Theoretical and practical applications of signomial rings to polynomial optimization

Riley Murray

University of California, Berkeley

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Joint work with Mareike Dressler

What are signomials?

Start with "monomial" basis functions, for $\boldsymbol{\alpha} \in \mathbb{R}^n$

$$\mathrm{e}^{\boldsymbol{\alpha}} : \mathbb{R}^n \to \mathbb{R}_{++} \quad \text{takes values} \quad \mathrm{e}^{\boldsymbol{\alpha}}(\boldsymbol{x}) := \exp\langle \boldsymbol{\alpha}, \boldsymbol{x} \rangle.$$

A signomial supported on $\mathcal{A} \subset \mathbb{R}^n$ is a linear combination

$$f = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} c_{\boldsymbol{\alpha}} \mathrm{e}^{\boldsymbol{\alpha}}.$$

For modeling reasons, write as *generalized polynomials* in $t_i = \exp x_i$:

$$\boldsymbol{t} \mapsto \sum_{\boldsymbol{\alpha} \in \mathcal{A}} c_{\boldsymbol{\alpha}} \, t_1^{\alpha_1} \cdots t_n^{\alpha_n}$$

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A template for nonnegativity certificates

Characterize nonnegative functions

$$\sum_{\boldsymbol{\alpha} \in \mathcal{A}} c_{\boldsymbol{\alpha}} \boldsymbol{t}^{\boldsymbol{\alpha}} + c_{\boldsymbol{\beta}} \boldsymbol{t}^{\boldsymbol{\beta}} \geq 0 \quad \text{for all} \quad \boldsymbol{t} \in \mathsf{S}$$

with one free term ($c_{\boldsymbol{\alpha}} \boldsymbol{t}^{\boldsymbol{\alpha}} \geq 0$ on S "trivially"). Then take sums!

Example. $t^{-3} + t^{-2} + 4t + t^2 - 4t^{-1} - 1 - t^3 \geq 0$ for all $t \in (0, 1]$.

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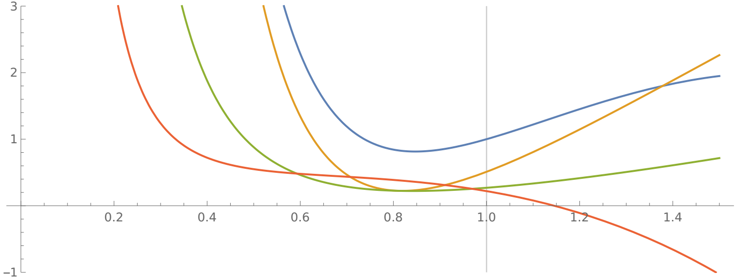

Manifestations of the template

Who	Method name	S	am/gm	convex duality
Reznick [1]	agiforms	$\mathbb{R}^n$	yes	no
Pantea, Koeppl, and Craciun [2]	monomial domination	$\mathbb{R}^n_{++}$	yes	no
Iliman and de Wolff [3]	SONC	$\mathbb{R}^n$	yes	no
Chandrasekaran and Shah [4]	SAGE signomials	$\mathbb{R}^n_{++}$	yes	yes
MCW [5]	SAGE polynomials	$\mathbb{R}^n$	yes	yes
Katthän, Naumann, and Theobald [6]	$\mathcal{S}$-cone*	$\mathbb{R}^n$	yes	yes
MCW [7]	conditional SAGE	$\log$ S convex	no**	yes

Call them what you will, but use the efficient relative entropy formulations in [5, 7]! They work out of the box!

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High-degree and non-polynomial models.

Aircraft design [8, 9, 10, 11, 12] and structural engineering [13, 14, 15, 16].

