Optimization with Polynomials in Diverse Forms

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Outline

1. Optimization with polynomials in diverse forms
2. Positivstellensatz and the moment-SOS hierarchy
3. Improve scalability by exploiting structures

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Optimization with polynomials in diverse forms

Commutative polynomial optimization

- commutative polynomial optimization:

$$\begin{cases} \inf_{\mathbf{x}\in\mathbb{R}^n} & f(\mathbf{x}) \\ \text{s.t.} & g_i(\mathbf{x}) \ge 0, \quad i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0, \quad j = 1, \ldots, \ell \end{cases}$$

- cover a board class of continuous and discrete nonconvex optimization problems

➤ optimal power flow, computer vision, combinatorial optimization, neutral network verification, sensor network localization

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Sum-of-rational-functions optimization

- sum-of-rational-functions optimization:

$$\begin{cases} \inf\limits_{\mathbf{x}\in\mathbb{R}^n} & \sum_{i=1}^N \frac{p_i(\mathbf{x})}{q_i(\mathbf{x})} \\ \text{s.t.} & g_i(\mathbf{x}) \ge 0, \quad i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0, \quad j = 1, \ldots, \ell \end{cases}$$

➤ computer vision, signal processing

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Polynomial matrix optimization

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$$\begin{cases} \inf\limits_{\mathbf{x}\in\mathbb{R}^n} & \lambda_{\min}(F(\mathbf{x})) \\ \text{s.t.} & G_i(\mathbf{x}) \succeq 0, \quad i = 1, \ldots, m \end{cases}$$

➤ control theory, program verification

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Complex polynomial optimization

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$$\begin{cases} \inf\limits_{\mathbf{z}\in\mathbb{C}^n} & f(\mathbf{z},\overline{\mathbf{z}}) \\ \text{s.t.} & g_i(\mathbf{z},\overline{\mathbf{z}}) \ge 0, \quad i = 1,\ldots,m \\ & h_j(\mathbf{z},\overline{\mathbf{z}}) = 0, \quad j = 1,\ldots,\ell \end{cases}$$

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Trigonometric polynomial optimization

- trigonometric polynomial optimization:

$$\begin{cases} \inf\limits_{\mathbf{x}\in[0,2\pi)^n} & f(\sin x_1,\ldots,\sin x_n,\cos x_1,\ldots,\cos x_n) \\ \text{s.t.} & g_i(\sin x_1,\ldots,\sin x_n,\cos x_1,\ldots,\cos x_n)\ge 0, \quad i=1,\ldots,m \\ & h_j(\sin x_1,\ldots,\sin x_n,\cos x_1,\ldots,\cos x_n)=0, \quad j=1,\ldots,\ell \end{cases}$$

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Eigenvalue optimization with noncommutative polynomials

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Trace optimization with noncommutative polynomials

- (normalized) trace optimization with noncommutative polynomials:

$$\begin{cases} \inf\limits_{\mathbf{x}\in\cup_{k\geq 1}(\mathbb{S}_k)^n} & \mathrm{tr}(f(\mathbf{x})) \quad (\mathrm{tr}(A) := \frac{1}{k}\sum_{i=1}^k A_{ii}) \\ \text{s.t.} & g_i(\mathbf{x}) \geq 0, \quad i = 1, \ldots, m \\ & h_j(\mathbf{x}) = 0, \quad j = 1, \ldots, \ell \end{cases}$$

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Trace polynomial optimization

- trace polynomial: $\mathrm{tr}(x_1^2)x_2x_1 + \mathrm{tr}(x_1)\mathrm{tr}(x_2x_1x_2)$, $x_1, \ldots, x_n \in \mathcal{B}(\mathcal{H})$
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State polynomial optimization

- state polynomial: $\varsigma(x_1^2)x_2x_1 + \varsigma(x_1)\varsigma(x_2x_1x_2)$, $x_1, \ldots, x_n \in \mathcal{B}(\mathcal{H})$, ς is a formal state (i.e., a positive unital linear functional) on $\mathcal{B}(\mathcal{H})$
- state polynomial optimization:

$$\begin{cases} \inf\limits_{(\mathcal{H},\varsigma,\mathbf{x})} & \varsigma(f(\varsigma;\mathbf{x})) \\ \text{s.t.} & g_i(\varsigma;\mathbf{x}) \geq 0, \quad i = 1, \ldots, m \\ & h_j(\varsigma;\mathbf{x}) = 0, \quad j = 1, \ldots, \ell \end{cases}$$

