Theoretical and practical applications of signomial rings to polynomial optimization

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University of California, Berkeley

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Joint work with Mareike Dressler
What are signomials?

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

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

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

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

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

$$t \mapsto \sum_{\alpha \in A} c_\alpha t_1^{\alpha_1} \cdots t_n^{\alpha_n}.$$
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A signomial supported on $\mathcal{A} \subset \mathbb{R}^n$ is a linear combination

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A template for nonnegativity certificates

Characterize nonnegative functions

\[ \sum_{\alpha \in A} c_{\alpha} t^{\alpha} + c_{\beta} t^{\beta} \geq 0 \quad \text{for all} \quad t \in S \]

with one free term \((c_{\alpha} t^{\alpha} \geq 0 \text{ on } S \text{ “trivially”}). \]

Then take sums!

Example. \( t^{-3} + t^{-2} + 4t + t^2 - 4t^{-1} - 1 - t^3 \geq 0 \text{ for all } t \in (0, 1]. \)
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What’s this all good for?

*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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Outline for the talk

This talk is about “conditional SAGE.”

1. Basics of conditional SAGE.
   Definition $\rightarrow$ dual perspective $\rightarrow$ an application

2. A Positivstellensatz which respects signomial rings
   An earlier SAGE Positivstellensatz $\rightarrow$ our result $\rightarrow$ proof outline

3. Grading signomial rings by “A-degree”

4. A new hierarchy
   Definition $\rightarrow$ signomial example $\rightarrow$ polynomial example

All numerical convex optimization examples use MOSEK 9.2.
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All numerical convex optimization examples use MOSEK 9.2.
For finite $A \subset \mathbb{R}^n$, define

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

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

$$\sum_{\alpha \in A} c_\alpha e^\alpha \iff c \in \mathbb{R}^A.$$

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

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

The support of a signomial

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

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Definition [7, MCW]. A signomial \( f = \sum_{\alpha \in A} c_{\alpha} e^{\alpha} \) is called X-AGE if

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

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

Take sums to get X-SAGE signomials.

\[
C_X(A) = \left\{ c \in \mathbb{R}^A \left| \begin{array}{l}
\sum_{\alpha \in A} c_{\alpha} e^{\alpha}(x) = \sum_i f_i(x) \\
each f_i \text{ is an X-AGE signomial}
\end{array} \right. \right\}
\]

Sparsity preservation ([5, MCW] and [7, MCW]):

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

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The dual perspective

Introduce X-AGE cones

\[ C_X(A, \beta) := \left\{ c \in \mathbb{R}^A \left| \begin{array}{c} \ c_\alpha \geq 0 \ \text{for all } \alpha \neq \beta \\ \sum_{\alpha \in A} c_\alpha e^\alpha \geq 0 \ \text{on } X \end{array} \right. \right\}. \]

The dual X-SAGE cone can be represented as

\[ C_X(A)^\dagger = \bigcap_{\beta \in A} C_X(A, \beta)^\dagger. \]

Theorem [7, MCW]. If \( X \) is convex, then

\[ C_X(A, \beta)^\dagger = \text{cl} \left\{ v \in \mathbb{R}^A_{++} : \text{some } z \text{ satisfies } z/v_\beta \in X \right\} \]

\[ \text{and } v_\beta \log \left( \frac{v_\alpha}{v_\beta} \right) \geq \langle \alpha - \beta, z \rangle \ \forall \alpha \in A \].
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Chemical dynamics

Concentrations of chemical species are described by an ODE

\[ \frac{d}{dt} s(t) = R_k(s(t)). \]

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


Consider various boxes B.

Is \( R_k \) injective \( \forall k \in B \)?

Apply conditional SAGE

Yes, \( R_k \) always injective

No, some \( R_k \) not injective

0.05 seconds per B
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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 $\{e^\alpha\}_{\alpha \in \mathcal{A}}$.

Chandrasekaran and Shah [4, Theorem 4.2].

