

Sparse (Non)commutative Polynomial Optimization

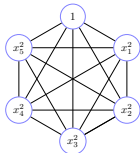
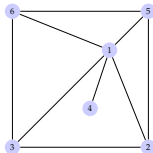
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Joint commutative work with J.-B. Lasserre, H. N. A. Mai & J. Wang

Joint Noncommutative work with I. Klep & J. Povh

Real Algebraic Geometry with a View Toward Hyperbolic
Programming and Free Probability, Oberwolfach

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The Moment-Sums of Squares Hierarchy

NP-hard NON CONVEX Problem $f^* = \inf f(x)$

Theory

(Primal)		(Dual)
$\inf \int f d\mu$		$\sup \lambda$
with μ proba \Rightarrow	INFINITE LP	\Leftarrow with $f - \lambda \geq 0$

The Moment-Sums of Squares Hierarchy

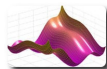
NP-hard NON CONVEX Problem $f^* = \inf f(x)$

Practice

(Primal **Relaxation**)

$$\text{moments } \int x^\alpha d\mu$$

finite number \Rightarrow



SDP

(Dual **Strengthening**)

$$f - \lambda = \text{sum of squares}$$

\Leftarrow **fixed** degree

LASSERRE'S HIERARCHY of **CONVEX PROBLEMS** $\uparrow f^*$
[Lasserre/Parrilo 01]

degree d & n vars $\Rightarrow \binom{n+2d}{n}$ **SDP** VARIABLES

Numeric solvers \Rightarrow **Approx** Certificate



Exploiting correlative sparsity

Exploiting term sparsity

Exploiting correlative sparsity

Exploiting term sparsity

SDP for Polynomial Optimization

NP hard General Problem: $f^* := \min_{\mathbf{x} \in \mathbf{K}} f(\mathbf{x})$

- Semialgebraic set

$$\mathbf{K} := \{\mathbf{x} \in \mathbb{R}^n : g_1(\mathbf{x}) \geq 0, \dots, g_l(\mathbf{x}) \geq 0\}$$

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$$\underbrace{f}_{x_1 x_2} =$$

$$-\frac{1}{8} + \frac{1}{2} \overbrace{\left(x_1 + x_2 - \frac{1}{2}\right)^2}^{\sigma_0} + \frac{1}{2} \overbrace{x_1(1 - x_1)}^{g_1} + \frac{1}{2} \overbrace{x_2(1 - x_2)}^{g_2}$$

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- Sums of squares (SOS) σ_j

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- Sums of squares (SOS) σ_j
- Bounded degree:

$$\mathcal{M}(\mathbf{K})_d := \left\{ \sigma_0 + \sum_{j=1}^l \sigma_j g_j, \text{ with } \deg \sigma_j g_j \leq 2d \right\}$$

SDP for Polynomial Optimization

- **Hierarchy of SDP relaxations:**

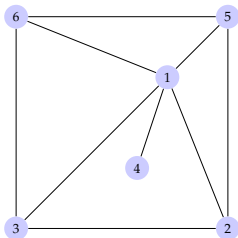
$$\lambda_d := \sup_{\lambda} \left\{ \lambda : f - \lambda \in \mathcal{M}(\mathbf{K})_d \right\}$$

- Convergence guarantees $\lambda_d \uparrow f^*$ [Lasserre 01]
- Can be computed with SDP solvers (CSDP, SDPA, MOSEK)
- **“No Free Lunch” Rule:** $\binom{n+2d}{n}$ SDP variables

Sparse polynomial optimization [Waki, Lasserre 06]

- Correlative sparsity pattern (csp) of vars

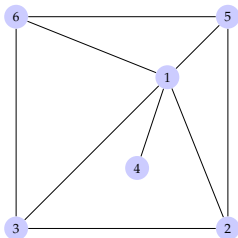
$$x_2x_5 + x_3x_6 - x_2x_3 - x_5x_6 + x_1(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6)$$