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Difficult to solve

- Non-convex
- Various natures of variables
- No classical derivatives
- NP-hard

Positivstellensatz and the moment-SOS hierarchy

Various nonnegativity

- real polynomial $f \geq 0$ if $f(\mathbf{x}) \geq 0$, $\forall \mathbf{x} \in \mathbb{R}^n$
- polynomial matrix $F \geq 0$ if $F(\mathbf{x}) \succeq 0$, $\forall \mathbf{x} \in \mathbb{R}^n$
- complex polynomial $f \geq 0$ if $f(\mathbf{z}, \bar{\mathbf{z}}) \geq 0$, $\forall \mathbf{z} \in \mathbb{C}^n$
- noncommutative polynomial $f \geq 0$ if $f(\mathbf{x}) \succeq 0$, $\forall \mathbf{x} \in \cup_{k\geq 1}(\mathbb{S}_k)^n$
- noncommutative polynomial $\mathrm{tr}(f) \geq 0$ if $\mathrm{tr}(f(\mathbf{x})) \geq 0$, $\forall \mathbf{x} \in \cup_{k\geq 1}(\mathbb{S}_k)^n$
- trace polynomial $\mathrm{tr}(f) \geq 0$ if $\mathrm{tr}(f(\mathbf{x})) \geq 0$, $\forall \mathbf{x} \in \cup_{k\geq 1}(\mathbb{S}_k)^n$
- state polynomial $f \geq 0$ if $\varsigma(f(\varsigma; \mathbf{x})) \geq 0$, $\forall (\mathcal{H}, \varsigma, \mathbf{x})$

Sum of squares

- Sum of squares (SOS):

$$f = f_1^2 + \cdots + f_t^2 \quad \rightsquigarrow \quad f \geq 0$$

- Hilbert, 1888: "nonnegativity = SOS" $\iff$ $n = 1 || d = 2 || n = 2, d = 4$
- Artin, 1927: "nonnegative polynomials = rational SOS"
- Matrix sum of squares: $F(\mathbf{x}) = P(\mathbf{x})^\intercal P(\mathbf{x})$
- Hermitian sum of squares: $f = |f_1|^2 + \cdots + |f_t|^2$
- Sum of Hermitian squares: $f = f_1^* f_1 + \cdots + f_t^* f_t$

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Gram matrix and semidefinite programming

- $\deg(f) = 2d$, $[\mathbf{x}]_d := [1, x_1, \ldots, x_n, x_1^d, \ldots, x_n^d]$
- f is an SOS $\iff$ there exists a PSD matrix G s.t.

$$f = [\mathbf{x}]_d \cdot G \cdot [\mathbf{x}]_d^\intercal \quad \rightsquigarrow \quad \text{SDP}$$

- G is called a Gram matrix of f, which is of size $\binom{n+d}{n} = \binom{n+d}{d}$

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Quadratic module

- $\Sigma(\mathbf{x}) := \{f \in \mathbb{R}[\mathbf{x}] \mid f = \sum_i f_i^2, f_i \in \mathbb{R}[\mathbf{x}]\}$
- Quadratic module: Given $\mathbf{g} = \{g_i\}_{i=1}^m \subseteq \mathbb{R}[\mathbf{x}]$,

$$\mathcal{Q}(\mathbf{g}) := \left\{\sigma_0 + \sum_{i=1}^m \sigma_i g_i \,\middle|\, \sigma_i \in \Sigma(\mathbf{x}), i = 0, 1, \ldots, m\right\}$$

- Truncated quadratic module:

$$\mathcal{Q}(\mathbf{g})_{2r} := \left\{\sigma_0 + \sum_{i=1}^m \sigma_i g_i \,\middle|\, \sigma_i \in \Sigma(\mathbf{x}), \deg(\sigma_i g_i) \le 2r, i = 0, 1, \ldots, m\right\}$$

- Archimedean's condition ($\approx$ compactness): there exists $N > 0$ s.t.

