Trace optimization of nc polynomials

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nc polynomials

- $\mathbb{R}\langle \underline{X} \rangle$ free algebra on $\underline{X} = (X_1, \dots, X_n)$
- Polynomials in the non-commuting variables $X_1, \dots, X_n$
  - $f = \sum_w f_w w$, $w \in \langle \underline{X} \rangle, f_w \in \mathbb{R}$
- $\mathbb{R}\langle \underline{X} \rangle_k = \{ f \in \mathbb{R}\langle \underline{X} \rangle \mid \deg f \leq k \}$

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- Evaluation in symmetric matrices $\underline{A} = (A_1, \ldots, A_n) \in (\mathcal{S}\mathbb{R}^{s \times s})^n$
  - $f(\underline{A}) = f_1 \mathbf{1}_s + f_{X_1} A_1 + f_{X_2} A_2 + \ldots + f_{X_1^2 X_3 X_2^3} A_1^2 A_3 A_2^3 + \ldots$
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1. What is the minimal trace a polynomial $f \in \mathbb{R}\langle \underline{X} \rangle$ can attain?

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Questions

1. What is the minimal trace a polynomial $f \in \mathbb{R}\langle \underline{X} \rangle$ can attain?
2. Can we find a relaxation to compute a bound via an SDP?

$\rightarrow$ Sums of hermitian squares and commutators

Sums of hermitian squares

- Involution $^* : \mathbb{R}\langle \underline{X} \rangle \to \mathbb{R}\langle \underline{X} \rangle$ compatible with transposition ^{T}:

$$f^*(\underline{A}) = f(\underline{A})^T \text{ for all } \underline{A} \in \mathcal{S}^n$$

Definition

$$\Sigma^2 := \{f \in \mathbb{R}\langle \underline{X} \rangle \mid f = \sum_{i=1}^{r} {g_i}^* g_i \text{ for some } g_i \in \mathbb{R}\langle \underline{X} \rangle, r \in \mathbb{N}_0\}$$

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Fact 1

If $f \in \Sigma^2$, then $f(\underline{A})$ is positive semidefinite for all $\underline{A} \in \mathcal{S}^n$.

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If $f \in \Sigma^2$, then $f(\underline{A})$ is positive semidefinite for all $\underline{A} \in \mathcal{S}^n$.

Fact 2

For all $p, q \in \mathbb{R}\langle \underline{X}\rangle$: $\mathrm{Tr}((pq - qp)(\underline{A})) = 0$ for all $\underline{A} \in \mathcal{S}^n$.

- We call $[p, q] = pq - qp$ for $p, q \in \mathbb{R}\langle \underline{X}\rangle$ a commutator.

Cyclic equivalence

Definition

$f, g \in \mathbb{R}\langle \underline{X} \rangle$ are cyclically equivalent ($f \overset{\text{cyc}}{\sim} g$) if

$$f - g = \sum_{i=1}^{r} [p_i, q_i] \text{ for some } r \in \mathbb{N}_0, p_i, q_i \in \mathbb{R}\langle \underline{X} \rangle.$$

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Example

$f = 2XY^2X - Y^2X^2 + 2YXY \overset{\text{cyc}}{\sim} g = X^2Y^2 + 2XY^2$:

$$f - g = [XY^2, X] + [X, Y^2X] + 2[Y, XY].$$

Fact 2'

If $f \overset{\text{cyc}}{\sim} g$, then $\mathrm{Tr}(f(\underline{A})) = \mathrm{Tr}(g(\underline{A}))$ for all $\underline{A} \in \mathcal{S}^n$.