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1 Index sets I_1, \dots, I_p

2 Average size $\kappa \rightsquigarrow \binom{\kappa+2d}{\kappa}$ vars

$$I_1 = \{1, 4\}$$

$$I_2 = \{1, 2, 3, 5\}$$

$$I_3 = \{1, 3, 5, 6\}$$

Dense SDP: 210 vars

Sparse SDP: 115 vars

Sparse polynomial optimization [Waki, Lasserre 06]

Sparse $f = f_1 + \dots + f_p$ with $f_k \in \mathbb{R}[x, I_k]$

Sparse $\mathbf{K} = \{\mathbf{x} : g_j(\mathbf{x}) \geq 0\}$ with $g_j \in \mathbb{R}[x, I_{k(j)}]$ for some $k(j)$

Additional constraints $n_k - \sum_{i \in I_k} x_i^2 \geq 0$ in \mathbf{K}

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$$\forall k = 2, \dots, p \quad I_k \cap \bigcup_{j < k} I_j \subseteq I_i \quad \text{for some } i < k$$

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Theorem: Sparse Putinar's representation [Lasserre 06]

$$f > 0 \text{ on } \mathbf{K} + \text{RIP} \implies f = \sigma_{01} + \dots + \sigma_{0p} + \sum_{j=1}^m \sigma_j g_j$$

with $\sigma_{0k} \in \Sigma[x, I_k]$, $\sigma_j \in \Sigma[x, I_{k(j)}]$

Sparse examples

- Chained singular function:

$$f_{\text{CS}} = \sum_{i \in J} ((x_i + 10x_{i+1})^2 + 5(x_{i+2} - x_{i+3})^2 + (x_{i+1} - 2x_{i+2})^4 + 10(x_i - x_{i+3})^4)$$

where $J = \{1, 3, 4, \dots, n - 3\}$ and n is a multiple of 4

💡 $I_k = \{k, k + 1, k + 2, k + 3\}$

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- Generalized Rosenbrock function:

$$f_{\text{gR}} = 1 + \sum_{i=1}^{n-1} \left(100(x_{i+1} - x_i^2)^2 + (1 - x_{i+1})^2 \right)$$

💡 $I_k = \{k, k + 1\}$

Roundoff Errors

- Exact:

$$f(\mathbf{x}) := x_1x_2 + x_3x_4$$

- Floating-point:

$$\hat{f}(\mathbf{x}, \mathbf{e}) := [x_1x_2(1 + e_1) + x_3x_4(1 + e_2)](1 + e_3)$$

- $\mathbf{x} \in \mathbf{X}$, $|e_i| \leq 2^{-\delta}$ $\delta = 24$ (single) or 53 (double)

Roundoff Errors

Input: exact $f(\mathbf{x})$, floating-point $\hat{f}(\mathbf{x}, \mathbf{e})$

Output: Bounds for $f - \hat{f}$

1: Error $r(\mathbf{x}, \mathbf{e}) := f(\mathbf{x}) - \hat{f}(\mathbf{x}, \mathbf{e}) = \sum_{\alpha} r_{\alpha}(\mathbf{e}) \mathbf{x}^{\alpha}$

2: Decompose $r(\mathbf{x}, \mathbf{e}) = \ell(\mathbf{x}, \mathbf{e}) + h(\mathbf{x}, \mathbf{e})$, ℓ **linear** in \mathbf{e}

3: Bound $h(\mathbf{x}, \mathbf{e})$ with interval arithmetic

4: Bound $\ell(\mathbf{x}, \mathbf{e})$ with **SPARSE SUMS OF SQUARES**

Exploiting sparsity for roundoff error bounds

$$l(\mathbf{x}, \mathbf{e}) = \sum_{i=1}^m s_i(\mathbf{x})e_i$$

I_1, \dots, I_m correspond to $\{\mathbf{x}, e_1\}, \dots, \{\mathbf{x}, e_m\}$

Dense relaxation: $\binom{n+m+2d}{n+m}$ SDP variables

Sparse relaxation: $m \binom{n+1+2d}{n+1}$ SDP variables

Simple comparison [M.-Constantinides-Donaldson 17]

$$f(\mathbf{x}) := x_2x_5 + x_3x_6 - x_2x_3 - x_5x_6 + x_1(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6)$$

$$\mathbf{x} \in [4.00, 6.36]^6, \quad \mathbf{e} \in [-\epsilon, \epsilon]^{15}, \quad \epsilon = 2^{-53}$$

