Algebraic Perspectives on Signomial Programming with Applications to Polynomial Optimization

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(Joint work with R. Murray)

Workshop POP23:
Future Trends in Polynomial Optimization

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**Signomial**: A weighted exponential sum supported on $A \subseteq \mathbb{R}^n$:

$$f(x) = \sum_{\alpha \in A} c_\alpha \exp\langle x, \alpha \rangle, \quad c_\alpha \in \mathbb{R} \text{ for all } \alpha \in A.$$ 

E.g., $f(x) = 2.7 \exp(2x_1 - \frac{1}{3} x_2 + 0.7 x_3) - \sqrt{3} \exp(-4x_1 + \frac{2}{5} x_3)$.

**Signomial Programming**:
Given a signomial $f$ and a signomial constraint set $K$, then consider the **optimization problem**

$$f^K_* := \inf \{ f(x) : x \in K \}.$$ 

- Nonconvex optimization problem.
- Computationally intractable (NP-hard).
- Problem has many applications, e.g., chemical engineering, aircraft design, communications networks.
Problem is equivalent to

\[ f_K^* = \sup\{\gamma \in \mathbb{R} : f(x) - \gamma \geq 0 \text{ for all } x \in K\} \]

**Algebraic Question:** Is \( f \) NONNEGATIVE on \( K \) ?

- Key Problem in real algebraic geometry.
- Problem is NP-hard in general.

**Usual approach:** Find inner/outer approximations of cones of signomials that are nonnegative on \( K \) for which membership can be checked efficiently (usually based on Positivstellensätze).
Different nonnegativity certificates

- *Prominent example for polynomials*: Sums of squares (SOS), which can be tested via semidefinite programming (SDP). More tractable relaxations via DSOS and SDSOS certificates, detectable via LP and SOCP (Ahmadi, Majumdar, 2017).

- Alternative certificates adapted to *sparse* settings:
  - Sums of Nonnegative Circuit (SONC) Polynomials (Iliman, de Wolff, 2016)
  - Sums of AM/GM Exponentials (SAGE) (Chandrasekaran, Shah, 2016)

Detected via relative entropy programming (REP) or in specific cases via geometric programming (GP).

**My Talk**: Approximations via “conditional SAGE”.
Outline for the talk

1. Introduction into the concept of signomial rings.
2. Basics of conditional SAGE.
3. A Positivstellensatz which respects signomial rings.
4. Grading signomial rings by “A-degree”.
5. A complete hierarchy of lower bounds.
7. Outlook: Complete Hierarchy of upper bounds (that builds on signomial moment theory and outer approximations.)
Let $\mathcal{A} \subseteq \mathbb{R}^n$ be a finite set containing 0.

To every $\alpha \in \mathcal{A}$ associate a “monomial” basis function

$$e^\alpha: \mathbb{R}^n \to \mathbb{R}_{++} \text{ that takes values } e^\alpha(x) = \exp\langle \alpha, x \rangle.$$
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A signomial supported on $\mathcal{A} \subseteq \mathbb{R}^n$ is a linear combination

$$f(x) = \sum_{\alpha \in \mathcal{A}} c_\alpha e^\alpha(x),$$

where the support of a signomial is given by

$$\text{supp}(f) = \text{ the smallest set } \mathcal{A} \subseteq \mathbb{R}^n \text{ for which } f \in \text{span}\{e^\alpha\}_{\alpha \in \mathcal{A}}.$$
Let $A \subseteq \mathbb{R}^n$ be a finite set containing 0.

To every $\alpha \in A$ associate a “monomial” basis function

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A posynomial is a signomial with only nonnegative terms.
The *signomial ring* \( \mathbb{R}[A] \) is the \( \mathbb{R} \)-algebra generated by basis functions \( \{ e^\alpha \}_{\alpha \in A} \).
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For modeling reasons, signomials are usually written in geometric form

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

where $t \in \mathbb{R}_{++}^n$ has the correspondence $t_i = \exp(x_i)$.

