1 \in P + Pp$ and $-1 \in P + Pq$, i.e., there are $a, b, c, d \in P$ such that

$$\left. \begin{aligned} -1 &= a + bp \implies a + 1 = -bp \\ -1 &= c + dq \implies c + 1 = -dq \end{aligned} \right\}$$

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If $-pq \in P, p \notin P$ and $q \notin P$, then $-1 \in P + Pp$ and $-1 \in P + Pq$, i.e., there are $a, b, c, d \in P$ such that

$$\left. \begin{array}{l} -1 = a + bp \implies a + 1 = -bp \\ -1 = c + dq \implies c + 1 = -dq \end{array} \right\} \implies -1 = ac + a + c - bdpq \in P.$$

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This is wrong. **What to do?**

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$$\mathbb{R} \rightarrow \mathbb{R}[X]/I \subseteq \text{qf}(\mathbb{R}[X]/I) =: K.$$

The ordering \leq on K is defined via P such that

$$\forall p \in \mathbb{R}[X] : (p + I \geq 0 \iff p \in P).$$

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Have $y \in K^n$. Want $x \in \mathbb{R}^n$!

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Artin and Schreier: Every ordered field K can be extended to a real closed field.

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- $\mathbb{R}[X] := \mathbb{R}[X_1, \dots, X_n]$ polynomial ring
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- . . . and the preorder $T := \sum \mathbb{R}[X]^2 + \sum \mathbb{R}[X]^2 g$

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Konrad Schmüdgen: The K -moment problem for compact semi-algebraic sets

Math. Ann. **289**, No. 2, 203–206 (1991)

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- **Denominatorfree version** of following formulation of the **Positivstellensatz**:

$$f > 0 \text{ on } S \iff \exists \varepsilon > 0 : \exists q \in T : qf \in \varepsilon + T$$

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$$\frac{M + 1}{2} \pm X_i = \frac{1}{2} \left((X_i \pm 1)^2 + \left(M - \sum_{j=1}^n X_j^2 \right) + \sum_{j \neq i} X_j^2 \right).$$

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Marshall Stone, Donald Dubois, Richard Kadison, Eberhard Becker

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- When applying the Positivstellensatz on f , we know already that the bad case in its proof cannot occur.
- Nevertheless, the application on f is the bad one for applications in optimization.

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George Pólya: Über positive Darstellung von Polynomen
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Jesús De Loera, Francisco Santos: **An effective version of Pólya's theorem on positive definite forms**

J. Pure Appl. Algebra **108**, No. 3, 231–240 (1996)

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Victoria Powers, Bruce Reznick: A new bound for Pólya's theorem with applications to polynomials positive on polyhedra
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But $f_\varepsilon := \sum_{|\alpha|=d} a_\alpha (X_1)_\varepsilon^{\alpha_1} \cdots (X_n)_\varepsilon^{\alpha_n} \rightarrow f$ uniformly on Δ for $\varepsilon \rightarrow 0$.

Notation for the whole week (recapitulation)

- $X := (X_1, \dots, X_n)$ variables
- $\mathbb{R}[X] := \mathbb{R}[X_1, \dots, X_n]$ polynomial ring
- $f \in \mathbb{R}[X]$ an arbitrary polynomial
- $g \in \mathbb{R}[X]$ the polynomial defining. . .
- . . . the set $S := \{x \in \mathbb{R}^n \mid g(x) \geq 0\}$. . .
- . . . and the preorder $T := \sum \mathbb{R}[X]^2 + \sum \mathbb{R}[X]^2 g$

Remember that S is assumed
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Weak version $\xRightarrow{\text{Pólya}}$ Strong version
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Proof.

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- Main idea was introduction of new coordinates lying in T and summing up to a natural number N (barycentric coordinates).
- The fact that these coordinates sum up to N allowed **rewriting** f as a homogeneous polynomial in the new coordinates and made the denominator from Pólya's Theorem harmless.

- Rewriting did not change the values of f on

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Lemma. Suppose $C \subseteq \mathbb{R}^n$ is compact and $g \leq 1$ on C . Then

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- Need other coordinates satisfying **more algebraic relations**. In addition, S must inside Δ be defined by an equation since any rewrite step which lets f invariant on S , lets f invariant on the Zariski-closure of S .
- Idea: Try to take g itself as an additional coordinate.