Suppose we have rational exponents $\mathcal{A} = \{0, \alpha_1, \ldots, \alpha_\ell\} \subset \mathbb{Q}^n$ and constraint signomials $\{g_1, \ldots, g_{2\ell+m}\} \subset \mathbb{R}[\mathcal{A}]$ that include

\[ g_i(x) = U - e^{\alpha_i}(x) \quad \text{for } i \in \{1, \ldots, \ell\}, \text{ and} \]
\[ g_i(x) = e^{\alpha_i}(x) - L \quad \text{for } i \in \{\ell + 1, \ldots, 2\ell\} \]

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

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

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

\[ f = \sum_{j \in \mathbb{N}^M} \lambda_j \cdot g_1^{j_1} \cdots g_M^{j_M} \quad \text{for finitely many } \mathbb{R}^n\text{-SAGE } \lambda_j \in \mathbb{R}[\mathcal{A}]. \]
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Chandrasekaran and Shah [4, Theorem 4.2].

*Suppose we have rational exponents $\mathcal{A} = \{0, \alpha_1, \ldots, \alpha_\ell\} \subset \mathbb{Q}^n$ and constraint signomials $\{g_1, \ldots, g_{2\ell+m}\} \subset \mathbb{R}[\mathcal{A}]$ that include*

\[
g_i(x) = U - e^{\alpha_i}(x) \quad \text{for } i \in \{1, \ldots, \ell\}, \quad \text{and}
\]

\[
g_i(x) = e^{\alpha_i}(x) - L \quad \text{for } i \in \{\ell+1, \ldots, 2\ell\}
\]

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

\[
K = \{x \mid g_i(x) \geq 0 \quad \text{for all} \quad i \in \{1, \ldots, M\}\}.
\]

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

\[
f = \sum_{j \in \mathbb{N}^M} \lambda_j \cdot g_1^{j_1} \cdots g_M^{j_M} \quad \text{for finitely many } \mathbb{R}^n\text{-SAGE } \lambda_j \in \mathbb{R}[\mathcal{A}].
\]
Our result

Theorem

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

$$K = \{ x \in X \mid g_i(x) \geq 0 \text{ for all } i \in \{1, \ldots, m\}\}.$$ 

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

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

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

Points of note

- No products of constraint functions.
- Neither $X$ nor $\{\exp x \mid x \in X\}$ need be semi-algebraic.
- No assumptions on $A$. 

Riley Murray
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Corollary

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

\[
(\sum_{\alpha \in \mathcal{A}} e^{\alpha})^r f \text{ is } X\text{-SAGE for large enough } r \in \mathbb{N}.
\]

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

1. Represent \( f(x) = p(\exp \mathcal{A}x) \) with a homogeneous polynomial \( p \):
   \[
   f > 0 \text{ on } X \iff p > 0 \text{ on } Y := \{ \exp \mathcal{A}x \mid x \in X \}.
   \]

2. Represent \( Y \) by infinitely many homogeneous binomial inequalities and one normalization constraint (\( y_0 = 1 \)).

3. Apply Dickinson-Povh Positivstellensatz [21] to \((p, Y)\).

4. Map the Dickinson-Povh certificate to an \( X\text{-SAGE} \) certificate.
**Corollary**

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

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

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Grading certificates from the Positivistensatz

We can use REP to search for an identity

\[(\sum_{\alpha \in A} e^{\alpha})^r f = \lambda_0 + \sum_{i=1}^{m} \lambda_i \cdot g_i\]

once we’ve decided \(r\) and \textbf{permissible supports} \(S_i \supset \text{supp}(\lambda_i)\).

By sparsity preservation, we don’t need to explicitly bound \(\text{supp}(\lambda_0)\).

We have to decide \(S_i\) for \(i \geq 1\).

How should we go about doing this?

Complexity of \(\lambda_i\) would be with consideration to \(f, r, \) and \(g_i\).

Signomials have no concept of “degree!”
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Signomials have no concept of “degree!”
Consider a sequence of nested sets

$$A_d := \left\{ \sum_{\alpha \in A} w_\alpha \alpha : w \in \mathbb{N}^A, \langle 1, w \rangle \leq d \right\}$$

for $d \geq 1$.

**Definition**

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

Denote this by $\text{deg}_A(f)$.

- *Not intrinsic to a signomial.*

  Setting $A = \text{supp}(f)$, we have $\text{deg}_A(f) = 1$.

- Co-variant with affine changes of coordinates.