Signomials in $\mathbb{R}[A]$ are “like” polynomials on $\mathbb{R}_+^A$. 
Consider a signomial \( f = \sum_{\alpha \in A} c_{\alpha} e^{\alpha} \).

**Question:** Signomial Nonnegativity?
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**Easy case**: If all \( c_\alpha \geq 0 \), then \( \sum_{\alpha \in A} c_\alpha e^{\alpha x}(x) \geq 0 \) for all \( x \in \mathbb{R}^n \).
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What about signomials with at most one negative term?
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What about signomials with at most one negative term?

**Definition** (Chandrasekaran, Shah, 2014)

A (globally) nonnegative signomial with at most one negative term is called an “AM/GM Exponential” or an “AGE function”.
Sums of AM/GM Exponentials

**Example**

Let \( f = e^{\alpha_1} + e^{\alpha_2} + e^{\alpha_3} - 3e^{\alpha_4} \), for

\[
\alpha_1 = (2, 4, 0), \quad \alpha_2 = (4, 2, 0), \quad \alpha_3 = (0, 0, 6), \quad \alpha_4 = (2, 2, 2).
\]

Use \( e^\alpha(x) = \exp\langle \alpha, x \rangle = e^x(\alpha) \) and convexity to bound the negative term

\[
\frac{1}{3}\alpha_1 + \frac{1}{3}\alpha_2 + \frac{1}{3}\alpha_3 = \alpha_4 \quad \Rightarrow \quad e^{\alpha_1} + e^{\alpha_2} + e^{\alpha_3} \geq 3e^{\alpha_4}.
\]

**Note:** Convexity of \( \exp \) is equivalent to AM/GM inequality:

Let \( t_1, \ldots, t_m > 0 \) and weights \( \lambda_1, \ldots, \lambda_m \in [0, 1] \) with \( \sum \lambda_i = 1 \), then

\[
\lambda_1 t_1 + \cdots + \lambda_m t_m \geq t_1^{\lambda_1} \cdots t_m^{\lambda_m}.
\]
For signomials with more negative terms ...

**Definition** (Chandrasekaran, Shah, 2014)

A signomial is a "SAGE function" if it can be written as a sum of AGE functions.
Sums of AM/GM Exponentials

For signomials with more negative terms ...

**Definition** (Chandrasekaran, Shah, 2014)
A signomial is a “SAGE function” if it can be written as a sum of AGE functions.

**Facts:**
- Checking whether a signomial is SAGE can be done via *relative entropy programming* (REP).
- REPs are *convex* and involve constraints defining the relative entropy cone: \( \nu_j \log \left( \frac{\nu_j}{\zeta_j} \right) \leq \delta_j \).
- In general SAGE is only a *sufficient* condition for nonnegativity.  
  \( \rightarrow \) E.g., \( f = \exp(2x_1) + \exp(2x_2) + \exp(2x_3) - 2 \exp(x_1 + x_2) - 2 \exp(x_1 + x_3) + 2 \exp(x_2 + x_3) \) is nonnegative, but not SAGE.  
  Note: \( f = (\exp(x_1) - \exp(x_2) - \exp(x_3))^2 \).
Definition (Murray, Chandrasekaran, Wierman, 2019)

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 $\beta \in A$. 

Sparsity Preservation (Murray, Chandrasekaran, Wierman, 2018+2019)

If $f$ is supported on $A$ and has $k \geq 1$ negative coefficients, then $f \in \mathcal{C}_{X}^{P} \mathcal{A} \mathcal{Q}$ is a sum of $k$ X-AGE functions, each supported on $A$. 

