

# A new look at nonnegativity on closed sets

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- Positivstellensätze for semi-algebraic sets  $K \subset \mathbb{R}^n$  from the knowledge of **defining polynomials**
- → **inner approximations** of the cone of polynomials nonnegative on  $K$
- Optimization: Semidefinite relaxations yield **lower bounds**
- Another look at nonnegativity from knowledge of a **measure** supported on  $K$ .
- → **outer approximations** of the cone of polynomials nonnegative on  $K$
- Optimization: Semidefinite approximations yield **upper bounds**

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Let  $K \subseteq \mathbb{R}^n$  be closed



A basic question is:

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

and if possible ....

a characterization amenable to practical computation!  
Because then .....



**I'M HAPPY !**

# Positivstellensätze for basic semi-algebraic sets

Let  $\mathbf{K} := \{\mathbf{x} \in \mathbb{R}^n : g_j(\mathbf{x}) \geq 0, \quad j = 1, \dots, m\}$ , 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

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

The **preordering** associated with  $(g_j)$  is the set

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

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  $\sigma_J$  (or the  $\sigma_j$ ) provide **certificates** of nonnegativity on  $\mathbf{K}$ .

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# Truncated versions

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

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

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One may also define the convex cones

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



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

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

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

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

Hence, GIVEN  $f \in \mathbb{R}[\mathbf{x}]_d$ , checking 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

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

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## Schmüdgen's Positivstellensatz

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

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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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  $k \dots$

And so, the previous Positivstellensatz 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  $L_{\mathbf{y}} : \mathbb{R}[\mathbf{x}] \rightarrow \mathbb{R}$  by:

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

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

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

## 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 measure** 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  $\mathbb{N}_k^n = \{\alpha \in \mathbb{N}^n : \sum_i \alpha_i \leq k\}$ .

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

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

$$M_1(\mathbf{y}) = \begin{bmatrix} y_{00} & | & y_{10} & y_{01} \\ - & - & - \\ y_{10} & | & y_{20} & y_{11} \\ y_{01} & | & y_{11} & y_{02} \end{bmatrix}$$

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



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

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

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

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

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

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

# 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:

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

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

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  $\mathbf{y}^*$  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  $i = 1, \dots, n$ ,  $L_{\mathbf{y}^k}(\mathbf{x}_i) \rightarrow x_i^*$  as  $k \rightarrow \infty$ .

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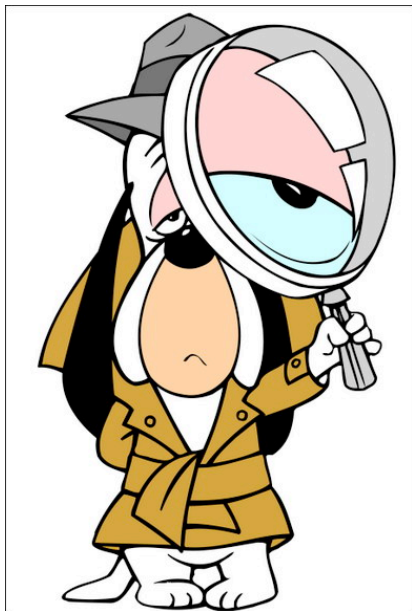
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# Another look at of nonnegativity



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

### Support of a measure

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

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

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

*A continuous function  $f : X \rightarrow \mathbb{R}$  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  $\nu$  is a positive measure then  $f(\mathbf{x}) \geq 0$  for  $\mu$ -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  $\mathbf{x}_k \rightarrow \mathbf{x}$  as  $k \rightarrow \infty$ . 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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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  $\mathbf{x}_k \rightarrow \mathbf{x}$  as  $k \rightarrow \infty$ . 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  $\mu$  be an arbitrary, fixed, finite Borel measure on  $\mathbf{K}$  with  $\text{supp } \mu = \mathbf{K}$ . Let  $f$  be a continuous function on  $\mathbb{R}^n$  and let  $\mathbf{z} = (\mathbf{z}_\alpha)$ ,  $\alpha \in \mathbb{N}^n$ , with

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

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

$$M_k(\mathbf{z}) \succeq 0, \quad k = 0, 1, \dots,$$

and if  $f \in \mathbb{R}[\mathbf{x}]$  then  $f \geq 0$  on  $\mathbf{K}$  if and only if

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# Sketch of proof

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

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

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

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

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Let identify  $f \in \mathbb{R}[\mathbf{x}]_d$  with its vector of coefficient  $f \in \mathbb{R}^{s(d)}$ , with  $s(d) = \binom{n+d}{n}$ .

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

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

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

↓

Inner approximations  
representation dependent

↓

Outer approximations  
independent of representation

## 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  $\mu$  be such that  $\text{supp } \mu = \mathbf{K}$  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  $u_k^*, u_k \downarrow f^* = \min_{\mathbf{x}} \{ f(\mathbf{x}) : \mathbf{x} \in \mathbf{K} \}$ .

recall that

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

whereas

$$U_k = \min_{\nu} \left\{ \int_{\mathbf{K}} f \underbrace{\sigma d\mu}_{d\nu} : \nu(\mathbf{K}) = 1, \nu(\mathbb{R}^n \setminus \mathbf{K}) = 0; \sigma \in \Sigma[\mathbf{x}]_k \right\}$$

that is, one optimizes over the subspace of Borel probability measures absolutely continuous with respect to  $\mu$ , 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  $\mu$  has to satisfy **Carleman-type** sufficient condition which limits the growth of the moments. For example, take

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

- The sequences of upper bounds  $(u_k, u_k^*)$  complement the sequences of lower bounds  $(\rho_k, \rho_k^*)$  obtained from SDP-relaxations.
- Of course, for practical computation, the previous semidefinite relaxations require **knowledge** of the moment sequence  $\mathbf{y} = (\mathbf{y}_\alpha), \alpha \in \mathbb{N}^n$ .

This is possible for relatively simple sets  $\mathbf{K}$  like a box, a simplex, the discrete set  $\{-1, 1\}^n$ , an ellipsoid, etc., where one can take  $\mu$  to be uniformly distributed, or  $\mathbf{K} = \mathbb{R}^n$  (or  $\mathbf{K} = \mathbb{R}_+^n$ ) with

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# Some experiments

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

$$y_{ij} = i!j!, \quad \forall i, j = 0, 1, \dots$$

- $\mathbf{x} \mapsto f(\mathbf{x}) := x_1^2 x_2^2 (x_1^2 + x_2^2 - 1)$  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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# THANK YOU!