Optimized Pulse Patterns [17]

Hyperloop Design [18]

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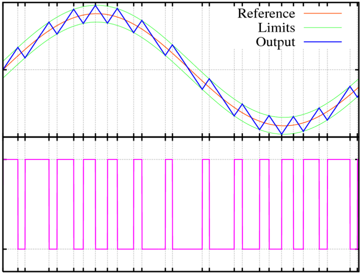

Illustration by Cyril Buttay

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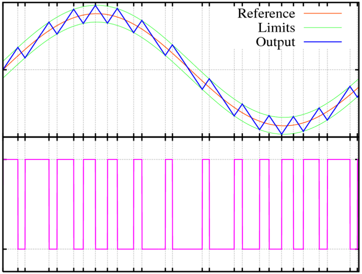

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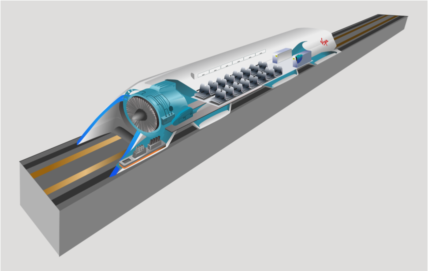

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Outline for the talk

This talk is about "**conditional SAGE**."

1. Basics of conditional SAGE.

   Definition → dual perspective → an application

2. A Positivstellensatz which respects *signomial rings*

   An earlier SAGE Positivstellensatz → our result → proof outline

3. Grading signomial rings by "$\mathcal{A}$-degree"

4. A new hierarchy

   Definition → signomial example → polynomial example

All numerical convex optimization examples use MOSEK 9.2.

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Notation

For finite $A \subset \mathbb{R}^n$, define

$$\mathbb{R}^A := \{\text{real } |A|\text{-tuples indexed by } \boldsymbol{\alpha} \in A\}.$$

Identify signomials w/ coefficients on basis functions $\{\mathrm{e}^{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha} \in A}$

$$\sum_{\boldsymbol{\alpha} \in A} c_{\boldsymbol{\alpha}} \mathrm{e}^{\boldsymbol{\alpha}} \quad \Leftrightarrow \quad \boldsymbol{c} \in \mathbb{R}^A.$$

Understand $A : \mathbb{R}^n \to \mathbb{R}^A$ as a linear operator

$$A\boldsymbol{x} = (\langle \boldsymbol{\alpha}, \boldsymbol{x} \rangle)_{\boldsymbol{\alpha} \in A}$$

The *support* of a signomial

$$\mathrm{supp}(f) = \text{the smallest } A \subset \mathbb{R}^n \text{ for which } f \in \mathrm{span}\{\mathrm{e}^{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha} \in A}.$$

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Conditional SAGE

Definition [7, **M**CW]. *A signomial* $f = \sum_{\boldsymbol{\alpha} \in A} c_{\boldsymbol{\alpha}} \mathrm{e}^{\boldsymbol{\alpha}}$ *is called* X-**AGE** *if*

(1) f *is nonnegative on* X, *and*

(2) at most one $c_{\boldsymbol{\beta}} < 0$ *for any* $\boldsymbol{\beta} \in A$.

Take sums to get X-**SAGE** signomials.

$$\mathcal{C}_{\mathsf{X}}(A) = \left\{ \boldsymbol{c} \in \mathbb{R}^A \;\middle|\; \begin{array}{c} \sum_{\boldsymbol{\alpha} \in A} c_{\boldsymbol{\alpha}} \mathrm{e}^{\boldsymbol{\alpha}}(\boldsymbol{x}) = \sum_i f_i(\boldsymbol{x}) \\ \text{each } f_i \text{ is an X-AGE signomial} \end{array} \right\}$$

Sparsity preservation ([5, **M**CW] and [7, **M**CW]):

If f *is an X-SAGE signomial supported on* A, *then* f *is a sum of X-AGE signomials* also supported on A.

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If f *is an* X-*SAGE signomial supported on* A, *then* f *is a sum of* X-*AGE signomials* also supported on A.

The dual perspective

Introduce X-AGE cones

$$\mathcal{C}_{\mathsf{X}}(A,\boldsymbol{\beta}) := \left\{ \boldsymbol{c} \in \mathbb{R}^A \;\middle|\; \begin{array}{c} c_{\boldsymbol{\alpha}} \geq 0 \text{ for all } \boldsymbol{\alpha} \neq \boldsymbol{\beta} \\ \sum_{\boldsymbol{\alpha}\in A} c_{\boldsymbol{\alpha}} e^{\boldsymbol{\alpha}} \geq 0 \text{ on } \mathsf{X} \end{array} \right\}.$$

