Noncommutative polynomial optimization and Bell inequalities

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Outline

1. Motivation: Linear Bell inequalities
2. Noncommutative polynomial optimization and the Navascués-Pironio-Acín hierarchy
3. Nonlinear Bell inequalities and state polynomial optimization

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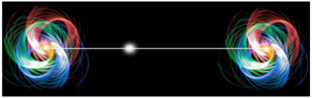
Classical correlations



Alice $\leftarrow$ Source $\rightarrow$ Bob

- Correlations = conditional joint probabilities:

$$P(ab \mid st) = P(\text{Alice, Bob answer } a, b \mid \text{Alice, Bob are asked } s, t)$$

- Deterministic strategies:

$$P(a \mid s), P(b \mid t) \in \{0,1\} \Rightarrow P(ab \mid st) = P(a \mid s)P(b \mid t) \in \{0,1\}$$

- Classical correlations: convex comb. of deterministic correlations

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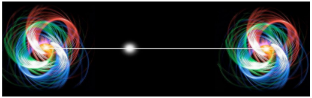

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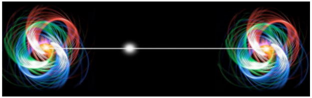

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Linear Bell inequalities

- Linear Bell inequalities: linear inequalities in terms of correlations (e.g., $P(ab \mid st)$) & marginals (e.g., $P(a \mid s)$, $P(b \mid t)$), valid for all classical correlations

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CHSH inequality

- Clauser-Horne-Shimony-Holt (CHSH) inequality:

$$P(11 \mid 00) + P(11 \mid 01) + P(11 \mid 10) - P(11 \mid 11) \leq 2$$

- Alice & Bob share a bipartite quantum state ψ and they answer a, b by performing quantum measurements on their part of ψ:

$$P(ab \mid st) = \psi^* A_s^a B_t^b \psi$$

for some commuting unitary operators $\{A_s^a\}, \{B_t^b\}$

- CHSH: $\psi^*(A_0^1 B_0^1 + A_0^1 B_1^1 + A_1^1 B_0^1 - A_1^1 B_1^1)\psi \leq 2$ is violated on the entangled state $\psi = \frac{1}{\sqrt{2}}(e_1 \otimes e_1 + e_2 \otimes e_2)$ (attaining the value $2\sqrt{2}$)

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Maximal quantum violation

- Question: Given a linear Bell inequality, how could we determine the maximal quantum violation?

- Reformulate as an optimization problem in operators:

$$\xi = \sup\{\langle f(A,B)\psi,\psi\rangle : A_i^2 = 1, B_j^2 = 1, A_iB_j = B_jA_i, \psi \in \mathcal{H}, \|\psi\| = 1\}$$
$$= \inf \lambda \ \text{ s.t. } \ \lambda I - f(A,B) \succeq 0, \text{ for all } A_i^2 = 1, B_j^2 = 1, A_iB_j = B_jA_i$$

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Noncommutative polynomial optimization

Noncommutative polynomials

- $\mathcal{H}$: a separable real Hilbert space (admitting a countable orthonormal basis)
- $\mathcal{B}(\mathcal{H})$: Banach algebra of bounded linear operators on $\mathcal{H}$
- Words/monomials: products of $x_1, \ldots, x_n \in \mathcal{B}(\mathcal{H})$
- Noncommutative (NC) polynomials: polynomials in $x_1, \ldots, x_n \in \mathcal{B}(\mathcal{H})$
  - $x_1^2 + x_1x_2x_1 + x_1x_3 + x_3x_1, x_1, x_2, x_3 \in \mathcal{B}(\mathcal{H})$
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Quantum states

- Quantum states: positive unital linear functionals on $\mathcal{B}(\mathcal{H})$, that is,

$$\varsigma : \mathcal{B}(\mathcal{H}) \to \mathbb{R} \text{ is linear, } \varsigma(w^* w) \geq 0, \varsigma(w^*) = \varsigma(w), \varsigma(1) = 1$$

