A new look at nonnegativity on closed sets

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- Positivstellensatze for semi-algebraic sets $\mathbf{K} \subset \mathbb{R}^n$ from the knowledge of defining polynomials
- $\rightarrow$ inner approximations of the cone of polynomials nonnegative on $\mathbf{K}$
- Optimization: Semidefinite relaxations yield lower bounds
- Another look at nonnegativity from knowledge of a measure supported on $\mathbf{K}$.
- $\rightarrow$ outer approximations of the cone of polynomials nonnegative on $\mathbf{K}$
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Let $\mathbf{K} \subseteq \mathbb{R}^n$ be closed

A basic question is:

Characterize the continuous functions $f : \mathbb{R}^n \to \mathbb{R}$ that are nonnegative on $\mathbf{K}$

and if possible ....

a characterization amenable to practical computation!

Because then .....

Positivstellensatze for basic semi-algebraic sets

Let $\mathbf{K} := \{\mathbf{x} \in \mathbb{R}^n : g_j(\mathbf{x}) \geq 0, \quad j = 1, \ldots, m\}$, for some polynomials $(g_j) \subset \mathbb{R}[\mathbf{x}]$.

Here, knowledge on $\mathbf{K}$ is through its defining polynomials $(g_j) \subset \mathbb{R}[\mathbf{x}]$.

Let $\mathcal{C}(\mathbf{K})_d$ be the CONVEX cone of polynomials of degree at most d, nonnegative on $\mathbf{K}$, and $\mathcal{C}_d$ the CONVEX cone of polynomials of degree at most d, nonnegative on $\mathbb{R}^n$.

Define

$$\mathbf{x} \mapsto g_J(\mathbf{x}) := \prod_{k \in J} g_k(\mathbf{x}), \qquad J \subseteq \{1, \ldots, m\}.$$

The preordering associated with (g_j) is the set

$$P(g) := \left\{ \sum_{J\subseteq\{1,\ldots,m\}} \sigma_J \, g_J \;:\; \sigma_J \in \Sigma[\mathbf{x}] \right\}$$

The quadratic module associated with (g_j) is the set

$$Q(g) := \left\{ \sum_{j=1}^{m} \sigma_j \, g_j \;:\; \sigma_j \in \Sigma[\mathbf{x}] \right\}$$

Of course every element of $P(g)$ or $Q(g)$ is nonnegative on $\mathbf{K}$, and the σ_J (or the σ_j) provide certificates of nonnegativity on $\mathbf{K}$.

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Truncated versions

The k-truncated preordering associated with (g_j) is the set

$$P_k(g) := \left\{ \sum_{J\subseteq\{1,\ldots,m\}} \sigma_J\, g_J \;:\; \sigma_J \in \Sigma[\mathbf{x}],\ \deg \sigma_J\, g_J \leq 2k \right\}$$

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d-Truncated versions

One may also define the convex cones

$$\begin{aligned} P_k^d(g) &:= P_k(g) \cap \mathbb{R}[\mathbf{x}]_d \\ Q_k^d(g) &:= Q_k(g) \cap \mathbb{R}[\mathbf{x}]_d \end{aligned}$$

Observe that

$$Q_k^d(g) \subset P_k^d(g) \subset \mathcal{C}(\mathbf{K})_d,$$

and so, the convex cones $Q_k^d(g)$ and $P_k^d(g)$ provide inner approximations of $\mathcal{C}(\mathbf{K})_d$.

... and ... TESTING whether $f \in P_k^d(g)$, or $f \in Q_k^d(g)$

IS SOLVING an SDP!

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Stengle's NichtNegativstellensatz

$$f \geq 0 \text{ on } \mathbf{K} \quad \Leftrightarrow \quad h\,f = f^{2s} + p$$

for some integer s, and polynomials $h, p \in P(g)$.

Moreover, bounds for s and degrees of h, p exist!

Hence, GIVEN $f \in \mathbb{R}[\mathbf{x}]_d$, cheking whether $f \geq 0$ on $\mathbf{K}$

... reduces to solve a SINGLE SDP! ......BUT

- .. its size is out of reach ....!!! (hence try small degree certificates)
- it does not provide a NICE characterization of $\mathcal{C}(\mathbf{K})_d$, and
- not very practical for optimization purpose

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Note in passing that

$$f \geq 0 \text{ on } \mathbb{R}^n \quad (i.e., f \in \mathcal{C}_d) \quad \Leftrightarrow \quad h f = p$$

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Schmüdgen's Positivstellensatz

$$[\,\mathbf{K} \text{ compact and } f > 0 \text{ on } \mathbf{K}\,] \quad \Rightarrow \quad f \in P_k(g)$$

for some integer k.