The dual X-SAGE cone can be represented as

$$\mathcal{C}_{\mathsf{X}}(A)^{\dagger} = \bigcap_{\boldsymbol{\beta}\in A} \mathcal{C}_{\mathsf{X}}(A,\boldsymbol{\beta})^{\dagger}.$$

Theorem [7, **M**CW]. *If* X *is convex, then*

$$\mathcal{C}_{\mathsf{X}}(A,\boldsymbol{\beta})^{\dagger} = \operatorname{cl}\Big\{ \boldsymbol{v} \in \mathbb{R}^A_{++} \,:\, \text{some } \boldsymbol{z} \text{ satisfies } \boldsymbol{z}/v_{\boldsymbol{\beta}} \in \mathsf{X} \text{ and } v_{\boldsymbol{\beta}} \log\left(\frac{v_{\boldsymbol{\alpha}}}{v_{\boldsymbol{\beta}}}\right) \geq \langle \boldsymbol{\alpha}-\boldsymbol{\beta}, \boldsymbol{z}\rangle \,\forall\, \boldsymbol{\alpha}\in A \Big\}.$$

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Chemical dynamics

Concentrations of *chemical species* are described by an ODE

$$\frac{\mathrm{d}}{\mathrm{dt}}\boldsymbol{s}(t) = R_{\boldsymbol{k}}(\boldsymbol{s}(t)).$$

At most one equilibrium point? See Pantea, Koeppl, Craciun [2].

Example. A system from [2] with six species.

Consider various boxes B.

Is $R_{\boldsymbol{k}}$ injective $\forall \boldsymbol{k} \in \mathrm{B}$?

Apply conditional SAGE

- Yes, $R_{\boldsymbol{k}}$ always injective
- No, some $R_{\boldsymbol{k}}$ not injective
- 0.05 seconds per B

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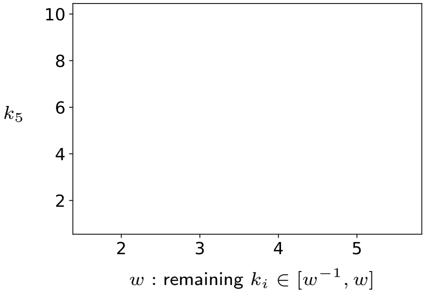

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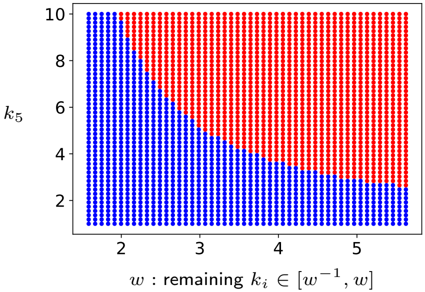

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Reinterpreting an earlier SAGE Positivstellensatz

Definition

For a finite set $\mathcal{A} \subset \mathbb{R}^n$ which contains the origin, the signomial ring $\mathbb{R}[\mathcal{A}]$ is the $\mathbb{R}$-algebra generated by $\{\mathrm{e}^{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha} \in \mathcal{A}}$.

Chandrasekaran and Shah [4, Theorem 4.2].

Suppose we have rational exponents $\mathcal{A} = \{\mathbf{0}, \boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_\ell\} \subset \mathbb{Q}^n$ *and constraint signomials* $\{g_1, \ldots, g_{2\ell+m}\} \subset \mathbb{R}[\mathcal{A}]$ *that include*

$$g_i(\boldsymbol{x}) = U - \mathrm{e}^{\boldsymbol{\alpha}_i}(\boldsymbol{x}) \text{ for } i \in \{1, \ldots, \ell\}, \text{ and}$$
$$g_i(\boldsymbol{x}) = \mathrm{e}^{\boldsymbol{\alpha}_i}(\boldsymbol{x}) - L \text{ for } i \in \{\ell+1, \ldots, 2\ell\}$$

for some $U, L > 0$. *Abbreviate* $M = 2\ell + m$ *and define the compact set*

$$\mathrm{K} = \{\boldsymbol{x} \,|\, g_i(\boldsymbol{x}) \geq 0 \;\; \text{for all} \;\; i \in \{1, \ldots, M\}\}.$$

If $f \in \mathbb{R}[\mathcal{A}]$ *is positive on* K, *then there is an identity*

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Reinterpreting an earlier SAGE Positivstellensatz

Definition

For a finite set $\mathcal{A} \subset \mathbb{R}^n$ which contains the origin, the signomial ring $\mathbb{R}[\mathcal{A}]$ is the $\mathbb{R}$-algebra generated by $\{\mathrm{e}^{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha} \in \mathcal{A}}$.