Proof. Suppose $f > 0$ on S . **To show:** $f \in T$. By weak version, w.l.o.g. $X_1, \dots, X_n \in T$ and we find $N \in \mathbb{N}$ such that $N - (X_1 + \dots + X_n + g) \in T$.

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g for Y and $N - (X_1 + \dots + X_n + g)$ for Z .

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- The proof is again an effective construction, in particular, it avoids the Positivstellensatz.
- Degree of $h := f + \lambda(Y - g)^2$ depends **only** on $\deg f$ and $\deg g$ and **not** on geometric properties of f .

First proof:

Optimization of polynomials on compact semialgebraic sets
preprint

Second proof:

An algorithmic approach to Schmüdgen's Positivstellensatz
Journal of Pure and Applied Algebra **166**, 307–319 (2002)

Consequences of second proof:

On the complexity of Schmüdgen's Positivstellensatz
to appear in Journal of Complexity

Notation for the whole week (recapitulation)

- $X := (X_1, \dots, X_n)$ variables
- $\mathbb{R}[X] := \mathbb{R}[X_1, \dots, X_n]$ polynomial ring
- $f \in \mathbb{R}[X]$ an arbitrary polynomial
- $g \in \mathbb{R}[X]$ the polynomial defining. . .
- . . . the set $S := \{x \in \mathbb{R}^n \mid g(x) \geq 0\}$. . .
- . . . and the preorder $T := \sum \mathbb{R}[X]^2 + \sum \mathbb{R}[X]^2 g$

Remember that S is assumed
to be compact.

The S -moment problem

Given a family $(a_\alpha)_{\alpha \in \mathbb{N}^n}$ of real numbers, when is it true that they are the **moments** of some probability measure on S ?

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To be more precise, denote by $\mathcal{M}^1(A)$ the set of all probability measures on a subset A of \mathbb{R}^n . Then the question is:

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To be more precise, denote by $\mathcal{M}^1(A)$ the set of all probability measures on a subset A of \mathbb{R}^n . Then the question is:

For which real families $(a_\alpha)_{\alpha \in \mathbb{N}^n}$ is it true that

$$\exists \mu \in \mathcal{M}^1(S) : \forall \alpha \in \mathbb{N}^n : a_\alpha = \int X^\alpha d\mu$$

holds?

Schmüdgen's solution to the moment problem. Write $g = \sum_{\alpha \in \mathbb{N}^n} c_\alpha X^\alpha$, $c_\alpha \in \mathbb{R}$. For every real family $(a_\alpha)_{\alpha \in \mathbb{N}^n}$ are equivalent:

(1) $a_0 = 1$ and for all real families $(b_\alpha)_{\alpha \in \mathbb{N}^n}$ with finite support,

$$\sum_{\alpha, \beta \in \mathbb{N}^n} b_\alpha b_\beta a_{\alpha+\beta} \geq 0 \quad \text{and} \quad \sum_{\alpha, \beta, \gamma \in \mathbb{N}^n} b_\alpha b_\beta c_\gamma a_{\alpha+\beta+\gamma} \geq 0.$$

(2) $\exists \mu \in \mathcal{M}^1(S) : \forall \alpha \in \mathbb{N}^n : a_\alpha = \int X^\alpha d\mu$

Konrad Schmüdgen: The K -moment problem for compact semi-algebraic sets

Math. Ann. **289**, No. 2, 203–206 (1991)

Schmüdgen's solution to the moment problem. Write $g = \sum_{\alpha \in \mathbb{N}^n} c_\alpha X^\alpha$, $c_\alpha \in \mathbb{R}$. For every linear map $L : \mathbb{R}[X] \rightarrow \mathbb{R}$ are equivalent:

(1) $L(1) = 1$ and for all real families $(b_\alpha)_{\alpha \in \mathbb{N}^n}$ with finite support,

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Proof sketch. For the nontrivial implication, it suffices to show

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Best known strategy for minimization:

Go downhill!





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- Take a **dual standpoint**:

$$f^* = \sup\{a \in \mathbb{R} \mid f - a \geq 0 \text{ on } S\} = \sup\{a \in \mathbb{R} \mid f - a > 0 \text{ on } S\}$$

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Schmüdgen's solution \Downarrow to the moment problem

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Schmüdgen's \Downarrow Positivstellensatz

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Introduce finite-dimensional approximations $T_k \subseteq \mathbb{R}[X]_k$ of $T \subseteq \mathbb{R}[X]$.