$N - \|\mathbf{x}\|^2 \in \mathcal{Q}(\mathbf{g}) + \mathcal{I}(\mathbf{h})$

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Commutative Positivstellensatz

- $S := \{\mathbf{x} \in \mathbb{R}^n \mid g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0, h_1(\mathbf{x}) = 0, \ldots, h_\ell(\mathbf{x}) = 0\}$

Theorem (Putinar's Positivstellensatz, 1993)

Assume $\mathcal{Q}(\mathbf{g}) + \mathcal{I}(\mathbf{h})$ satisfies Archimedean's condition. If f is positive on S, then

$$f = \sigma_0 + \sigma_1 g_1 + \cdots + \sigma_m g_m + \tau_1 h_1 + \cdots + \tau_\ell h_\ell,$$

where $\sigma_0, \ldots, \sigma_m$ are SOS, and $\tau_1, \ldots, \tau_\ell$ are polynomials.

Matrix Positivstellensatz

- $S := \{\mathbf{x} \in \mathbb{R}^n \mid G(\mathbf{x}) \succeq 0\}$

Theorem (Scherer and Hol, 2006)

Assume that $\mathcal{Q}(G)$ satisfies Archimedean's condition and $F(\mathbf{x}) \in \mathbb{S}[\mathbf{x}]^p$ is positive definite on S. Then there exist SOS polynomial matrices $\Sigma_0(\mathbf{x}) \in \mathbb{S}[\mathbf{x}]^p$ and $\Sigma_1(\mathbf{x}) \in \mathbb{S}[\mathbf{x}]^{pq}$ such that

$$F(\mathbf{x}) = \Sigma_0(\mathbf{x}) + (\Sigma_1(\mathbf{x}), G(\mathbf{x}))_p.$$

Complex Positivstellensatz

- $S := \{\mathbf{z} \in \mathbb{C}^n \mid g_1(\mathbf{z}, \overline{\mathbf{z}}) \geq 0, \ldots, g_m(\mathbf{z}, \overline{\mathbf{z}}) \geq 0, |z_1|^2 + \cdots + |z_n|^2 = R\}$

Theorem (D'Angelo and Putinar, 2009)

If f is positive on S, then

$$f = \sigma_0 + \sigma_1 g_1 + \cdots + \sigma_m g_m + \tau(|z_1|^2 + \cdots + |z_n|^2 - R),$$

where $\sigma_0, \ldots, \sigma_m$ are Hermitian SOS, and τ is a self-conjugate complex polynomial.

Noncommutative Positivstellensatz

- $S := \{\mathbf{x} \in \mathcal{B}(\mathcal{H})^n \mid g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0\}$

Theorem (Helton and McCullough, 2004)

Assume that $\{g_i\}_{i=1}^m$ satisfies Archimedean's condition. If f is positive on S, then

$$f = \sum_{g \in \{1\} \cup \{g_i\}_{i=1}^m} s_g^* g s_g, \quad \textit{for some } \{s_g\}_g \subseteq \mathbb{R}\langle \mathbf{x} \rangle.$$

Reformulate POPs with nonnegative polynomials

- $S = \{\mathbf{x} \in \mathbb{R}^n \mid g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0, h_1(\mathbf{x}) = 0, \ldots, h_\ell(\mathbf{x}) = 0\}$

$$f_{\min} \coloneqq \sup_{\lambda} \{\lambda : f(\mathbf{x}) - \lambda \geq 0, \forall \mathbf{x} \in S\}$$

- $P_S(\mathbf{x}) \coloneqq \{g \in \mathbb{R}[\mathbf{x}] \mid g \geq 0 \text{ on } S\} \rightsquigarrow$ intractable

- Replace $P_S(\mathbf{x})$ by tractable subsets $\rightsquigarrow \mathcal{Q}(\mathbf{g})_{2r} + \mathcal{I}(\mathbf{h})_{2r}$

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The hierarchy of dual SOS relaxations

- The hierarchy of dual SOS relaxations (Parrilo 2000 & Lasserre 2001)

$$\theta_r^* := \begin{cases} \sup\limits_{\lambda} & \lambda \\ \text{s.t.} & f - \lambda \in \mathcal{Q}(\mathbf{g})_{2r} + \mathcal{I}(\mathbf{h})_{2r} \end{cases}$$