Putinar Positivstellensatz

Assume that for some $M > 0$, the quadratic polynomial $\mathbf{x} \mapsto M - \|\mathbf{x}\|^2$ is in $Q(g)$. Then:

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for some integer k.

Observe that if $f \geq 0$ on $\mathbf{K}$ then for every $\epsilon > 0$, there exists k such that $f + \epsilon \in Q_k^d(g)$ (or $f + \epsilon \in Q_k^d(g)$) for some k ...

And so, the previous Positivstellensatze state that

$$\overline{\left(\bigcup_{k=0}^{\infty} P_k^d(g)\right)} = \mathcal{C}(\mathbf{K})_d$$

and if $\mathbf{x} \mapsto M - \|\mathbf{x}\|^2$ is in $Q(g)$

$$\overline{\left(\bigcup_{k=0}^{\infty} Q_k^d(g)\right)} = \mathcal{C}(\mathbf{K})_d$$

Duality

Given a sequence $\mathbf{y} = (\mathbf{y}_\alpha)$, $\alpha \in \mathbb{N}^n$, define the linear functional $L_{\mathbf{y}} : \mathbb{R}[\mathbf{x}] \to \mathbb{R}$ by:

$$f \left(= \sum_\alpha f_\alpha \, \mathbf{x}^\alpha\right) \mapsto L_{\mathbf{y}}(f) := \sum_\alpha f_\alpha \, \mathbf{y}_\alpha, \qquad \forall\, f \in \mathbb{R}[\mathbf{x}]$$

A sequence $\mathbf{y}$ has a representing Borel measure on $\mathbf{K}$ if there exists a finite Borel measure μ supported on $\mathbf{K}$, such that

$$\mathbf{y}_\alpha = \int_{\mathbf{K}} \mathbf{x}^\alpha \, d\mu(\mathbf{x}), \qquad \forall \alpha \in \mathbb{N}^n.$$

Theorem (Dual version of Putinar's theorem)

Let $\mathbf{K}$ be compact and assume that the polynomial $M - \|\mathbf{x}\|^2$ belongs to $Q(g)$. Then $\mathbf{y}$ has a representing mesure supported on $\mathbf{K}$ if

$$L_{\mathbf{y}}(h^2) \geq 0, \quad L_{\mathbf{y}}(h^2\, g_j) \geq 0, \quad \forall\, h \in \mathbb{R}[\mathbf{x}]$$

Moment matrix $M_k(\mathbf{y})$

with rows and columns indexed in $\mathbb{N}^n_k = \{\alpha \in \mathbb{N}^n : \sum_i \alpha_i \leq k\}$.

$$M_k(\mathbf{y})(\alpha,\beta) \;:=\; L_{\mathbf{y}}(\mathbf{x}^{\alpha+\beta}) \;=\; \mathbf{y}_{\alpha+\beta}, \quad \alpha,\beta \in \mathbb{N}^n_k$$

For instance in $\mathbb{R}^2$:

$$M_1(y) \;=\; \left[\begin{array}{c|cc} y_{00} & y_{10} & y_{01} \\ \hline y_{10} & y_{20} & y_{11} \\ y_{01} & y_{11} & y_{02} \end{array}\right]$$

Then $\left[L_{\mathbf{y}}(f^2) \geq 0, \quad \forall f,\ \deg(f) \leq k \right] \quad \Leftrightarrow \quad M_k(\mathbf{y}) \succeq 0$

Localizing matrix $M_r(\theta y)$ with respect to $\theta \in \mathbb{R}[\mathbf{x}]$

With $\mathbf{x} \mapsto \theta(\mathbf{x}) = \sum_\gamma \theta_\gamma \, \mathbf{x}^\gamma$

$$M_r(\theta\,\mathbf{y})(\alpha,\beta) \;=\; L_{\mathbf{y}}(\theta\,\mathbf{x}^{\alpha+\beta}) \;=\; \sum_{\gamma\in\mathbb{N}^n} \theta_\gamma\,\mathbf{y}_{\alpha+\beta+\gamma}, \quad \alpha,\beta \in \mathbb{N}^n_k$$