- If $\mathcal{H}$ is finite-dim then a quantum state ς = PSD matrix with unit trace
- Pure state: rank-1 state = $\psi\psi^*$ for $\psi \in \mathcal{H}$

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Noncommutative polynomial optimization

- $f, g_i \in \mathbb{R}[\mathbf{x}]$ (ring of noncommutative polynomials):

$$\xi := \begin{cases} \inf\limits_{\mathbf{x}\in\mathcal{B}(\mathcal{H})^n} & \lambda_{\min}(f(\mathbf{x}))\ (= \langle\psi|f(\mathbf{x})|\psi\rangle \text{ where } \psi\in\mathcal{H}, \|\psi\|=1) \\ \text{s.t.} & g_i(\mathbf{x}) \succeq 0, \quad i=1,\ldots,m \end{cases}$$

☞ The Navascués-Pironio-Acín hierarchy of semidefinite relaxations

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Reformulation with nonnegative NC polynomials

- $\mathcal{D} := \left\{ \mathbf{x} \in \mathcal{B}(\mathcal{H})^n \,\middle|\, g_i(\mathbf{x}) \succeq 0,\ i = 1, \ldots, m \right\}$

$$\xi = \sup_{\lambda} \{\lambda : f(\mathbf{x}) - \lambda I \succeq 0,\ \forall \mathbf{x} \in \mathcal{D}\}$$

- **Problem:** characterize the set of NC polynomials that are positive semidefinite over $\mathcal{D}$

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Sum of Hermitian squares

- Sum of Hermitian squares (SOHS): $f = f_1^* f_1 + \cdots + f_t^* f_t$
- $[\mathbf{x}]_d := [1, x_1, \ldots, x_n, x_1^d, \ldots, x_n^d]$
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Noncommutative Positivstellensatz

Theorem (Helton and McCullough, 2004)

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

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

SOHS relaxations

- *r*-th order SOHS relaxation:

$$\theta_r^* := \begin{cases} \sup\limits_{\lambda, s_g} & \lambda \\ \text{s.t.} & f - \lambda = \sum_{g \in \{1\} \cup \{g_i\}_{i=1}^m} s_g^* g s_g \\ & \deg(s_g^* g s_g) \le 2r \end{cases} \quad \rightsquigarrow \quad \text{SDP}$$

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Reformulation with linear functionals

- Consider a linear functional $L : \mathbb{R}[\mathbf{x}] \to \mathbb{R}$ such that $L(w^*) = L(w)$
- r-th order moment matrix $\mathbf{M}_r(L)$:

$$[\mathbf{M}_r(L)]_{uv} := L(u^* v), \quad \forall |u|, |v| \le r$$

- r-th order localizing matrix $\mathbf{M}_r(gL)$ associated to $g = \sum_w g_w w$:

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The Navascués-Pironio-Acín hierarchy

$$
\begin{array}{ccccccc}
 & & & \xi & & & \\
 & & \rotatebox{-45}{$\leq$} & & \rotatebox{45}{$\geq$} & & \\
 & & \vdots & & \vdots & & \\
 & & \geq & & \geq & & \\
\text{(Moment relaxation)} & & \theta_r & \text{“}=\text{”} & \theta_r^* & & \text{(dual SOHS relaxation)} \\
 & & \geq & & \geq & & \\
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Detecting global optimality and extracting an optimal solution

- Global optimality is certified (i.e., $\theta_r = \xi$) if

$$\operatorname{rank} \mathbf{M}_r(L) = \operatorname{rank} \mathbf{M}_{r-d_{\mathcal{D}}}(L) \quad \textbf{(flatness condition)}$$

$\rightsquigarrow$ There is a cheap algorithm for extracting an optimal solution as well as the corresponding optimal state

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Exploiting structures

- The size of SDPs arising from the hierarchy rapidly grows
- Exploiting structures:
  - Using a customized monomial basis
  - Equality constraints
  - Symmetry
  - Correlative sparsity
  - Term sparsity