Sums of hermitian squares and commutators

Recall: $\Sigma^2 = \{f \in \mathbb{R}\langle \underline{X} \rangle \mid f = \sum_i {g_i}^* g_i \text{ for some } g_i \in \mathbb{R}\langle \underline{X} \rangle\}$

Definition

$$\Theta^2 := \{f \in \mathbb{R}\langle \underline{X} \rangle \mid f \overset{\text{cyc}}{\sim} g \text{ for some } g \in \Sigma^2\}$$

Example

$f = X^2Y^2 - XYXY$:

$$f \overset{\text{cyc}}{\sim} \frac{1}{2}(XY^2X + YX^2Y - XYXY - YXYX)$$
$$= \frac{1}{2}(XY - YX)^*(XY - YX) \in \Sigma^2$$

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Recall: $\Sigma^2 = \{f \in \mathbb{R}\langle \underline{X} \rangle \mid f = \sum_i {g_i}^* g_i \text{ for some } g_i \in \mathbb{R}\langle \underline{X} \rangle\}$

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Fact 1 + Fact 2'

If $f \in \Theta^2$, then $\mathrm{Tr}(f(\underline{A})) \geq 0$ for all $\underline{A} \in \mathcal{S}^n$.

Trace optimization

Let $f \in \mathbb{R}\langle \underline{X} \rangle$.

- Optimization problem

$$f_* := \inf\{\mathrm{Tr}\left(f(\underline{A})\right) \mid \underline{A} \in \mathcal{S}^n\}.$$

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- "SOS" -Relaxation

$$f_{\text{sos}} := \sup\{a \in \mathbb{R} \mid f - a \in \Theta^2\}.$$

Tracial Gram matrix method

Proposition (Klep, Schweighofer)

Let $f \in \mathbb{R}\langle \underline{X} \rangle$. Then $f \in \Theta^2$ if and only if there is a $G \succeq 0$ such that

$$f \overset{\text{cyc}}{\sim} \mathbf{v}^* G \mathbf{v},$$

where $\mathbf{v}$ is a vector consisting of all words $w \in \langle \underline{X} \rangle$ with

$$\operatorname{mindeg}(f) \leq 2 \deg(w) \leq \deg(f).$$

Given such a $G \succeq 0$ of rank r, one can construct $g_1, \ldots, g_r \in \mathbb{R}\langle \underline{X} \rangle$ such that

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and vice versa.

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and vice versa.

The degree bound can be improved using a tracial version of the Newton polytope.

Example

- $f = X^2Y^2 - XYXY$
- $\mathbf{v} = [X^2, XY, YX, Y^2]^T$ $\qquad \mathbf{v}^* = [X^2, YX, XY, Y^2]$

$$\mathbf{v}^*\mathbf{v} = \begin{bmatrix} X^4 & X^3Y & X^2YX & X^2Y^2 \\ YX^3 & YX^2Y & YXYX & YXY^2 \\ XYX^2 & XYXY & XY^2X & XY^3 \\ Y^2X^2 & Y^2XY & Y^3X & Y^4 \end{bmatrix}$$

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- $f \overset{\text{cyc}}{\sim} \mathbf{v}^* G \mathbf{v}$

$$G = \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \succeq 0$$

- $f \overset{\text{cyc}}{\sim} \frac{1}{2}(XY - YX)^*(XY - YX)$

Back to trace optimization

- Let $f \in \mathbb{R}\langle \underline{X} \rangle$
  - Problem:

$$f_* = \inf\{\operatorname{Tr}\left(f(\underline{A})\right) \mid \underline{A} \in \mathcal{S}^n\}$$

Back to trace optimization

- Let $f \in \mathbb{R}\langle \underline{X} \rangle$
  - Problem:
    $$f_* = \inf\{\operatorname{Tr}\left(f(\underline{A})\right) \mid \underline{A} \in \mathcal{S}^n\}$$
  - SOS relaxation:
    $$\boxed{\begin{array}{lll} f_{\mathrm{sos}} = & \sup & a \\ & \text{s. t.} & f - a \in \Theta^2. \end{array}}$$
  - Formulation as SDP
    $$\boxed{\begin{array}{lllll} f_{\mathrm{sos}} = & \sup & f_1 - \langle E_{11}, G \rangle & & \\ & \text{s. t.} & f - f_1 & \overset{\mathrm{cyc}}{\sim} & \mathbf{v}^T(G - g_{11}E_{11})\mathbf{v} \\ & & G & \succeq & 0. \end{array}}$$

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Fact

Let $f \in \mathbb{R}\langle \underline{X} \rangle$. Then $f_{\mathrm{sos}} \leq f_*$.