- **Dense SDP:** $\binom{6+15+4}{6+15} = 12650$ variables \leadsto **Out of memory**

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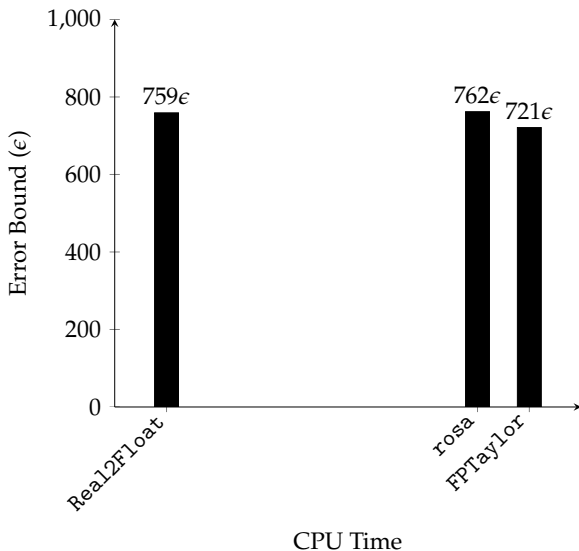
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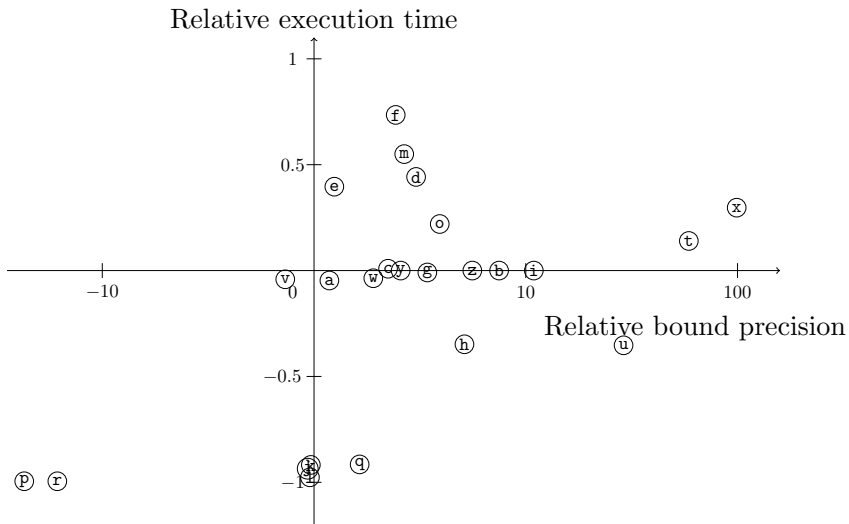
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- **Symbolic Taylor** FPTaylor tool: 721ϵ ($21 \times$ more CPU)
- **SMT-based** rosa tool: 762ϵ ($19 \times$ more CPU)