- $\cdots \le \theta_r^* \le \theta_{r+1}^* \le \cdots \le f_{\min}$

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Measures and moments

- For a finite Borel measure μ, $y_{\boldsymbol{\alpha}} = \int_S \mathbf{x}^{\boldsymbol{\alpha}} \, \mathrm{d}\mu \rightsquigarrow$ moment
- Reformulation using measures and moments:

$$\inf_{\mu \in \mathcal{M}(S)_+} \left\{ \int_S f(\mathbf{x}) \, \mathrm{d}\mu : \mu(S) = 1 \right\}$$

$$\Updownarrow$$

$$\inf_{\mathbf{y}} \left\{ L_{\mathbf{y}}(f) = \sum_{\alpha \in \mathrm{supp}(f)} f_\alpha y_\alpha : \exists \mu \in \mathcal{M}(S)_+ \text{ s.t. } \mathbf{y} \sim \mu \text{ and } y_{\mathbf{0}} = 1 \right\}$$

Question: When does a sequence $\mathbf{y} = (y_\alpha)_{\alpha \in \mathbb{N}^n}$ admits a finite Borel measure representation with support contained in S?

Measures and moments

- For a finite Borel measure μ, $y_{\boldsymbol{\alpha}} = \int_S \mathbf{x}^{\boldsymbol{\alpha}} \, \mathrm{d}\mu \rightsquigarrow$ moment
- Reformulation using measures and moments:

$$\inf_{\mu \in \mathcal{M}(S)_+} \left\{ \int_S f(\mathbf{x}) \, \mathrm{d}\mu : \mu(S) = 1 \right\}$$

$$\Updownarrow$$

$$\inf_{\mathbf{y}} \left\{ L_{\mathbf{y}}(f) = \sum_{\boldsymbol{\alpha} \in \mathrm{supp}(f)} f_{\boldsymbol{\alpha}} y_{\boldsymbol{\alpha}} : \exists \mu \in \mathcal{M}(S)_+ \text{ s.t. } \mathbf{y} \sim \mu \text{ and } y_{\mathbf{0}} = 1 \right\}$$

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Moment matrix and localizing matrix

- $\mathbb{N}^n_r := \{\boldsymbol{\beta} = (\beta_i) \in \mathbb{N}^n \mid \sum_{i=1}^n \beta_i \le r\}$
- r-th order moment matrix $\mathbf{M}_r(\mathbf{y})$:

$$[\mathbf{M}_r(\mathbf{y})]_{\beta\gamma} := y_{\beta+\gamma}, \quad \forall \boldsymbol{\beta}, \boldsymbol{\gamma} \in \mathbb{N}^n_r$$

- Given $g = \sum_\alpha g_\alpha \mathbf{x}^\alpha$, r-th order localizing matrix $\mathbf{M}_r(g\mathbf{y})$:

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- $\mathbf{x} = x$, $g = 1 - x^2$:

$$\mathbf{M}_2(\mathbf{y}) = \begin{array}{c|c} & \begin{array}{ccc} 1 & x & x^2 \end{array} \\ \begin{array}{c} 1 \\ x \\ x^2 \end{array} & \begin{bmatrix} y_0 & y_1 & y_2 \\ y_1 & y_2 & y_3 \\ y_2 & y_3 & y_4 \end{bmatrix} \end{array}, \quad \mathbf{M}_1(g\mathbf{y}) = \begin{array}{c|c} & \begin{array}{cc} 1 & x \end{array} \\ \begin{array}{c} 1 \\ x \end{array} & \begin{bmatrix} y_0 - y_2 & y_1 - y_3 \\ y_1 - y_3 & y_2 - y_4 \end{bmatrix} \end{array}$$

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Sequences admitting a Borel representing measure

Theorem (The dual to Putinar's Positivstellensatz)

Assume that Archimedean's condition holds. The sequence $\mathbf{y} = (y_{\boldsymbol{\alpha}})_{\boldsymbol{\alpha} \in \mathbb{N}^n}$ *admits a finite Borel representing measure with support contained in* S *if and only if* $\mathbf{M}_r(\mathbf{y}) \succeq 0, \mathbf{M}_{r-d_i}(g_i \mathbf{y}) \succeq 0, L_{\mathbf{y}}(\mathbf{x}^{\boldsymbol{\alpha}} h_j) = 0$ *for all* i, j, r *and* $\boldsymbol{\alpha} \in \mathbb{N}^n$.