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Conditional SAGE

**Definition** *(Murray, Chandrasekaran, Wierman, 2019)*

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.
- The cone of **X-SAGE** signomials supported on \( A \):

\[
C_X(A) := \left\{ f : f(x) = \sum_i f_i(x) \text{ each } f_i \text{ is an X-AGE signomial} \right\}
\]

- Membership in \( C_X(A) \) can again be tested via REP.
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Sparsity Preservation: (Murray, Chandrasekaran, Wierman, 2018+2019)
If \( f \) is supported on \( A \) and has \( k \geq 1 \) negative coefficients, then \( f \in C_X(A) \iff f \) is a sum of \( k \) X-AGE functions, each supported on \( A \).
A univariate example

\[ f(x) = e^{-3x} + e^{-2x} + 4e^x + e^{2x} - 4e^{-x} - 1 - e^{3x} \text{ over } x \leq 0. \]
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\( f(x) = e^{-3x} + e^{-2x} + 4e^x + e^{2x} - 4e^{-x} - 1 - e^{3x} \) over \( x \leq 0 \).

\[ f_1(x) = 0.88 \cdot e^{-3x} + 0.82 \cdot e^{-2x} + 2.69 \cdot e^x + 0.12 \cdot e^{2x} - 4e^{-x} \]

\[ f_2(x) = 0.10 \cdot e^{-3x} + 0.15 \cdot e^{-2x} + 0.90 \cdot e^x + 0.12 \cdot e^{2x} - 1 \]

\[ f_3(x) = 0.02 \cdot e^{-3x} + 0.03 \cdot e^{-2x} + 0.41 \cdot e^x + 0.76 \cdot e^{2x} - e^{3x} \]
Chandrasekaran, Shah, 2014:
Suppose we have *rational* exponents $A = \{0, \alpha_1, \ldots, \alpha_\ell\} \subseteq \mathbb{Q}^n$ and constraint signomials $\{g_1, \ldots, g_{2\ell+m}\} \subseteq \mathbb{R}[A]$ that include

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

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

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

$$K = \{x : g_i(x) \geq 0 \text{ for all } i = 1, \ldots, M\}.$$
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$$g_i(x) = U - e^{\alpha_i}(x) \quad \text{for } i = 1, \ldots, \ell,$$  
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for some $U, L > 0$. Let $M = 2\ell + m$ and define the compact set

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

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

$$f = \sum_{j \in \mathbb{N}^M} \lambda_j \cdot g_1^{j_1} \cdots g_M^{j_M},$$

for finitely many $\mathbb{R}^n$-SAGE $\lambda_j \in \mathbb{R}[A]$. 
**Theorem** (Positivstellensatz; D., Murray, 2021)

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

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

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

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

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

**Note**: No products of constraint functions. Neither $X$ nor $t^x$ need to be semialgebraic. No assumption on $A$. 

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Our Positivstellensatz for X-SAGE

**Theorem** (Positivstellensatz; D., Murray, 2021)

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

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

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

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

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

**Note:**

- No products of constraint functions.
- Neither $X$ nor $\{\exp x : x \in X\}$ need to be semialgebraic.
- No assumption on $\mathcal{A}$.
Our Positivstellensatz for X-SAGE

Corollary (D., Murray, 2021)

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

\[
\left( \sum_{\alpha \in A} e^{\alpha} \right)^r f 
\]

is X-SAGE for large enough \( r \in \mathbb{N} \).
Our Positivstellensatz for X-SAGE

**Corollary** (D., Murray, 2021)

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

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\]

**Theorem** (A. Wang et al., 2020)

Suppose the exponents \( \alpha \in A \) are rational and that \( f \) has “\( A \)-degree” one. If \( f \) is positive on \( X \), then there exists a natural number \( r \) for which \( (\sum_{\alpha \in A} e^{\alpha})^r f \) is X-SAGE.
Our Positivstellensatz for X-SAGE

**Corollary** (D., Murray, 2021)

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

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\[
(\sum_{\alpha \in A} e^{\alpha})^r f \quad \text{is X-SAGE.}
\]

**Note**: Our Positivstellensatz naturally generalizes A. Wang at al.’s to allow nonconvex constraints, to possibly irrational exponents \( A \), and to \( f \) having arbitrary “\( A \)-degree”.
Corollary (D., Murray, 2021)

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

$$(\sum_{\alpha \in \mathcal{A}} e^{\alpha})^r f$$

is X-SAGE for large enough $r \in \mathbb{N}$.