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Ground state energy of quantum many-body systems

- The Heisenberg chain is defined by the Hamiltonian:

$$H = \sum_{i=1}^{N} \sum_{a \in \{x,y,z\}} \sigma_i^a \sigma_{i+1}^a$$

- Computing ground state energy of the Heisenberg chain can be formulated as a noncommutative polynomial optimization problem:

$$\begin{cases} \min\limits_{\{|\psi\rangle, \sigma_i^a\}} & \langle\psi|H|\psi\rangle \\ \text{s.t.} & (\sigma_i^a)^2 = 1, \quad i = 1, \ldots, N, a \in \{x, y, z\} \\ & \sigma_i^x \sigma_i^y = \mathbf{i}\sigma_i^z, \sigma_i^y \sigma_i^z = \mathbf{i}\sigma_i^x, \sigma_i^z \sigma_i^x = \mathbf{i}\sigma_i^y, \quad i = 1, \ldots, N \\ & \sigma_i^a \sigma_j^b = \sigma_j^b \sigma_i^a, \quad 1 \le i \ne j \le N, a, b \in \{x, y, z\} \end{cases}$$

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Structures of the Heisenberg model

1. sparsity
2. sign symmetry
3. translation symmetry
4. permutation symmetry
5. mirror symmetry

☞ 100 spins, accuracy 10^{-5} [Wang et al., PRX 2024]

From linearity to nonlinearity

Covariance Bell inequalities

- Binary random variables A and B
- Covariance on a classical model:

$$\mathrm{cov}(A, B) = \int AB\mathrm{d}\mu - \int A\mathrm{d}\mu \int B\mathrm{d}\mu = E(AB) - E(A)E(B)$$

➤ max over all probas μ = classical bound

- Covariance on a quantum model:

$$\mathrm{cov}(A, B) = \varsigma(AB) - \varsigma(A)\varsigma(B)$$

where ς is a state

➤ max over all states ς = maximal quantum violation

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$$\mathrm{cov}_{3322} = \mathrm{cov}(A_1, B_1) + \mathrm{cov}(A_1, B_2) + \mathrm{cov}(A_1, B_3) + \mathrm{cov}(A_2, B_1) + \mathrm{cov}(A_2, B_2) - \mathrm{cov}(A_2, B_3) + \mathrm{cov}(A_3, B_1) - \mathrm{cov}(A_3, B_2)$$

- Concrete μ yields $\mathrm{cov}_{3322} = 4.5$
  $$\mu = \frac{3}{8}(+++/+++) + \frac{3}{8}(--+/--+) + \frac{1}{4}(-+-/-+-)$$
- $(A_1A_2A_3/B_1B_2B_3)$: strategy where Alice and Bob deterministically output A_x and B_y for inputs x and y
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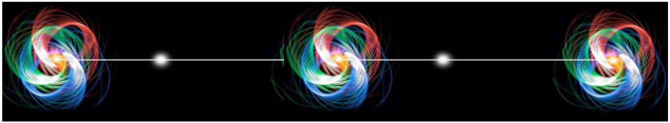

Alice $\leftarrow$ Source 1 $\rightarrow$ Bob $\leftarrow$ Source 2 $\rightarrow$ Charlie

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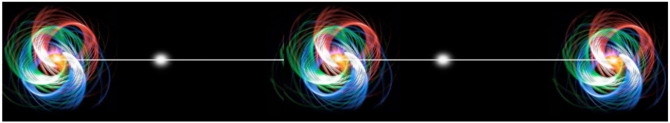

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State polynomial optimization