For instance, in $\mathbb{R}^2$, and with $X \mapsto \theta(\mathbf{x}) := 1 - x_1^2 - x_2^2$,

$$M_1(\theta\,\mathbf{y}) = \left[\begin{array}{ccc} y_{00}-y_{20}-y_{02}, & y_{10}-y_{30}-y_{12}, & y_{01}-y_{21}-y_{03} \\ y_{10}-y_{30}-y_{12}, & y_{20}-y_{40}-y_{22}, & y_{11}-y_{21}-y_{12} \\ y_{01}-y_{21}-y_{03}, & y_{11}-y_{21}-y_{12}, & y_{02}-y_{22}-y_{04} \end{array}\right].$$

Then $\left[L_{\mathbf{y}}(f^2\,\theta) \geq 0, \quad \forall f, \deg(f) \leq k\right] \quad \Leftrightarrow \quad M_k(\theta\,y) \succeq 0$

Optimization: Hierarchy of semidefinite relaxations

Consider the global optimization problem

$$f^* = \min\{f(\mathbf{x}) \,:\, \mathbf{x} \in \mathbf{K}\}$$

For every j, let $v_j := \lceil \deg(g_j)/2 \rceil$.

Theorem

Let $\mathbf{K}$ be compact and assume that the polynomial $M - \|\mathbf{x}\|^2$ belongs to $Q(g)$. Consider the semidefinite programs:

$$\rho_k^* := \max\,\{\, \lambda \,:\, f - \lambda \in Q_k(g) \,\}$$

$$\begin{array}{rll} \rho_k := \min_{\mathbf{y}} & L_{\mathbf{y}}(f) & \\ s.t. & L_{\mathbf{y}}(1) = 1 & \\ & M_k(\mathbf{y}),\, M_{k-v_j}(g_j\,\mathbf{y}) \succeq 0, & j = 1, \ldots, m \end{array}$$

Then $\rho_k^* \leq \rho_k$ for all k, and $\rho_k^*, \rho_k \uparrow f^* := \min\,\{\, f(\mathbf{x}) \,:\, \mathbf{x} \in \mathbf{K} \,\}$

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Notice that the primal semidefinite program

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is a relaxation of

$$f^* = \min_{\mu \in M(\mathbf{K})} \left\{ \int_{\mathbf{K}} f\, d\mu \ :\ \mu(\mathbf{K}) = 1 \right\}$$

where $M(\mathbf{K})$ is the space of finite Borel measures on $\mathbf{K}$.

Let $\mathbf{y}^k$ be an optimal solution of the primal SDP

If there is a unique global minimizer $\mathbf{x}^* \in \mathbf{K}$ then $\mu^* = \delta_{\mathbf{x}^*}$ and for every $i = 1, \ldots, n$, $L_{\mathbf{y}^k}(\mathbf{x}_i) \to x_i^*$ as $k \to \infty$.

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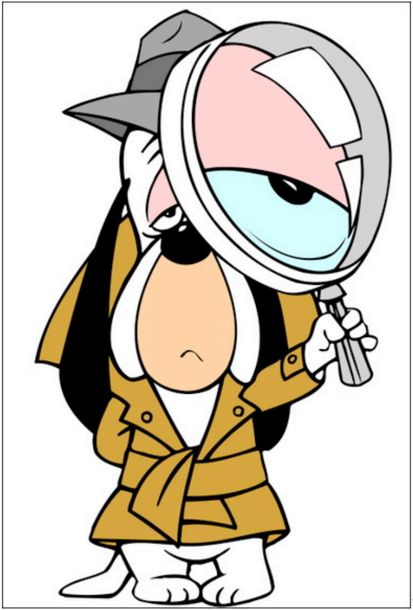
Another look at of nonnegativity



Let $\mathbf{K} \subseteq \mathbb{R}^n$ be an arbitrary closed set, and let $f : \mathbb{R}^n \to \mathbb{R}$ be a continuous function.

Support of a measure

On a separable metric space X, the support $\mathrm{supp}\,\mu$ of a Borel measure μ is the (unique) smallest closed set such that $\mu(X \setminus \mathbf{K}) = 0$.

Here the knowledge on $\mathbf{K}$ is through a measure μ with $\mathrm{supp}\,\mu = \mathbf{K}$, and is independent of the representation of $\mathbf{K}$.

Lemma (Let μ be such that $\mathrm{supp}\,\mu = \mathbf{K}$)

A continuous function $f : X \to \mathbb{R}$ is nonnegative on $\mathbf{K}$ if and only if the signed Borel measure $\nu(B) = \int_{\mathbf{K}\cap B} f\, d\mu$, $B \in \mathcal{B}$, is a positive measure.