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

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

$$f > 0 \text{ on } X \iff p > 0 \text{ on } Y := \{\exp A x : x \in X\}.$$

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

3. Apply Dickinson-Povh Positivstellensatz to $(p, Y)$.

4. Map the Dickinson-Povh certificate to an X-SAGE certificate.
We can use REP to search for an identity

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

once we have decided $r \in \mathbb{N}$ and *permissible supports* $S_i \supseteq \text{supp}(\lambda_i)$.

**Note:** By sparsity preservation, we do NOT need to explicitly bound $\text{supp}(\lambda_0)$!

We have to decide $S_i$ for $i \geq 1$. 
Grading certificates from the Positivstellensatz

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**Note:** By sparsity preservation, we do NOT need to explicitly bound \(\text{supp}(\lambda_0)\)!

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

**Question:** 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”!
Define the $A$-degree of a signomial $f \in \mathbb{R}[A]$ as

$$\text{deg}_A(f) = \min \# \text{ of products of } \{e^\alpha \}_{\alpha \in A} \text{ to express } f.$$
Define the $\mathcal{A}$-degree of a signomial $f \in \mathbb{R}[\mathcal{A}]$ as

$$\text{deg}_\mathcal{A}(f) = \min \# \text{ of products of } \{e^\alpha\}_{\alpha \in \mathcal{A}} \text{ to express } f.$$ 

Using $\mathcal{A}_d = \{\text{sums of } \leq d \text{ vectors from } \mathcal{A}\}$, we express

$$\text{deg}_\mathcal{A}(f) = \inf\{d : \text{ supp}(f) \subseteq \mathcal{A}_d\}.$$
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**Example**

For $\mathcal{A} = \{0, 1, 3\}$, we have

$$\text{deg}_\mathcal{A}(\exp(x)) = 1, \quad \text{deg}_\mathcal{A}(\exp(2x)) = 2, \quad \text{deg}_\mathcal{A}(\exp(3x)) = 1.$$
Signomial $\mathcal{A}$-degree

Define the $\mathcal{A}$-degree of a signomial $f \in \mathbb{R}[\mathcal{A}]$ as

$$\deg_{\mathcal{A}}(f) = \min \# \text{ of products of } \{e^{\alpha}\}_{\alpha \in \mathcal{A}} \text{ to express } f.$$  

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- Not intrinsic to signomials.

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

- Co-variant with affine changes of coordinates.
Define the $\mathcal{A}$-degree of a signomial $f \in \mathbb{R}[\mathcal{A}]$ as
\[ \deg_{\mathcal{A}}(f) = \min \# \text{ of products of } \{e^{\alpha}\}_{\alpha \in \mathcal{A}} \text{ to express } f. \]

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- Not intrinsic to signomials.
  
  Setting $\mathcal{A} = \text{supp}(f)$, we have $\deg_{\mathcal{A}}(f) = 1$.

- Co-variant with affine changes of coordinates.

Let $\mathbb{R}[\mathcal{A}]_d$ denote the signomials in $\mathbb{R}[\mathcal{A}]$ of $\mathcal{A}$-degree at most $d$. 
The following inequality always holds. It can be strict

\[ \deg_A(fg) \leq \deg_A(f) + \deg_A(g). \]
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\[ \deg_{\mathcal{A}}(fg) \leq \deg_{\mathcal{A}}(f) + \deg_{\mathcal{A}}(g). \]

**Example**

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

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

So, \( \deg_{\mathcal{A}}(fg) < \deg_{\mathcal{A}}(f). \)
The following inequality always holds. It can be strict

\[ \deg_A(fg) \leq \deg_A(f) + \deg_A(g). \]

**Example**

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If \( g \in \{c \exp(-x) : c \in \mathbb{R}\} \), then \( \deg_A(gf) = 1 \).

So, \( \deg_A(fg) < \deg_A(f) \).