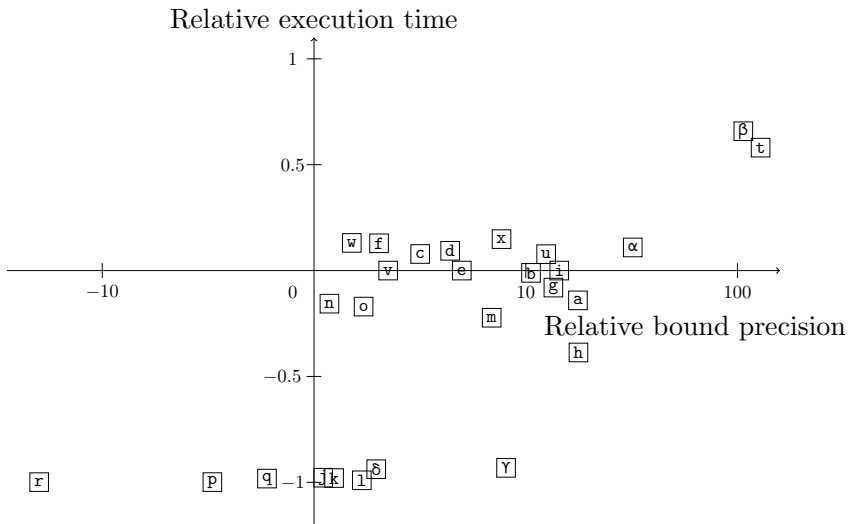
Simple comparison [M.-Constantinides-Donaldson 17]



SOS versus rosa [M.-Constantinides-Donaldson 17]



SOS versus FPTaylor [M.-Constantinides-Donaldson 17]



Noncommutative (NC) polynomials

Symmetric **Matrix** variables X_i, Y_j

$$f = X_1(Y_1 + Y_2 + Y_3) + X_2(Y_1 + Y_2 - Y_3) + X_3(Y_1 - Y_2) - X_1 - 2Y_1 - Y_2$$

with $X_1X_2 \neq X_2X_1$, **involution** $(X_1Y_3)^* = Y_3X_1$

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Constraints $\mathbf{K} = \{(X, Y) : X_i, Y_j \succcurlyeq 0, X_i^2 = X_i, Y_j^2 = Y_j, X_iY_j = Y_jX_i\}$

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MINIMAL EIGENVALUE OPTIMIZATION

$$\lambda_{\min} = \inf \{ \langle f(X, Y) \mathbf{v}, \mathbf{v} \rangle : (X, Y) \in \mathbf{K}, \|\mathbf{v}\| = 1 \}$$

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$$\begin{aligned}\lambda_{\min} &= \inf \{ \langle f(X, Y)\mathbf{v}, \mathbf{v} \rangle : (X, Y) \in \mathbf{K}, \|\mathbf{v}\| = 1 \} \\ &= \sup \lambda \\ &\text{s.t. } f(X, Y) - \lambda \mathbf{I} \succcurlyeq 0, \quad \forall (X, Y) \in \mathbf{K}\end{aligned}$$

Putinar's representation

“Archimedean” constraint in $\mathbf{K} = \{X : g_j(X) \succcurlyeq 0\}$:

$$N - \sum_i X_i^2 \succcurlyeq 0$$

Theorem: NC Putinar's representation [Helton-McCullough 02]

$$f \succcurlyeq 0 \text{ on } \mathbf{K} \implies f = \sum_i s_i^* s_i + \sum_j \sum_i t_{ji}^* g_j t_{ji} \text{ with } s_i, t_{ji} \in \mathbb{R}\langle X \rangle$$

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NC variant of Lasserre's Hierarchy for λ_{\min} :

💡 replace “ $f - \lambda \mathbf{I} \succcurlyeq 0$ on \mathbf{K} ” by $f - \lambda \mathbf{I} = \sum_i s_i^* s_i + \sum_j \sum_i t_{ji}^* g_j t_{ji}$
with s_i, t_{ji} of **bounded** degrees

Sparse Putinar's representation [Klep-M.-Povh 19]

Sparse $f = f_1 + \cdots + f_p$ with $f_k \in \mathbb{R}\langle X, I_k \rangle$

Sparse $\mathbf{K} = \{X : g_j(X) \succcurlyeq 0\}$ with $g_j \in \mathbb{R}\langle X, I_{k(j)} \rangle$ for some $k(j)$

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$$\forall k = 2, \dots, p \quad I_k \cap \bigcup_{j < k} I_j \subseteq I_i \quad \text{for some } i < k$$