Duality

- Let $f \in \mathbb{R}\langle \underline{X} \rangle_{2d}$
  - SOS relaxation:

$$\boxed{\begin{array}{rll} f_{\mathrm{sos}} = & \sup & a \\ & \text{s. t.} & f - a \in \Theta^2. \end{array}}$$

  - Dual SDP

$$\boxed{\begin{array}{rll} f^{\mathrm{sos}} = & \inf & L(f) \\ & \text{s. t.} & L : \mathbb{R}\langle \underline{X} \rangle_{2d} \to \mathbb{R} \text{ is a linear } *\text{-map} \\ & & L(1) = 1 \\ & & L(p) \geq 0 \text{ for all } p \in \Theta^2 \cap \mathbb{R}\langle \underline{X} \rangle_{2d}. \end{array}}$$

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Theorem

We have strong duality, i.e. $f^{\mathrm{sos}} = f_{\mathrm{sos}}$.

Optimality

- In general f_{sos} might be different from f_*
  - Let
$$f = X_1^2 X_2^4 + X_1^4 X_2^2 - 3X_1^2 X_2^2 + 1,$$
then $f_* = 0$ but $f_{\text{sos}} = -\infty$.

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Question

When is the relaxation optimal, i.e. $f_{\mathrm{sos}} = f_*$?

The truncated tracial moment problem

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f^{\mathrm{sos}} = & \inf & L(f) \\
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- L is tracial, i.e. $L(pq - qp) = 0$ for all $p, q \in \mathbb{R}\langle \underline{X} \rangle_{2d}$.

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- L is tracial, i.e. $L(pq - qp) = 0$ for all $p, q \in \mathbb{R}\langle \underline{X} \rangle_{2d}$.

Definition (Truncated tracial moment problem)

For which tracial linear functionals $L \in (\mathbb{R}\langle \underline{X} \rangle_{2d})^*$ exist some $s \in \mathbb{N}$ and a probability measure μ on $(\mathcal{S}\mathbb{R}^{s \times s})^n$, such that for all $g \in \mathbb{R}\langle \underline{X} \rangle_{2d}$:

$$L(g) = \int \mathrm{Tr}(g(\underline{A}))\, d\mu(\underline{A})?$$

- $s = 1$: Classical moment problem
- μ can be chosen to be finitely atomic

Optimality criterion

$$\boxed{\begin{array}{lll} f^{\mathrm{sos}} = & \inf & L(f) \\ & \text{s.t.} & L : \mathbb{R}\langle \underline{X} \rangle_{2d} \to \mathbb{R} \text{ is a linear } *\text{-map} \\ & & L(1) = 1 \\ & & L(p) \geq 0 \text{ for all } p \in \Theta^2 \cap \mathbb{R}\langle \underline{X} \rangle_{2d}. \end{array}}$$

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Theorem

If L^{sos} has a representation

$$L^{\text{sos}}(g) = \int \operatorname{Tr}(g(\underline{A}))\, d\mu(\underline{A}) \quad (g \in \mathbb{R}\langle \underline{X} \rangle_{2d})$$

for some $s \in \mathbb{N}$ and a probability measure μ on $(\mathcal{S}\mathbb{R}^{s\times s})^n$, then the SOS relaxation is exact: $f_{\text{sos}} = f^{\text{sos}} = f_*$.