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$$= \left\{ \sigma + \tau g \mid \sigma, \tau \in \sum \mathbb{R}[X]^2, \deg \sigma \leq k, \deg(\tau g) \leq k \right\}$$

for arbitrary $k \in \mathcal{N} := \{s \in \mathbb{N} \mid s \geq \max\{\deg g, \deg f\}\}$.

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Warning: Never confuse T_k with $T \cap \mathbb{R}[X]_k \supseteq T_k$.

We saw that

$$f^* = \inf\{L(f) \mid L : \mathbb{R}[X] \rightarrow \mathbb{R} \text{ is linear, } L(1) = 1, L(T) \subseteq [0, \infty)\} \quad \text{and}$$

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In analogy to this, we set

$$P_k^* = \inf\{L(f) \mid L : \mathbb{R}[X]_k \rightarrow \mathbb{R} \text{ is linear, } L(1) = 1, L(T_k) \subseteq [0, \infty)\} \quad \text{and}$$

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$P_k^* \in \mathbb{R} \cup \{\pm\infty\}$ and $D_k^* \in \mathbb{R} \cup \{\pm\infty\}$ are the optimal values of the following pair of optimization problems. . .

(P_k) minimize $L(f)$ subject to $L : \mathbb{R}[X]_k \rightarrow \mathbb{R}$ is linear,
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Theorem (Lasserre). $(D_k^*)_{k \in \mathcal{N}}$ and $(P_k^*)_{k \in \mathcal{N}}$ are increasing sequences that converge to f^* and satisfy $D_k^* \leq P_k^* \leq f^*$ for all $k \in \mathcal{N}$.

Proof.

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$$(P_k) \quad \text{minimize} \quad L(f) \quad \text{subject to} \quad \begin{array}{l} L : \mathbb{R}[X]_k \rightarrow \mathbb{R} \text{ is linear,} \\ L(1) = 1 \text{ and} \\ L(T_k) \subseteq [0, \infty) \end{array}$$

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Clear: P_k^* and D_k^* increase. $\lim_{k \rightarrow \infty} D_k^* \rightarrow f^*$: If $a < f^*$, then $f - a \in T_k$ for some $k \in \mathcal{N}$ by Schmüdgen's Positivstellensatz.

$$(P_k) \quad \text{minimize} \quad L(f) \quad \text{subject to} \quad \begin{array}{l} L : \mathbb{R}[X]_k \rightarrow \mathbb{R} \text{ is linear,} \\ L(1) = 1 \text{ and} \\ L(T_k) \subseteq [0, \infty) \end{array}$$

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Clear: P_k^* and D_k^* increase. $\lim_{k \rightarrow \infty} D_k^* \rightarrow f^*$: If $a < f^*$, then $f - a \in T_k$ for some $k \in \mathcal{N}$ by **Schmüdgen's Positivstellensatz**. Then a is feasible for (D_k) whence $a \leq D_k^*$.

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Theorem. There exists $C \in \mathbb{N}$ depending on f and g and $c \in \mathbb{N}$ depending on f such that

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On the complexity of Schmüdgen's Positivstellensatz
to appear in Journal of Complexity

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In practice: Convergence usually very fast,
 often $D_k^* = P_k^* = f^*$ for small k .

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What can we know from Schmüdgen's solution to the moment problem?

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A priori nothing! But with additional compactness arguments involving Tychonoff's Theorem, the following. . .

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Theorem. Suppose that L_k solves (P_k) nearly to optimality ($k \in \mathcal{N}$).

$$\forall d \in \mathbb{N} : \forall \varepsilon > 0 : \exists k_0 \in \mathcal{N} \cap [d, \infty) : \forall k \geq k_0 : \exists \mu \in \mathcal{M}^1(S^*) :$$

$$\left\| \left(L_k(X^\alpha) - \int X^\alpha d\mu \right)_{|\alpha| \leq d} \right\| < \varepsilon.$$

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Theorem (Lasserre). If S has nonempty interior, then $D_k^* = P_k^*$.

- “Strong duality”

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- “Strong duality”
- “Weak duality” $D_k^* \leq P_k^*$ always holds.
- First proved by using duality theory from semidefinite programming since (P_k) and (D_k) can be translated into semidefinite programs and are as such dual to each other.