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

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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

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

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

$$\text{supp}(g) \subset \text{invsupp}_d(f) \implies \deg_{\mathcal{A}}(g) \leq d \text{ and } \deg_{\mathcal{A}}(fg) \leq d.$$
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**Definition**

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

$$\deg_A(e^{\alpha}f) \leq d \text{ for all } \alpha \text{ in } B.$$  

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$$\text{supp}(g) \subset \text{invsupp}_d(f) \Rightarrow \deg_A(g) \leq d \text{ and } \deg_A(fg) \leq d.$$
A hierarchy of lower bounds

We want to compute

$$f_K^* = \inf_{x \in K} f(x) \quad \text{where} \quad K = \{x \in X | g(x) \geq 0\}.$$  

**Definition**

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

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

$$\lambda_i \in \mathcal{C}_X(\text{invsupp}_d(g_i)) \quad \forall \ i \in \{1, \ldots, m\},$$

$$\lambda_0 \in \mathcal{C}_X(\mathcal{A}_d), \text{ and } \gamma \in \mathbb{R}.$$  

Otherwise, $f_K^{(d)} = -\infty$.  

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\[ \lambda_i \in C_X(\text{invsupp}_d(g_i)) \forall i \in \{1, \ldots, m\}, \]

\[ \lambda_0 \in C_X(A_d), \text{ and } \gamma \in \mathbb{R}. \]

Otherwise, \( f^{(d)}_K = -\infty \).
A chemical reactor design problem

\[
\begin{align*}
\min_{t \in \mathbb{R}_+^8} & \quad 2.0425 t_1^{0.782} + 52.25 t_2 + 192.85 t_2^{0.9} + 5.25 t_2^3 + 61.465 t_6^{0.467} \\
& \quad + 0.01748 t_3^{1.33}/t_4^{0.8} + 100.7 t_4^{0.546} + 3.66 \cdot 10^{-10} t_3^{2.85}/t_4^{1.7} \\
& \quad + 0.00945 t_5 + 1.06 \cdot 10^{-10} t_5^{2.8}/t_4^{1.8} + 116 t_6 - 205 t_6 t_7 - 278 t_2^2 t_7
\end{align*}
\]

s.t. Five nonconvex constraints of the form

\[
1 - (\text{posynomial in } t) = 0.
\]

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

Work in the naive ring

\[ A = \text{all monomial exponents in the problem.} \]

Handling equality constraints

Infer valid convex constraints “\(1 - (\text{posynomial in } t) \geq 0\)” for X.

“Lagrange multipliers” \(\lambda_i\) only constrained by their supports.
A chemical reactor design problem

$$\begin{align*}
\min_{t \in \mathbb{R}^8_{++}} & \quad 2.0425 \, t_1^{0.782} + 52.25 \, t_2 + 192.85 \, t_2^{0.9} + 5.25 \, t_2^3 + 61.465 \, t_6^{0.467} \\
& \quad + 0.01748 \, t_3^{1.33} / t_4^{0.8} + 100.7 \, t_4^{0.546} + 3.66 \cdot 10^{-10} \, t_3^{2.85} / t_4^{1.7} \\
& \quad + 0.00945 \, t_5 + 1.06 \cdot 10^{-10} \, t_5^{2.8} / t_4^{1.8} + 116 \, t_6 - 205 \, t_6 \, t_7 - 278 \, t_2^3 \, t_7 \\
\text{s.t.} \quad & \quad 1 - (\text{posynomial in } t) = 0.
\end{align*}$$

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 “$1 - (\text{posynomial in } t) \geq 0$” for $X$.

“Lagrange multipliers” $\lambda_i$ only constrained by their supports.
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Results for the chemical reactor design problem

Compute SAGE bounds

\[ f_K^{(1)} = 16377.32 \quad \text{in} \quad 0.13 \text{ seconds, and} \]
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Solution recovery yields \( f(x') = 17485.99 \) and \( \|g(x')\|_\infty = 5.85 \cdot 10^{-15} \).

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

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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 \( f(x) = p(\exp x) \), considered 2,500 different “X.”

Here: consider the X with largest gap \( f^*_x - \sup\{\gamma \mid f - \gamma \text{ is X-SAGE}\} \).

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Moment-SOS approaches

- Lasserre hierarchy via YALMIP: 572 s, computes \( f^*_x \approx 22.8 \)

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   The most general signomial Positivstellensatz to-date.

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Extra slides