- $d_i := \lceil \deg(g_i)/2 \rceil, i = 1, \ldots, m$
- Riesz linear functional $L_{\mathbf{y}} : \mathbb{R}[\mathbf{x}] \to \mathbb{R}$, $f = \sum_{\boldsymbol{\alpha}} f_{\boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\alpha}} \mapsto \sum_{\boldsymbol{\alpha}} f_{\boldsymbol{\alpha}} y_{\boldsymbol{\alpha}}$

The hierarchy of moment relaxations

- The hierarchy of moment relaxations (Lasserre, 2001)

$$\theta_r := \begin{cases} \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ \text{s.t.} & \mathbf{M}_r(\mathbf{y}) \succeq 0 \\ & \mathbf{M}_{r-d_i}(g_i\mathbf{y}) \succeq 0, \quad i = 1, \ldots, m \\ & L_{\mathbf{y}}(\mathbf{x}^{\boldsymbol{\alpha}} h_j) = 0, \quad |\boldsymbol{\alpha}| \le 2r - \deg(h_j), j = 1, \ldots, \ell \\ & y_{\mathbf{0}} = 1 \end{cases}$$

- $\cdots \le \theta_r \le \theta_{r+1} \le \cdots \le f_{\min}$

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The Moment-SOS/Lasserre's hierarchy

$$
\begin{array}{ccccccc}
 & & & f_{\min} & & & \\
 & & \rotatebox{45}{$\leq$} & & \rotatebox{-45}{$\geq$} & & \\
 & & \vdots & & \vdots & & \\
 & & \geq & & \geq & & \\
\textcolor{red}{\text{(Moment relaxation)}} & & \theta_r & \text{“}=\text{”} & \theta_r^* & & \textcolor{red}{\text{(dual SOS relaxation)}} \\
 & & \geq & & \geq & & \\
 & & \vdots & & \vdots & & \\
 & & \geq & & \geq & & \\
 & & \theta_{r_{\min}} & \text{“}=\text{”} & \theta_{r_{\min}}^* & &
\end{array}
$$

Asymptotical convergence and finite convergence

- Under Archimedean's condition ($\approx$ compactness)

  ➤ $\theta_r \nearrow f_{\min}$ and $\theta_r^* \nearrow f_{\min}$ as $r \to \infty$ (**Putinar's Positivstellensatz**)

  ➤ Finite convergence happens generically (**Nie, 2014**)

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Detecting global optimality

- Global optimality certified ($\theta_r = f_{\min}$) when one of the following conditions holds:
  - There exists r' with $r_0 \leq r' \leq r$, $\operatorname{rank} \mathbf{M}_{r'-r_0}(\mathbf{y}) = \operatorname{rank} \mathbf{M}_{r'}(\mathbf{y})$

    $\rightsquigarrow$ A simple algorithm for extracting $\operatorname{rank} \mathbf{M}_{r'}(\mathbf{y})$ optimal solutions
  - $\operatorname{rank} \mathbf{M}_{r_{\min}}(\mathbf{y}) = 1$

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Improve scalability by exploiting structures

Rapidly growing size of the moment-SOS hierarchy

- The size of SDP corresponding to the r-th SOS relaxation:
  1. Size of PSD constraints: $\binom{n+r}{r}$
  2. Number of equality constraints: $\binom{n+2r}{2r}$
- $r = 2$, $n < 30$ (Mosek)
- Exploiting structures:
  - POP
  - SDP

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Quotient ring

- Equality constraints: $h_j(\mathbf{x}) = 0, \quad j = 1, \ldots, \ell$

- Build the moment-SOS hierarchy in the quotient ring

$$\mathbb{R}[\mathbf{x}]/(h_1(\mathbf{x}), \ldots, h_\ell(\mathbf{x}))$$

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Symmetries

- permutation symmetry: $(x_1, \ldots, x_n) \to (x_{\tau(1)}, \ldots, x_{\tau(n)})$
- translation symmetry: $(x_1, \ldots, x_n) \to (x_{1+i}, \ldots, x_{n+i})$, $x_{n+i} = x_i$
- sign symmetry: $(x_{i_1}, \ldots, x_{i_k}) \to (-x_{i_1}, \ldots, -x_{i_k})$
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➤ Use group theory to derive block-diagonal moment-SOS relaxations