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with $s_{ki} \in \mathbb{R}\langle X, I_k \rangle$, $t_{ji} \in \mathbb{R}\langle X, I_{k(j)} \rangle$

Proof outline: by contradiction

$f \succ 0$ on \mathbf{K} and

$$f \notin \underbrace{\left\{ \sum_k \sum_i s_{ki}^* s_{ki} + \sum_j \sum_i t_{ji}^* g_j t_{ji} : s_{ki} \in \mathbb{R}\langle X, I_k \rangle, t_{ji} \in \mathbb{R}\langle X, I_{k(j)} \rangle \right\}}_{\mathcal{M}(\mathbf{K})^{\text{sparse}}}$$

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💡 Separation argument \implies there exists $L : \mathbb{R}\langle X \rangle \rightarrow \mathbb{R}$ with $L(f) \leq 0$ and $L(\mathcal{M}(\mathbf{K})^{\text{sparse}}) \subseteq \mathbb{R}^{\geq 0}$

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💡 Gelfand-Naimark-Segal (GNS) construction:

Find $A \in \mathbf{K}$ and $\mathbf{v} \neq 0$ such that

$$L(f) = \langle f(A)\mathbf{v}, \mathbf{v} \rangle$$

Proof outline: induction on p & amalgamation

- $p = 1 \rightarrow$ NC Putinar's representation of f

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- $p = 2$ & $I_1 \cap I_2 = \emptyset \rightarrow$ NC Putinar's representation of f_1 & f_2

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- $p = 1 \rightarrow$ NC Putinar's representation of f
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- $p = 2$ and $I_1 \cap I_2 \neq \emptyset$

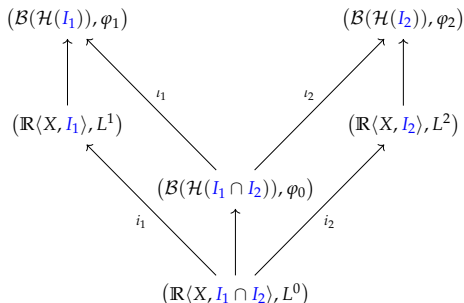
GNS construction on

$$L^k = L |_{\mathbb{R}\langle X, I_k \rangle}$$

\Downarrow

$$L^k(g) = \langle g(A^k) \mathbf{w}^k, \mathbf{w}^k \rangle \text{ for}$$

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- A^k (\times operator)
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Proof outline: induction on p & amalgamation

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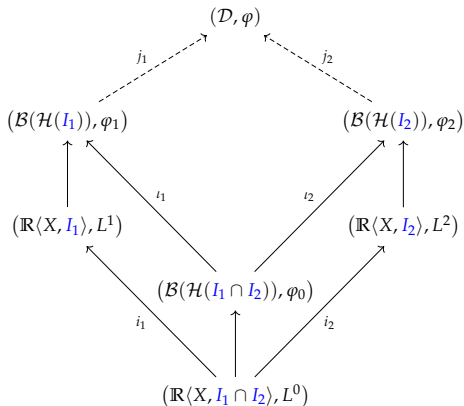
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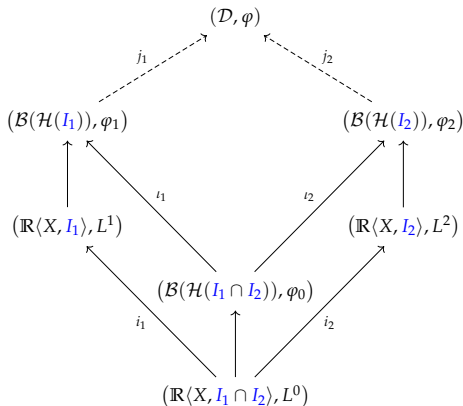
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GNS on $\mathcal{D} \implies A \in \mathbf{K}$ and $\mathbf{v} \neq 0$