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Sketch of Marshall's direct proof.

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Sketch of Marshall's direct proof. It suffices to show that T_k is closed in $\mathbb{R}[X]_k$. For s big (see below), M_k is image of $\mathbb{R}[X]_d^s \times \mathbb{R}[X]_e^s \rightarrow \mathbb{R}[X]_k$:

$$(p_1, \dots, p_s, q_1, \dots, q_s) \mapsto \sum_{i=1}^s p_i^2 + \sum_{i=1}^s q_i^2 g.$$

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This map is quadratically homogeneous and injective.

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Notation for the whole week (recapitulation)

- $X := (X_1, \dots, X_n)$ variables
- $\mathbb{R}[X] := \mathbb{R}[X_1, \dots, X_n]$ polynomial ring
- $f \in \mathbb{R}[X]$ an arbitrary polynomial
- $g \in \mathbb{R}[X]$ the polynomial defining. . .
- . . . the set $S := \{x \in \mathbb{R}^n \mid g(x) \geq 0\}$. . .
- . . . and the preorder $T := \sum \mathbb{R}[X]^2 + \sum \mathbb{R}[X]^2 g$

Remember that S is assumed
to be compact.

Optimization

We consider the problem of **minimizing** f on S . So we want to compute **numerically** the **infimum** (minimum if $S \neq \emptyset$)

$$f^* := \inf\{f(x) \mid x \in S\} \in \mathbb{R} \cup \{\infty\}$$

and, if possible, a **minimizer**, i.e., an element of the set

$$S^* := \{x^* \mid \forall x \in S : f(x^*) \leq f(x)\}.$$

Introduce finite-dimensional approximations $T_k \subseteq \mathbb{R}[X]_k$ of $T \subseteq \mathbb{R}[X]$.

$$\mathbb{R}[X]_k := \{p \mid p \in \mathbb{R}[X], \deg p \leq k\} \quad \text{real vector space}$$

$$T_k := \sum \mathbb{R}[X]_d^2 + \sum \mathbb{R}[X]_e^2 g \quad \text{convex cone}$$

$$= \left\{ \sigma + \tau g \mid \sigma, \tau \in \sum \mathbb{R}[X]^2, \deg \sigma \leq k, \deg(\tau g) \leq k \right\}$$

for arbitrary $k \in \mathcal{N} := \{s \in \mathbb{N} \mid s \geq \max\{\deg g, \deg f\}\}$.

Here $d := \max\{m \in \mathbb{N} \mid 2m \leq k\}$ and $e := \max\{m \in \mathbb{N} \mid 2m + \deg g \leq k\}$.

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Denote the optimal values of these optimization problems by $P_k^* \in \mathbb{R} \cup \{\pm\infty\}$ and $D_k^* \in \mathbb{R} \cup \{\pm\infty\}$, respectively.

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Additional instruments for detecting optimality and extracting solutions

- If L is an optimal solution of (P_k) , $x := (L(X_1), \dots, L(X_n)) \in S$ and $L(f) = f(x)$, then $L(f) = P_k^* \leq f^* \leq f(x) = L(f)$

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Trans. Am. Math. Soc. **352**, No. 6, 2825–2855 (2000)

Additional instruments for detecting optimality and extracting solutions

- If L is an optimal solution of (P_k) , $x := (L(X_1), \dots, L(X_n)) \in S$ and $L(f) = f(x)$, then $L(f) = P_k^* \leq f^* \leq f(x) = L(f)$, i.e., $L(f) = f(x) = f^*$ and therefore $x \in S^*$.
- If L is an optimal solution of (P_k) which comes from a measure μ on S (criteria of Curto and Fialkow for the **truncated** S -moment problem), then $L(f) = P_k^* \leq f^* \leq \int f d\mu = L(f)$, i.e., $L(f) = f^*$ and $\mu \in \mathcal{M}^1(S^*)$. In case that μ has finite support $\text{supp}(\mu)$, it seems that often (?) numerical linear algebra methods can obtain all elements of $\text{supp}(\mu) \subseteq S^*$ from the moments $L(X^\alpha)$, $|\alpha| \leq k$ of the measure μ ?