Chandrasekaran and Shah [4, Theorem 4.2].

Suppose we have rational exponents $\mathcal{A} = \{\mathbf{0}, \boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_\ell\} \subset \mathbb{Q}^n$ *and constraint signomials* $\{g_1, \ldots, g_{2\ell+m}\} \subset \mathbb{R}[\mathcal{A}]$ *that include*

$$g_i(\boldsymbol{x}) = U - \mathrm{e}^{\boldsymbol{\alpha}_i}(\boldsymbol{x}) \text{ for } i \in \{1, \ldots, \ell\}, \text{ and}$$
$$g_i(\boldsymbol{x}) = \mathrm{e}^{\boldsymbol{\alpha}_i}(\boldsymbol{x}) - L \text{ for } i \in \{\ell+1, \ldots, 2\ell\}$$

for some $U, L > 0$. *Abbreviate* $M = 2\ell + m$ *and define the compact set*

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Our result

Theorem

Consider a compact convex set X, *signomials* $g_1, \ldots, g_m \in \mathbb{R}[\mathcal{A}]$, *and*

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If $f \in \mathbb{R}[\mathcal{A}]$ *is positive on* K, *then there is an identity*

$$\left(\textstyle\sum_{\boldsymbol{\alpha} \in \mathcal{A}} \mathrm{e}^{\boldsymbol{\alpha}}\right)^r f = \lambda_0 + \textstyle\sum_{i=1}^{m} \lambda_i \cdot g_i$$

for X*-SAGE* $\lambda_0 \in \mathbb{R}[\mathcal{A}]$, *posynomials* $\lambda_i \in \mathbb{R}[\mathcal{A}]$, *and* $r \in \mathbb{N}$.

Points of note

- No products of constraint functions.
- Neither X nor $\{\exp \boldsymbol{x} \,|\, \boldsymbol{x} \in \mathsf{X}\}$ need be semi-algebraic.
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Corollary

If $f \in \mathbb{R}[\mathcal{A}]$ is positive on a compact convex set X, then

$$\left(\sum_{\boldsymbol{\alpha}\in\mathcal{A}} \mathrm{e}^{\boldsymbol{\alpha}}\right)^r f \text{ is X-SAGE for large enough } r \in \mathbb{N}.$$

We combine signomial rings with strategy of A. Wang et al [20].

1. Represent $f(\boldsymbol{x}) = p(\exp \mathcal{A}\boldsymbol{x})$ with a homogeneous polynomial p:

$$f > 0 \text{ on X} \quad \Leftrightarrow \quad p > 0 \text{ on Y} := \{\exp \mathcal{A}\boldsymbol{x} \,|\, \boldsymbol{x} \in \text{X}\}.$$

2. Represent Y by **infinitely many** homogeneous binomial inequalities and one normalization constraint ($y_0 = 1$).
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Grading certificates from the Positivstellensatz

We can use REP to search for an identity

$$\left(\sum_{\boldsymbol{\alpha}\in\mathcal{A}} \mathrm{e}^{\boldsymbol{\alpha}}\right)^r f = \lambda_0 + \sum_{i=1}^m \lambda_i \cdot g_i$$

once we've decided r and permissible supports $S_i \supset \mathrm{supp}(\lambda_i)$.

By sparsity preservation, we don't need to explicitly bound $\mathrm{supp}(\lambda_0)$.

We have to decide S_i for $i \geq 1$.

How should we go about doing this?

Complexity of λ_i would be with consideration to f, r, and g_i.

Signomials have no concept of "degree!"