Sparsity & no RIP \Rightarrow no sparse representation

$$f = (X_1 + X_2 + X_3)^2 = f_1 + f_2 + f_3$$

$$f_1 = \frac{1}{2}X_1^2 + \frac{1}{2}X_2^2 + X_1X_2 + X_2X_1 \in \mathbb{R}\langle X_1, X_2 \rangle$$

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$$\mathbf{K} = \{X : 1 - X_i^2 \succcurlyeq 0\}$$

$f \succcurlyeq 0$ on \mathbf{K} but $f + \lambda \in \mathcal{M}(\mathbf{K})^{\text{sparse}} \Leftrightarrow \lambda \geq 3$

Sparsity & no RIP \Rightarrow no sparse representation

$$f + 3 = (X_1 + X_2)^2 + (X_1 + X_3)^2 + (X_2 + X_3)^2 + \sum_i (1 - X_i^2) \in \mathcal{M}(\mathbf{K})^{\text{sparse}}$$

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💡 Duality argument: find $L_k : \mathbb{R}\langle X, I_k \rangle \rightarrow \mathbb{R}$ such that

1 $L_k(1) = 1$

2 $L_k(h^*h) \geq 0 \quad L_k(h^*(1 - X_k^2)h) \geq 0 \quad \forall h \in \mathbb{R}\langle X, I_k \rangle$

3 $\sum_k L_k(f_k) = -3$

4 $L_j = L_k$ on $\mathbb{R}\langle X, I_j \cap I_k \rangle$

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Answer:

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad B = -A$$

$$L_k(g) = \text{tr } g(A, B) \quad \text{for } g \in \mathbb{R}\langle X, I_k \rangle$$

A sparse Helton-McCullough's theorem?

Theorem [Helton-McCullough 02]

$$f \succcurlyeq 0 \Leftrightarrow f \in \Sigma\langle \underline{X} \rangle$$

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Lemma [Klep-M.-Povh 19]

There is no sparse analog of the Helton-McCullough's theorem

A counter-example

$$v = \begin{bmatrix} X_1 & X_1X_2 & X_2 & X_3 & X_3X_2 \end{bmatrix}$$
$$G = \begin{bmatrix} 1 & -1 & -1 & 0 & \alpha \\ -1 & 2 & 0 & -\alpha & 0 \\ -1 & 0 & 3 & -1 & 9 \\ 0 & -\alpha & -1 & 6 & -27 \\ \alpha & 0 & 9 & -27 & 142 \end{bmatrix} \quad \alpha \in \mathbb{R}$$

$$\begin{aligned} f &= vGv^* \\ &= X_1^2 - X_1X_2 - X_2X_1 + 3X_2^2 - 2X_1X_2X_1 + 2X_1X_2^2X_1 - X_2X_3 \\ &\quad - X_3X_2 + 6X_3^2 + 9X_2^2X_3 + 9X_3X_2^2 - 54X_3X_2X_3 + 142X_3X_2^2X_3 \end{aligned}$$

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$$\dots G \succcurlyeq 0 \Leftrightarrow 0.27 \lesssim \alpha \lesssim 1.11 \Rightarrow \boxed{f \notin \Sigma\langle X_1, X_2 \rangle + \Sigma\langle X_2, X_3 \rangle}$$

Sparse positive definite forms [Mai-Lasserre-M. 20]

Thm: Reznick's representation [Reznick 95]

$$\text{pd form } f \implies f = \frac{\sigma}{\|\mathbf{x}\|_2^{2d}} \text{ with } \sigma \in \Sigma[\mathbf{x}], d \in \mathbb{N}$$

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Sparse $f = f_1 + \dots + f_p$ with $f_k \in \mathbb{R}[\mathbf{x}, I_k]$

RUNNING INTERSECTION PROPERTY (RIP)

$$\forall k = 2, \dots, p \quad I_k \cap \underbrace{\bigcup_{j < k} I_j}_{\hat{I}_k} \subseteq I_{s_k} \quad \text{for some } s_k < k$$