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The *only if part* is straightforward. For the *if part*, if ν is a positive measure then $f(\mathbf{x}) \geq 0$ for μ-almost all $\mathbf{x} \in \mathbf{K}$. That is, there is a Borel set $G \subset \mathbf{K}$ such that $\mu(G) = 0$ and $f(\mathbf{x}) \geq 0$ on $\mathbf{K} \setminus G$.

Next, observe that $\overline{\mathbf{K} \setminus G} \subset \mathbf{K}$ and $\mu(\overline{\mathbf{K} \setminus G}) = \mu(\mathbf{K})$. Therefore $\overline{\mathbf{K} \setminus G} = \mathbf{K}$ by minimality of $\mathbf{K}$.

Hence, let $\mathbf{x} \in \mathbf{K}$ be fixed, arbitrary. As $\mathbf{K} = \overline{\mathbf{K} \setminus G}$, there is a sequence $(\mathbf{x}_k) \subset \mathbf{K} \setminus G$, $k \in \mathbb{N}$, with $\mathbf{x}_k \to \mathbf{x}$ as $k \to \infty$. But since f is continuous and $f(\mathbf{x}_k) \geq 0$ for every $k \in \mathbb{N}$, we obtain the desired result $f(\mathbf{x}) \geq 0$. $\square$

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Theorem

Let $\mathbf{K} \subseteq [-1,1]^n$ *be compact and let* μ *be an arbitrary, fixed, finite Borel measure on* $\mathbf{K}$ *with* $\mathrm{supp}\,\mu = \mathbf{K}$. *Let* f *be a continuous function on* $\mathbb{R}^n$ *and let* $\mathbf{z} = (\mathbf{z}_\alpha)$, $\alpha \in \mathbb{N}^n$, *with*

$$\mathbf{z}_\alpha = \int_{\mathbf{K}} \mathbf{x}^\alpha f(\mathbf{x}) d\mu(\mathbf{x}), \qquad \forall\, \alpha \in \mathbb{N}^n.$$

(a) $f \geq 0$ *on* $\mathbf{K}$ *if and only if*

$$M_k(\mathbf{z}) \succeq 0, \qquad k = 0, 1, \ldots,$$

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Let $\mathbf{K} \subseteq [-1,1]^n$ *be compact and let* μ *be an arbitrary, fixed, finite Borel measure on* $\mathbf{K}$ *with* $\mathrm{supp}\,\mu = \mathbf{K}$*. Let* f *be a continuous function on* $\mathbb{R}^n$ *and let* $\mathbf{z} = (\mathbf{z}_\alpha)$*,* $\alpha \in \mathbb{N}^n$*, with*

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Sketch of proof

Consider the signed measure $d\nu = f\,d\mu$. As $\mathbf{K} \subseteq [-1,1]^n$,

$$|z_\alpha| = \left|\int_{\mathbf{K}} \mathbf{x}^\alpha f d\mu\right| \le \int_{\mathbf{K}} |f| d\mu = \|f\|_1, \qquad \forall \alpha \in \mathbb{N}^n.$$

and so z is the moment sequence of a finite (positive) Borel measure ψ on $[-1,1]^n$.

As $\mathbf{K}$ is compact this implies $\nu = \psi$, and so, ν is a positive Borel measure, and with support equal to $\mathbf{K}$.

By the Lemma that we have seen, $f \ge 0$ on $\mathbf{K}$. $\square$

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Observe that, for every $k = 1, \ldots$

$\Delta_k := \{f \in \mathbb{R}^{s(d)} \; : \; M_k(f\,\mathbf{y}) \succeq 0\}$ is a spectrahedron in $\mathbb{R}^{s(d)}$,

that is, ...

one obtains a nested hierarchy of spectrahedra

$$\Delta_0 \supset \Delta_1 \cdots \supset \Delta_k \cdots \supset \mathcal{C}(\mathbf{K})_d,$$

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So we get the sandwich $P_k^d(g) \subset \mathcal{C}(\mathbf{K})_d \subset \Delta_k$ for all k, and

$$\overline{\left(\bigcup_{k=0}^{\infty} P_k^d(g)\right)} \;=\; \mathcal{C}(\mathbf{K})_d \;=\; \left(\bigcap_{k=0}^{\infty} \Delta_k\right)$$

$\downarrow$ Inner approximations, representation dependent

$\downarrow$ Outer approximations, independent of representation

Application to optimization

Theorem (A hierarchy of upper bounds)