**Definition** (D., Murray, 2021)

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

\[ \deg_A(e^\beta f) \leq d \quad \text{for all} \ \beta \in B. \]

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

\[ \text{supp}(g) \subseteq \text{invsupp}_d(f) \quad \Rightarrow \quad \deg_A(g) \leq d \quad \text{and} \quad \deg_A(fg) \leq d. \]
We want to compute:

\[ f^{*}_K = \inf_{x \in K} f(x) \quad \text{where} \quad K = \{ x \in X : g_i(x) \geq 0 \text{ for all } i = 1, \ldots, m \}. \]
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**Idea:** Grade certificates according to largest $A$-degree of the constituent signomials.
A Complete Hierarchy of Lower bounds

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**Idea:** Grade certificates according to largest \( \mathcal{A} \)-degree of the constituent signomials.

**Definition**

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

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

\[ \lambda_i \in C_X (\text{invsupp}_d(g_i)) \quad \text{for all } i = 1, \ldots, m, \]

\[ \lambda_0 \in C_X (\mathcal{A}_d), \quad \text{and} \quad \gamma \in \mathbb{R}. \]

Otherwise, \( f_K^{(d)} = -\infty \).
A Complete Hierarchy of Lower bounds

- \( f_K^* = \inf_{x \in K} f(x) \) where \( K = \{ x \in X : g_i(x) \geq 0 \text{ for all } i = 1, \ldots, m \} \)
- \( f_K^{(d)} := \sup \gamma \text{ s.t. } (\sum_{\alpha \in \mathcal{A}} e^{\alpha})^r (f - \gamma) = \lambda_0 + \sum_{i=1}^m \lambda_i g_i \)

**Corollary (D., Murray, 2021)**

The sequence \( f_K^{(1)}, f_K^{(2)}, \ldots \) is nondecreasing and bounded above by \( f_K^* \).
If \( \{f, g_1, \ldots, g_m\} \subseteq \mathbb{R}[\mathcal{A}] \) and \( X \) is compact, then

\[
\lim_{d \to \infty} f_K^{(d)} = f_K^*.
\]

**Note:** Bounds \( f_K^{(d)} \) can be computed via REPs.
Example 1: Chemical Reactor Design Problem, \( (t = \exp x) \)

We consider the design of a chemical reactor system as described by Blau and Wilde:

**Goal**: Find the best design of this chemical reactor system.

![Chemical reactor system diagram](image-url)
Example 1: Chemical Reactor Design Problem, \((t = \exp x)\)

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

s.t. Five nonconvex constraints of the form

\[
1 - \text{(posynomial in } t) = 0
\]
Example 1: Chemical Reactor Design Problem, \( (t = \exp x) \)

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

s.t. Five nonconvex constraints of the form
\[
1 - \text{(posynomial in } t) = 0
\]

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

Work in the *naive ring*

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

Handling *equality constraints*

- Infer valid constraints “1 – (posynomial in \( t \)) \geq 0” for \( X \).
- “Lagrange multipliers” \( \lambda_i \) only constrained by their supports.
Example 1: Chemical Reactor Design Problem, \((t = \exp x)\)

We compute

\[
\begin{align*}
    f_K^{(1)} &= 16377.32 \quad \text{in } 0.13 \text{ seconds, and} \\
    f_K^{(2)} &= 17462.73 \quad \text{in } 24.37 \text{ seconds.}
\end{align*}
\]

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.

<table>
<thead>
<tr>
<th></th>
<th>Using (t) as optimization variable</th>
<th>Using (x) as optimization variable</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>solver time (s) lower bound</td>
<td>solver time (s) lower bound</td>
</tr>
<tr>
<td>BARON</td>
<td>163 (-\infty)</td>
<td>7200 (-\infty)</td>
</tr>
<tr>
<td>ANTIGONE</td>
<td>145 (-16880.380)</td>
<td>7200 (-\infty)</td>
</tr>
<tr>
<td>LINDO</td>
<td>1468 17484.314</td>
<td>50 17485.988</td>
</tr>
</tbody>
</table>

All solvers above returned a solution with objective value \(\approx 17485.99\). SCIP returned no solution and no bound before timeout.
Example 2: Chemical dynamics

Concentration of chemical species are described by an ODE

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

Questions:

(i) When does a given CRN exhibit multistationarity (i.e., has multiple fixed points) over a set $S \subseteq \mathbb{R}^n_{++}$?