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Signomial $\mathcal{A}$-degree

Consider a sequence of nested sets

$$\mathcal{A}_d := \left\{ \sum_{\boldsymbol{\alpha} \in \mathcal{A}} w_{\boldsymbol{\alpha}} \boldsymbol{\alpha} \,:\, \boldsymbol{w} \in \mathbb{N}^{\mathcal{A}},\ \langle \mathbf{1}, \boldsymbol{w} \rangle \leq d \right\} \quad \text{for} \quad d \geq 1.$$

Definition

The *$\mathcal{A}$-degree* of $f \in \mathbb{R}[\mathcal{A}]$ is the smallest d for which $\operatorname{supp}(f) \subset \mathcal{A}_d$.

Denote this by $\deg_{\mathcal{A}}(f)$.

- *Not intrinsic to a signomial.*

  Setting $\mathcal{A} = \operatorname{supp}(f)$, we have $\deg_{\mathcal{A}}(f) = 1$.

- Co-variant with affine changes of coordinates.

Use $\mathbb{R}[\mathcal{A}]_d$ to denote the signomials in $\mathbb{R}[\mathcal{A}]$ of $\mathcal{A}$-degree at most d.

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Signomial $\mathcal{A}$-degree under multiplication

The following inequality always holds. It can be strict

$$\deg_{\mathcal{A}}(fg) \leq \deg_{\mathcal{A}}(f) + \deg_{\mathcal{A}}(g).$$

Consider $f(x) = \exp(3x)$ and $\mathcal{A} = \{-1, 0, 1, 2\}$.

If $g \in \{c \exp(-x) \mid c \in \mathbb{R}\}$, then $\deg_{\mathcal{A}}(fg) = 1$.

Definition

The *inverse support of* f *in* $\mathbb{R}[\mathcal{A}]_d$ is the largest $\mathcal{B} \subset \mathcal{A}_d$ that satisfies

$$\deg_{\mathcal{A}}(e^{\boldsymbol{\alpha}} f) \leq d \text{ for all } \boldsymbol{\alpha} \text{ in } \mathcal{B}.$$

Denote inverse support by $\operatorname{invsupp}_d(f)$. Operationally

$$\operatorname{supp}(g) \subset \operatorname{invsupp}_d(f) \quad \Rightarrow \quad \deg_{\mathcal{A}}(g) \leq d \text{ and } \deg_{\mathcal{A}}(fg) \leq d.$$

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$$\deg_{\mathcal{A}}(fg) \leq \deg_{\mathcal{A}}(f) + \deg_{\mathcal{A}}(g).$$

Consider $f(x) = \exp(3x)$ and $\mathcal{A} = \{-1, 0, 1, 2\}$.

If $g \in \{c\exp(-x) \,|\, c \in \mathbb{R}\}$, then $\deg_{\mathcal{A}}(fg) = 1$.

Definition

The *inverse support of f in* $\mathbb{R}[\mathcal{A}]_d$ is the largest $\mathcal{B} \subset \mathcal{A}_d$ that satisfies

$$\deg_{\mathcal{A}}(\mathrm{e}^{\boldsymbol{\alpha}} f) \leq d \text{ for all } \boldsymbol{\alpha} \text{ in } \mathcal{B}.$$

Denote inverse support by $\mathrm{invsupp}_d(f)$. Operationally

$$\mathrm{supp}(g) \subset \mathrm{invsupp}_d(f) \quad \Rightarrow \quad \deg_{\mathcal{A}}(g) \leq d \text{ and } \deg_{\mathcal{A}}(fg) \leq d.$$

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A hierarchy of lower bounds

We want to compute

$$f^\star_{\mathsf{K}} = \inf_{\boldsymbol{x} \in \mathsf{K}} f(\boldsymbol{x}) \quad \text{where} \quad \mathsf{K} = \{\boldsymbol{x} \in \mathsf{X} \,|\, g(\boldsymbol{x}) \geq \mathbf{0}\}.$$

Definition

If $r := d - \deg_{\mathcal{A}}(f) \geq 0$, the *$\mathcal{A}$-degree d SAGE bound* is defined as

$$f^{(d)}_{\mathsf{K}} := \sup \ \gamma \text{ s.t. } \left(\textstyle\sum_{\boldsymbol{\alpha} \in \mathcal{A}} \mathrm{e}^{\boldsymbol{\alpha}}\right)^r (f - \gamma) = \lambda_0 + \textstyle\sum_{i=1}^m \lambda_i g_i,$$

$$\lambda_i \in \mathcal{C}_{\mathsf{X}}(\mathrm{invsupp}_d(g_i)) \ \ \forall\, i \in \{1, \ldots, m\},$$