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How to solve the relaxations?

$$(P_k) \quad \text{minimize} \quad L(f) \quad \text{subject to} \quad \begin{array}{l} L : \mathbb{R}[X]_k \rightarrow \mathbb{R} \text{ is linear,} \\ L(1) = 1 \text{ and} \\ L(T_k) \subseteq [0, \infty) \end{array}$$

$$(D_k) \quad \text{maximize} \quad a \quad \text{subject to} \quad \begin{array}{l} a \in \mathbb{R} \text{ and} \\ f - a \in T_k \end{array}$$

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- When going downhill, we could hit the boundary. Therefore we need to be able to compute effectively a so called **barrier function** defined on the interior of the convex set.
- The cone $S\mathbb{R}_+^{s \times s}$ of positive semidefinite symmetric matrices has such a barrier function:

$$X \mapsto -\ln \det X$$

- Semidefinite programming is an extension of linear programming.
- Linear programming: Optimization of a linear function $\mathbb{R}^s \rightarrow \mathbb{R}$ on the intersection of the selfdual cone $[0, \infty)^s$ with an affine subspace of \mathbb{R}^s .

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- A lot of efficient semidefinite programming solvers are freely available.

Sums of squares and semidefinite matrices

Let v a column vector of length s whose entries generate the vector space $\mathbb{R}[X]_d$. Then $\sum \mathbb{R}[X]_d^2 = \{v^T G v \mid G \in S\mathbb{R}_+^{s \times s}\}$.

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$$\sum_{i=1}^t p_i^2 = (Av)^T Av = v^T \underbrace{(A^T A)}_{\in S\mathbb{R}_+^{s \times s}} v.$$

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Proof. “ \supseteq ” If $G \in SR_+^{s \times s}$, then $G = A^T D A$ for a real (orthogonal) $s \times s$ matrix A and an $s \times s$ diagonal matrix with nonnegative entries.

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Shows also what we used for showing strong duality.

Sums of squares and semidefinite matrices

Remember that, for $k \in \mathcal{N}$,

$$T_k = \sum \mathbb{R}[X]_d^2 + \sum \mathbb{R}[X]_e^2 g$$

where $d := \max\{m \in \mathbb{N} \mid 2m \leq k\}$ and
 $e := \max\{m \in \mathbb{N} \mid 2m + \deg g \leq k\}$.

Let v a column vector of length s whose entries generate the vector space $\mathbb{R}[X]_d$. Let w a column vector of length t whose entries generate the vector space $\mathbb{R}[X]_e$. Then

$$T_k = \{v^T G v + w^T H w g \mid G \in S\mathbb{R}^{s \times s}, H \in S\mathbb{R}^{t \times t}\}.$$

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With little elaborations this gives the translation of (P_k) into a semidefinite program.

Translation into a semidefinite program

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We just outlined how (P_k) can be formulated as a semidefinite program. **For (P_k) this is even easier.** To express that a linear map $L : \mathbb{R}[X]_k \rightarrow \mathbb{R}$ satisfies $L(T_k) \subset [0, \infty)$, one writes down that the matrices representing the following bilinear forms are positive semidefinite:

$$\mathbb{R}[X]_d \times \mathbb{R}[X]_d \rightarrow \mathbb{R} : (p, q) \mapsto L(pq) \quad \text{and}$$

$$\mathbb{R}[X]_e \times \mathbb{R}[X]_e \rightarrow \mathbb{R} : (p, q) \mapsto L(pqg)$$

Implementations

- [Henrion and Lasserre: GloptiPoly](http://www.laas.fr/~henrion/software/gloptipoly/)
`http://www.laas.fr/~henrion/software/gloptipoly/`
- [Prajna, Papachristodoulou, Parrilo: SOSTOOLS](http://control.ee.ethz.ch/~parrilo/sostools/)
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- Both use the free SeDuMi solver by Jos Sturm
- But they need MATLAB and the MATLAB Symbolic Toolbox

Example: The maximum cut problem

Given a graph, i.e., an $n \in \mathbb{N}$ (number of nodes) and a set

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$$\begin{array}{ll} \text{maximize} & \sum_{(i,j) \in E} \frac{1}{2}(1 - x_i x_j) \\ \text{subject to} & x_i^2 = 1 \text{ for all } i \in \{1, \dots, n\} \end{array}$$

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- The n -th relaxation yields the exact maximum cut value.