(ii) Has system capacity for multistationarity: can we add a constant vector-valued offset to $R_k$ so ODE has multiple fixed points in $S$?

Note, (ii) translates to specific injectivity criterion; see Pantea, Koeppel, Craciun [PKC].

Example: Consider system from [PKC] with six species and various boxes $B$. Is $R_k$ injective for all $k \in B$? ... Apply conditional SAGE.
Example 2: Minimizing the polynomial from before

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

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

<table>
<thead>
<tr>
<th>( r )</th>
<th>( A_{nat} )</th>
<th>( A_{int} )</th>
<th>( A_{naive} )</th>
<th>( A_{nat} )</th>
<th>( A_{int} )</th>
<th>( A_{naive} )</th>
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<tr>
<td>2</td>
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<td>-</td>
<td>-</td>
<td>49.2000</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Moment-SOS approaches:
- Lasserre hierarchy via YALMIP: 572 s, computes \( f_X^* \approx 22.8 \).
- TSSOS via TSSOS.jl: 567s, computes \( f_X^* \approx 22.8 \).
**Goal**: Complete hierarchy of upper bounds for

\[ f^*_K = \min \{ f(x) : x \in K \} . \]
**Goal:** Complete hierarchy of upper bounds for

\[ f^*_K = \min\{ f(x) : x \in K \}. \]

**Theorem (D., Murray, 2021)**

Let \( \text{span}(A) = \mathbb{R}^n \), \( K \) be compact, and \( \mu \) be a Borel measure with support \( K \).

Let \( (C_d)_{d \geq 1} \) be a nested sequence of closed convex cones where

1. \( C_d \subseteq \mathbb{R}[A]_d \) contains all posynomials in \( \mathbb{R}[A]_d \),
2. all signomials in \( C_d \) are nonnegative on \( K \), and
3. \( \bigcup_{d \geq 1} C_d \) includes every signomial in \( \mathbb{R}[A] \) that is positive on \( K \).
**Goal**: Complete hierarchy of upper bounds for

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For \( f \in \mathbb{R}[A] \) and integers \( d \geq 1 \), define

\[ \theta_d := \inf_{\psi} \left\{ \int f \psi \, d\mu : \int \psi \, d\mu = 1, \psi \in C_d \right\}. \]

The sequence \((\theta_d)_{d \geq 1}\) **monotonically converges** to \( f_K^* \) from **above**.
Outlook: Upper Bounds

**Goal:** Compl. hierarchy of upper bounds for \( f_K^* = \min\{f(x) : x \in K\} \).

**Theorem (D., Murray, 2021)**

Let \( \text{span}(A) = \mathbb{R}^n \), \( K \) be compact, and \( \mu \) be a Borel measure with support \( K \).

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\[
\theta_d := \inf_{\psi} \left\{ \int f\psi \, d\mu : \int \psi \, d\mu = 1, \psi \in C_d \right\}.
\]

The sequence \((\theta_d)_{d \geq 1}\) monotonically converges to \( f_K^* \) from above.

**Note:** No assumptions on the representation of \( K \) and agnostic to precise nature of \((C_d)_{d \geq 1}\).
Take-home message

1. Introduced a new Positivstellensatz.
   - Respects the structure of the new concept of signomial rings.
   - The most general signomial Positivstellensatz to-date.

2. Derived a canonical hierarchy based on $A$-degree.

3. Demonstrated the hierarchy’s practicality.
   - Competitive with BARON, ANTIGONE, LINDO on a hard SP.
   - Much faster than Moment-SOS methods on high-degree sparse POP.

4. There is more ...
   - Framework for signomial moments.
   - Hierarchical outer-approximations for the signomial nonnegativity cone.
   - Generic construction for complete hierarchy of upper bounds.
Open Problems

Open Questions

- How to choose “best” signomial ring $\mathbb{R}[A]$?
- Detailed study of signomial moment theory and upper bounds.
- Convergence rates for upper bounds.
Thank you for your attention!