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A chemical reactor design problem

$$\min_{\boldsymbol{t}\in\mathbb{R}^8_{++}} \quad 2.0425\, t_1^{0.782} + 52.25\, t_2 + 192.85\, t_2^{0.9} + 5.25\, t_2^3 + 61.465\, t_6^{0.467}$$
$$+ 0.01748\, t_3^{1.33}/t_4^{0.8} + 100.7\, t_4^{0.546} + 3.66{\cdot}10^{-10}\, t_3^{2.85}/t_4^{1.7}$$
$$+ 0.00945\, t_5 + 1.06{\cdot}10^{-10}\, t_5^{2.8}/t_4^{1.8} + 116\, t_6 - 205\, t_6 t_7 - 278\, t_2^3 t_7$$

s.t. Five nonconvex constraints of the form

$$1 - (\text{posynomial in } \boldsymbol{t}) = 0.$$

Invoke affine-invariance (in x) to rescale the problem!

Work in the *naive ring*

$$\mathcal{A} = \text{all monomial exponents in the problem.}$$

Handling **equality constraints**

Infer *valid convex constraints* "$1 - (\text{posynomial in } \boldsymbol{t}) \geq 0$" for X.

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Results for the chemical reactor design problem

Compute SAGE bounds

$$f_{\mathsf{K}}^{(1)} = 16377.32 \quad \text{in} \quad 0.13 \text{ seconds, and}$$

$$f_{\mathsf{K}}^{(2)} = 17462.73 \quad \text{in} \quad 24.37 \text{ seconds.}$$

Solution recovery yields $f(\boldsymbol{x}') = 17485.99$ and $\|g(\boldsymbol{x}')\|_\infty = 5.85 \cdot 10^{-15}$.

Apply global solvers in GAMS with two-hour time limit.

	Using t as optimization variable		Using x as optimization variable	
	solver time (s)	lower bound	solver time (s)	lower bound
BARON	163	$-\infty$	7200	$-\infty$
ANTIGONE	145	-16880.380	7200	$-\infty$
LINDO	1468	17484.314	50	17485.988

All solvers above returned a solution with objective ≈ 17485.99.

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Minimizing the polynomial from the CRN example

We were interested in injectivity of the CRN dynamics map.

- Checked if a certain polynomial p was > 0 on 2,500 subsets of $\mathbb{R}^9_+$.

  p was degree 6 and had about 50 terms.

- We signomialized $f(\boldsymbol{x}) = p(\exp \boldsymbol{x})$, considered 2,500 different "X."

Here: consider the X with largest gap $f^\star_X - \sup\{\gamma \,|\, f - \gamma \text{ is X-SAGE}\}$.

r	SAGE bounds $\mathcal{A}_{\text{nat}}$	SAGE bounds $\mathcal{A}_{\text{int}}$	SAGE bounds $\mathcal{A}_{\text{naive}}$	solver runtimes (s) $\mathcal{A}_{\text{nat}}$	solver runtimes (s) $\mathcal{A}_{\text{int}}$	solver runtimes (s) $\mathcal{A}_{\text{naive}}$
0	18.1596	18.1596	18.1596	0.0344	0.0301	0.0321
1	18.7188	22.8321	22.8321	1.0541	1.1123	3.4648
2	19.7375	-	-	49.2000	-	-

Moment-SOS approaches

- Lasserre hierarchy via `YALMIP`: 572 s, computes $f^\star_X \approx 22.8$
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Recap

1. Introduced a new Positivstellensatz.
   - Respects the structure of signomial rings.
   - The most general signomial Positivstellensatz to-date.
2. Derived a *canonical hierarchy* based on $\mathcal{A}$-degree.
3. Demonstrated the hierarchy's practicality.
   - Competitive with BARON, ANTIGONE, LINDO on a hard SP.
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Thank you!

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Extra slides