Let $f \in \mathbb{R}[\mathbf{x}]_d$ be fixed and $\mathbf{K} \subset \mathbb{R}^n$ be closed. Let μ be such that $\mathrm{supp}\,\mu = \mathbf{K}$ and with moment sequence $\mathbf{y} = (\mathbf{y}_\alpha)$, $\alpha \in \mathbb{N}^n$. Consider the hierarchy of semidefinite programs:

$$u_k = \min_{\sigma} \left\{ \int_{\mathbf{K}} f \underbrace{\sigma\, d\mu}_{d\nu} \;:\; \int_{\mathbf{K}} \underbrace{\sigma\, d\mu}_{d\nu} = 1;\ \sigma \in \Sigma[\mathbf{x}]_d \right\},$$

$$\begin{aligned} u_k^* &= \max_{\lambda} \{ \lambda \;:\; M_k(f - \lambda, \mathbf{y}) \succeq 0 \} \\ &= \max_{\lambda} \{ \lambda \;:\; \lambda\, M_k(\mathbf{y}) \preceq M_k(f, \mathbf{y}) \} \end{aligned}$$

Then $u_k^*, u_k \downarrow f^* = \min_{\mathbf{x}} \{ f(\mathbf{x}) \;:\; \mathbf{x} \in \mathbf{K} \}$.

Interpetation of u_k and u_k^*

- Computing u_k^* is a generalized eigenvalue problem!

- Next, recall that

$$f^* = \min_{\psi}\{\int_{\mathbf{K}} f\, d\psi \,:\, \psi(\mathbf{K}) = 1,\ \psi(\mathbb{R}^n \setminus \mathbf{K}) = 0\}$$

whereas

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that is, one optimizes over the subspace of Borel probability measures absolutely continuous with respect to μ, and with density $\sigma \in \Sigma[\mathbf{x}]_k$.

Ideally, when k is large, $\sigma(\mathbf{x}) > 0$ in a neighborhood of a global minimizer $\mathbf{x}^* \in \mathbf{K}$.

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• Also works for non-compact closed sets but then μ has to satisfy Carleman-type sufficient condition which limits the growth of the moments. For example, take

$$d\mu = \mathrm{e}^{-\|\mathbf{x}\|^2/2}\, d\mathbf{x}$$

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This is possible for relatively simple sets **K** like a box, a simplex, the discrete set, an ellipsoid, etc., where one can compute all moments of a measure μ whose support is **K**. For instancetake μ to be uniformly distributed, or $\mathbf{K} = \mathbb{R}^n$ (or $\mathbf{K} = \mathbb{R}^n_+$) with

$$d\mu = \mathrm{e}^{-\|\mathbf{x}\|^2/2}\, d\mathbf{x}, \qquad \mathbf{K} = \mathbb{R}^n$$

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$$d\mu = \; d\mathbf{x}, \left\{ \begin{array}{lcl} \mathbf{K} & = & [a_1, b_1] \times \cdots \times [a_n, b_n] \\ \mathbf{K} & = & \{\mathbf{x} \in \mathbb{R}^n_+ \; : \; \sum_{i=1}^n x_i \; \leq \; 1\} \end{array} \right.$$

For $\mathbf{K} = \{-1, 1\}^n$ or $\mathbf{K} = \{0, 1\}^n$ take μ to be uniformly distributed.

Some experiments

• $\mathbf{K} = \mathbb{R}^2_+$ with $d\mu = \mathrm{e}^{-\sum_i x_i} d\mathbf{x}$ so that

$$\mathbf{y}_{ij} \;=\; i!\,j!, \qquad \forall i,j = 0,1,\ldots$$

$\mathbf{x} \mapsto f(\mathbf{x}) := x_1^2 x_2^2\,(x_1^2 + x_2^2 - 1)$ with $f^* = -1/27 \approx -0.037$

u_k	15.6	4.3	1.5	0.6	0.27	0.13	0.0666
	0.03	0.017	0.008	0.004	0.0013	-0.0002	-0.0010

• $\mathbf{K} = \mathbb{R}^2_+$ and $\mathbf{x} \mapsto f(\mathbf{x}) = x_1 + (1 - x_1 x_2)^2$ with $f^* = 0$, not attained.

u_k	1.9	1.26	1.03	0.91	0.82	0.74	0.69
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- Numerical stability problems to be expected.
- Use bases different from the monomial basis.
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THANK YOU!