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- $\exists \lambda_i \in \mathbb{R}_{>0}$, with $\sum_i \lambda_i = 1$, and $\underline{A}^{(i)} \in (\mathcal{S}\mathbb{R}^{s\times s})^n$, such that

$$(f_{\text{sos}} =) f^{\text{sos}} = L^{\text{sos}}(f) = \sum_i \lambda_i \operatorname{Tr}(f(\underline{A}^{(i)})).$$

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$$(f_{\mathrm{sos}} =) f^{\mathrm{sos}} = L^{\mathrm{sos}}(f) = \sum_i \lambda_i \, \mathrm{Tr}(f(\underline{A}^{(i)})).$$

- Since $\mathrm{Tr}(f(\underline{A}^{(i)})) \geq f_{\mathrm{sos}}$ for each i, we get

$$f_* \leq \mathrm{Tr}(f(\underline{A}^{(i)})) = f_{\mathrm{sos}} \leq f_*.$$

Tracial Hankel matrix

- Associate to a tracial $L \in (\mathbb{R}\langle \underline{X} \rangle_{2d})^*$ the bilinear form

$$B_L : \mathbb{R}\langle \underline{X} \rangle_d \times \mathbb{R}\langle \underline{X} \rangle_d, (f, g) \mapsto L(f^* g).$$

Definition

The tracial Hankel matrix $M_k(L)$ of order k, indexed by $u, v \in \langle \underline{X} \rangle_k$, is given by

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Theorem (B.,Klep)

Let $L \in (\mathbb{R}\langle \underline{X} \rangle_{2d})^*$ be tracial with

1. $M_d(L) \succeq 0$
2. $\operatorname{rank} M_d(L) = \operatorname{rank} M_{d-1}(L) =: s$.

Then L has a representing measure on $(\mathcal{S}\mathbb{R}^{s \times s})^n$.

Optimality condition

Theorem

Let $f \in \mathbb{R}\langle \underline{X} \rangle_{2d}$ and let f^{sos} be attained. If the optimizer L^{sos} satisfies

1. $M_d(L^{\mathrm{sos}}) \succeq 0$
2. $\operatorname{rank} M_d(L^{\mathrm{sos}}) = \operatorname{rank} M_{d-1}(L^{\mathrm{sos}})$,

then the SOS relaxation is exact.
Furthermore, one can construct tracial optimizers.

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then the SOS relaxation is exact.
Furthermore, one can construct tracial optimizers.

- "finite GNS construction"
  - $L = L^{\text{sos}}$ induces a positive definite bilinear form on $E = \operatorname{ran} M_d$.
  - Let $\hat{X}_i$ be the right multiplication with X_i on E
  - $\hat{X}_i$ is well defined and symmetric $\to A_i \in \mathcal{S}\mathbb{R}^{s \times s}$
- Artin-Wedderburn block decomposition of $B(A_1, \dots, A_n)$
  - unitary U such that $U^T A_j U = \oplus_i A_j^{(i)}$
  - each $A^{(i)} = (A_1^{(i)}, \dots, A_n^{(i)})$ is a trace optimizer
- Implemented in `NCSOStools` (`http://ncsostools.fis.unm.si`)

Example

$$f = 3+X_1^2+2X_1^3+2X_1^4+X_1^6-4X_1^4X_2+X_1^4X_2^2+4X_1^3X_2+2X_1^3X_2^2-2X_1^3X_2^3$$
$$+ 2X_1^2X_2 - X_1^2X_2^2 + 8X_1X_2X_1X_2 + 2X_1^2X_2^3 - 4X_1X_2 + 4X_1X_2^2$$
$$+ 6X_1X_2^4 - 2X_2 + X_2^2 - 4X_2^3 + 2X_2^4 + 2X_2^6.$$