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Thm: Sparse Reznick's representation [Mai-Lasserre-M. 20]

$$\text{pd form } f + \text{RIP} \implies f = \sum_k \frac{\sigma_k}{H_k^d} \text{ with } \sigma_k \in \Sigma[\mathbf{x}, I_k], d \in \mathbb{N}$$

Uniform H_k involve products $\|\mathbf{x}(I)\|^2$ for $I \in \{I_k, \hat{I}_k, \hat{I}_i : s_i = k\}$

Proof ingredients

- 1 Induction on p as in [Grimm-Netzer-Schweighofer 07] for sparse positive polynomials on compact sets

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- 2 Similar ingredients used for generalized Schmüdgen's Positivstellensatz [Berr-Wörmann 01, Schweighofer 03]:

\mathbb{R} -algebra fin. generated by x_1, \dots, x_n & **fractions** $\frac{\mathbf{x}(I_k)^\alpha}{\|\mathbf{x}(I_k)\|_2^{2d_k}}$

The need for denominators

Commutative version of previous example:

$$f = x_1^2 - 2x_1x_2 + 3x_2^2 - 2x_1^2x_2 + 2x_1^2x_2^2 - 2x_2x_3 + 6x_3^2 + 18x_2^2x_3 + 88x_2^2x_3^2$$

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$$f \in \frac{\Sigma\langle x_1, x_2 \rangle}{1 + x_2^2} + \frac{\Sigma\langle x_2, x_3 \rangle}{1 + x_2^2}$$

Sparse example: I_{3322} Bell Inequality

Entanglement in quantum mechanics

→ **upper bounds** for violation levels of Bell inequalities

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I_{3322} Bell inequality

$$f = X_1(Y_1 + Y_2 + Y_3) + X_2(Y_1 + Y_2 - Y_3) + X_3(Y_1 - Y_2) - X_1 - 2Y_1 - Y_2$$

$$\mathbf{K} = \{(X, Y) : X_i, Y_j \succeq 0, X_i^2 = X_i, Y_j^2 = Y_j, X_i Y_j = Y_j X_i\}$$

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6	0.2508753977180	!!!!

Exploiting correlative sparsity

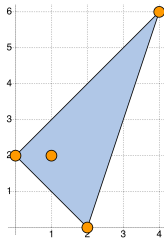
Exploiting term sparsity

Exploiting sparsity via Newton polytope

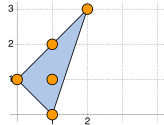
$$f = 4x^4y^6 + x^2 - xy^2 + y^2$$

$$\text{spt}(f) = \{(4, 6), (2, 0), (1, 2), (0, 2)\}$$

$$\text{Newton polytope } \mathcal{P} = \text{conv}(\text{spt}(f))$$



Squares in SOS decomposition $\subseteq \frac{\mathcal{P}}{2} \cap \mathbb{N}^n$
 [Reznick 78]



$$f = \left(x \quad y \quad xy \quad xy^2 \quad x^2y^3 \right) \underbrace{Q}_{\succeq 0} \begin{pmatrix} x \\ y \\ xy \\ xy^2 \\ x^2y^3 \end{pmatrix}$$

Exploiting term sparsity [Wang-M.-Lasserre 20]

$$f = x^2 - 2xy + 3y^2 - 2x^2y + 2x^2y^2 - 2yz \\ + 6z^2 + 18y^2z - 54yz^2 + 142y^2z^2$$

Newton polytope $\rightarrow f = (1 \ x \ y \ z \ xy \ yz) \underbrace{Q}_{\succeq 0}$

$\rightsquigarrow \frac{6 \times 7}{2} = 28$ “unknown” entries in Q

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Exploiting term sparsity [Wang-M.-Lasserre 20]

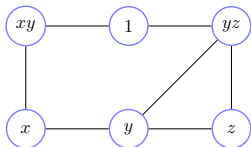
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💡 **Term sparsity pattern graph G**