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➤ Use group theory to derive block-diagonal moment-SOS relaxations

Correlative sparsity (Waki et al. 2006)

- Correlative sparsity pattern graph $G^{\mathrm{csp}}(V, E)$:
  - $V := \{x_1, \ldots, x_n\}$
  - $\{x_i, x_j\} \in E \iff x_i, x_j$ appear in the same term of f or in the same

constraint polynomial g_k

- For each maximal clique of $G^{\mathrm{csp}}(V, E)$, apply

$$I_k \longmapsto \mathbf{M}_r(\mathbf{y}, I_k), \mathbf{M}_{r-d_i}(g_i\mathbf{y}, I_k)$$

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Term sparsity (Wang & Magron & Lasserre, 2021)

- Term sparsity pattern graph $G^{\mathrm{tsp}}(V,E)$:
  - $V := [\mathbf{x}]_r = \{1, x_1, \ldots, x_n, x_1^r, \ldots, x_n^r\}$
  - $\{\mathbf{x}^{\boldsymbol{\alpha}}, \mathbf{x}^{\boldsymbol{\beta}}\} \in E \iff \mathbf{x}^{\boldsymbol{\alpha}} \cdot \mathbf{x}^{\boldsymbol{\beta}} = \mathbf{x}^{\boldsymbol{\alpha}+\boldsymbol{\beta}} \in \mathrm{supp}(f) \cup \bigcup_{i=1}^m \mathrm{supp}(g_i) \cup [\mathbf{x}]_r^2$
- Impose a sparsity pattern on $\mathbf{M}_r(\mathbf{y})$ using $G^{\mathrm{tsp}}(V,E)$

$$\begin{array}{cc} & \begin{array}{ccc} \cdots & \boldsymbol{\alpha} & \cdots \end{array} \\ \begin{array}{c} \vdots \\ \boldsymbol{\beta} \\ \vdots \end{array} & \begin{bmatrix} & \vdots & \\ \cdots & y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} & \cdots \\ & \vdots & \end{bmatrix} \end{array} = \mathbf{M}_r(\mathbf{y}), \quad y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} = 0 \iff \{\mathbf{x}^{\boldsymbol{\alpha}}, \mathbf{x}^{\boldsymbol{\beta}}\} \notin E$$

Structures of the moment problem

- Low-rank optimal solutions: $\mathrm{rank}(\mathbf{M}^{\mathrm{opt}}) \ll n$
- Unit diagonal: $\mathrm{diag}(\mathbf{M}) = \mathbf{1}$
- Unit trace: $\mathrm{tr}(\mathbf{M}) = 1$

Solving the moment problem via manifold optimization

- Low-rank: $\operatorname{rank} \mathbf{M}^{\mathrm{opt}} \ll n \rightsquigarrow \mathbf{M} = YY^{\intercal}$, $Y \in \mathbb{R}^{n\times p}$ **Burer-Monteiro**
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$\rightsquigarrow$ Efficient manifold optimization algorithms

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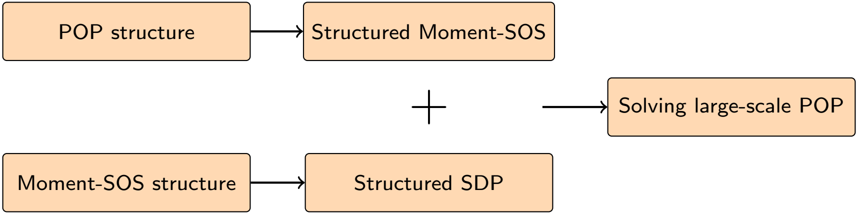
Solving large-scale polynomial optimization



Software

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  https://github.com/wangjie212/TSSOS

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Summary

- The moment-SOS hierarchy provides a power tool for **global optimization** of many difficult non-convex problems involving polynomials.
- The scalability of the moment-SOS hierarchy can be **significantly improved** by exploiting various structures.
- There are **tons of** applications in many different fields!

Thank You!

https://wangjie212.github.io/jiewang