Example

$$f = 3 + X_1^2 + 2X_1^3 + 2X_1^4 + X_1^6 - 4X_1^4X_2 + X_1^4X_2^2 + 4X_1^3X_2 + 2X_1^3X_2^2 - 2X_1^3X_2^3 + 2X_1^2X_2 - X_1^2X_2^2 + 8X_1X_2X_1X_2 + 2X_1^2X_2^3 - 4X_1X_2 + 4X_1X_2^2 + 6X_1X_2^4 - 2X_2 + X_2^2 - 4X_2^3 + 2X_2^4 + 2X_2^6.$$

- The trace-minimum f_* of f is 0.2842:
- Tracial Hankel matrix $M_3(L^{\text{sos}})$ is of rank 4 and satisfies the optimality condition.
- $\hat{X}_i$ is given by 4×4 matrices:

$$\hat{X}_1 = \begin{bmatrix} -1.0761 & 0.1802 & 0.5107 & 0.2590 \\ 0.1802 & -0.3393 & -0.1920 & 0.9428 \\ 0.5107 & -0.1920 & 0.5094 & 0.0600 \\ 0.2590 & 0.9428 & 0.0600 & -0.3020 \end{bmatrix},$$

$$\hat{X}_2 = \begin{bmatrix} 0.7108 & 0.7328 & 0.1043 & 0.4415 \\ 0.7328 & -0.3706 & 0.4757 & -0.2147 \\ 0.1043 & 0.4757 & 0.0776 & -0.9102 \\ 0.4415 & -0.2147 & -0.9102 & 0.1393 \end{bmatrix}.$$

Example – continued

- Artin-Wedderburn block decomposition of $\hat{X}_1, \hat{X}_2$

$$\begin{aligned} A_1 &= \begin{bmatrix} -1.1843 & 0 & -0.2095 & 0.3705 \\ 0 & -1.1843 & 0.3705 & 0.2095 \\ -0.2095 & 0.3705 & 0.5803 & 0 \\ 0.3705 & 0.2095 & 0 & 0.5803 \end{bmatrix}, \\ A_2 &= \begin{bmatrix} -0.1743 & 0 & 0.4851 & -0.8577 \\ 0 & -0.1743 & -0.8577 & -0.4851 \\ 0.4851 & -0.8577 & 0.4529 & 0 \\ -0.8577 & -0.4851 & 0 & 0.4529 \end{bmatrix}. \end{aligned}$$

Example – continued

- Artin-Wedderburn block decomposition of $\hat{X}_1, \hat{X}_2$

$$
\begin{aligned}
A_1 &= \begin{bmatrix} -1.1843 & 0 & -0.2095 & 0.3705 \\ 0 & -1.1843 & 0.3705 & 0.2095 \\ -0.2095 & 0.3705 & 0.5803 & 0 \\ 0.3705 & 0.2095 & 0 & 0.5803 \end{bmatrix}, \\
A_2 &= \begin{bmatrix} -0.1743 & 0 & 0.4851 & -0.8577 \\ 0 & -0.1743 & -0.8577 & -0.4851 \\ 0.4851 & -0.8577 & 0.4529 & 0 \\ -0.8577 & -0.4851 & 0 & 0.4529 \end{bmatrix}.
\end{aligned}
$$

- Unitary change gives real trace optimizers

$$
A_1' = \begin{bmatrix} 0.674861 & 0.0731923 \\ 0.0731923 & -1.27886 \end{bmatrix}, \quad A_2' = \begin{bmatrix} 0.0705101 & -1.03179 \\ -1.03179 & 0.20809 \end{bmatrix}.
$$

- $\mathrm{Tr}(f(A_1', A_2')) = 0.2842$

Conclusion

- SOS relaxation for trace optimization
  - Based on sums of hermitian squares and commutators
- Optimality criterion
  - Based on the truncated tracial moment problem
  - Rank condition on the bilinear form induced by optimizing linear form of dual SDP
  - Allows to extract trace optimizers

Conclusion

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Outline

- Rational SOS certificates using Peyrl/Parrilo
- SOS relaxation for trace optimization on semialgebraic sets
- Asymptotic convergence ?