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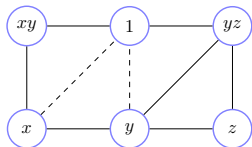
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💡 **Term sparsity pattern graph G**

Chordal extension



Replace Q by Q_G with nonzero entries at edges of G

$\rightsquigarrow 6 + 9 = 15$ “unknown” entries in Q_G

Lyapunov functions from networked systems

$$f = \sum_{i=1}^N a_i (x_i^2 + x_i^4) - \sum_{i,k=1}^N b_{ik} x_i^2 x_k^2 \quad a_i \in [1, 2] \quad b_{ik} \in \left[\frac{0.5}{N}, \frac{1.5}{N}\right]$$

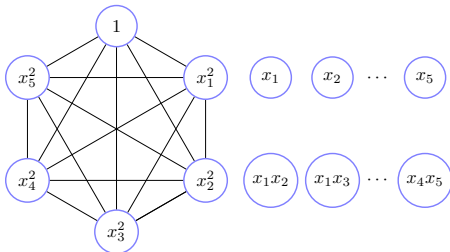
$\rightsquigarrow \binom{N+2}{2} (\binom{N+2}{2} + 1) / 2$ “unknown” entries in $\mathcal{Q} = 231$ for $N = 5$

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$\rightsquigarrow \binom{N+2}{2} \left(\binom{N+2}{2} + 1 \right) / 2$ “unknown” entries in $Q = 231$ for $N = 5$

💡 **tsp** graph G

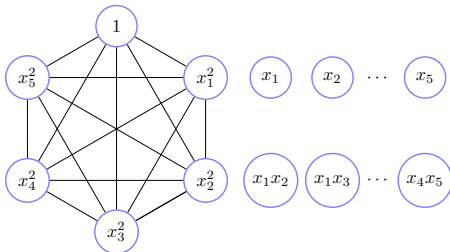


Lyapunov functions from networked systems

$$f = \sum_{i=1}^N a_i (x_i^2 + x_i^4) - \sum_{i,k=1}^N b_{ik} x_i^2 x_k^2 \quad a_i \in [1, 2] \quad b_{ik} \in \left[\frac{0.5}{N}, \frac{1.5}{N}\right]$$

$\rightsquigarrow \binom{N+2}{2} \left(\binom{N+2}{2} + 1 \right) / 2$ “unknown” entries in $Q = 231$ for $N = 5$

💡 **tsp** graph G



$\rightsquigarrow (N+1)^2$ “unknown” entries in $Q_G = 36$ for $N = 5$

Proof that $f \geq 0$ for $N = 80$ in ~ 10 seconds!

Conclusion and Perspectives

- Quest for efficiency

Commutative: **Roundoff error/Networked systems** $n \simeq 10^2$

Noncommutative: **Minimal eigenvalue** $n \simeq 20 - 30$

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💡 **DEGREE BOUNDS** of Sparse Reznick's representations?




💡 **SPARSE RATIONAL SOS** representations for sparse nonnegative polynomials?

💡 **SYMMETRIC** noncommutative problems?




💡 **Combine CORRELATIVE** and **TERM** sparsity

Conclusion and Perspectives



APPLICATIONS IN QUANTUM PHYSICS

- Quantum games: number of mutually unbiased bases in dim 6, OPEN FOR SEVERAL DECADES!!  **symmetric**
- Ground state energy of hamiltonians  **symmetric & sparse**
- Inflation for quantum correlations  **symmetric & sparse**

APPLICATIONS IN DYNAMICAL SYSTEMS

- learning, feedback design, decentralized stabilization  **sparse**
- Quantum Optimal Control  **sparse**
- Optimal power-flow  **sparse**

APPLICATIONS IN MACHINE LEARNING

- robustness of deep networks  **sparse**
- Lipschitz global/local constants of deep networks  **sparse**

Thank you for your attention!

<https://homepages.laas.fr/vmagron>



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