State polynomials

- States $\mathcal{S}(\mathcal{H})$: positive unital $\star$-linear functionals on $\mathcal{B}(\mathcal{H})$
- State polynomial: $\mathscr{S} := \mathbb{R}\left[\varsigma(w) \colon w \in [\mathbf{x}] \setminus \{1\}\right]$
  - $\varsigma(x_1^2)\varsigma(x_2x_1) + \varsigma(x_1)\varsigma(x_2x_1x_2)$, $x_1, \ldots, x_n \in \mathcal{B}(\mathcal{H})$, $\varsigma \in \mathcal{S}(\mathcal{H})$
- NC state polynomial: $\boldsymbol{\mathscr{S}} := \mathscr{S} \otimes \mathbb{R}[\mathbf{x}]$, the free $\mathscr{S}$-algebra on $[\mathbf{x}]$
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State polynomial optimization

- $f \in \mathscr{S}, g_i \in \mathscr{S}$:

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

Sum of Hermitian squares

- Sum of Hermitian squares (SOHS): $f = \varsigma(f_1^* f_1) + \cdots + \varsigma(f_t^* f_t)$
- NC state monomial: $\varsigma(u_1) \cdots \varsigma(u_s) w$
- $\langle \mathbf{x} \rangle_d$: vector of NC state monomials up to degree d
- f of degree $2d$ is an SOHS $\iff$ there exists a PSD matrix G s.t.

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State Positivstellensatz

- Define the feasible set

$$\mathcal{D} := \left\{(\varsigma, \mathbf{x}) \in \mathcal{S}(\mathcal{H}) \times \mathcal{B}(\mathcal{H})^n \,\middle|\, g_i(\varsigma; \mathbf{x}) \succeq 0,\ i = 1, \ldots, m\right\}$$

Theorem (Klep, Magron, Volčič, and Wang, 2024)

Assume that $\{g_i\}_{i=1}^m$ is algebraically bounded. If f is positive on $\mathcal{D}$, then

$$f = \sum_{g \in \{1\} \cup \{g_i\}_{i=1}^m} \varsigma(s_g^* g s_g), \quad \text{for some } \{s_g\}_g \subseteq \mathscr{S}.$$

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SOHS relaxations

- *r*-th order SOHS relaxation:

$$\theta_r^* := \begin{cases} \sup\limits_{\lambda, s_g} & \lambda \\ \text{s.t.} & f - \lambda = \sum_{g \in \{1\} \cup \{g_i\}_{i=1}^m} \varsigma(s_g^* g s_g) \\ & \deg(s_g^* g s_g) \le 2r \end{cases} \quad \rightsquigarrow \quad \text{SDP}$$

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Reformulation with linear functionals

- Consider a linear functional $L : \mathscr{S} \to \mathbb{R}$
- r-th order moment matrix $\mathbf{M}_r(L)$:

$$[\mathbf{M}_r(L)]_{uv} := L(\varsigma(u^* v)), \quad \forall |u|, |v| \leq r$$

- r-th order localizing matrix $\mathbf{M}_r(gL)$ associated to $g = \sum_w g_w w$:

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- For classical models: 3.375

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- Binary random variables A_i, B_j, C_k:

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➤ Bilocality constraints $E(A_1A_2A_3C_1C_2C_3)=E(A_1A_2A_3)E(C_1C_2C_3)+$ similar factorization constraints & vanishing constraints:

$$E(A_i)=E(B_i)=E(C_i)=0 \text{ for } i\in\{1,2,3\}$$

$$E(A_iB_j)=E(B_iC_j)=0 \text{ for } i\neq j$$

$$E(A_iB_jC_k)=0 \text{ for } |\{i,j,k\}|\leq 2$$

Bilocal Bell inequality

$$\begin{cases} \sup & \frac{1}{3}\sum_{i\in\{1,2,3\}}(\varsigma(b_ic_i)-\varsigma(a_ib_i))-\sum_{\{i,j,k\}=\{1,2,3\}}\varsigma(a_ib_jc_k) \\ \text{s.t.} & \varsigma(a_1a_2a_3c_1c_2c_3)=\varsigma(a_1a_2a_3)\varsigma(c_1c_2c_3) \\ & \varsigma(a_i)=\varsigma(b_i)=\varsigma(c_i)=0 \text{ for } i\in\{1,2,3\} \\ & \varsigma(a_ib_j)=\varsigma(b_ic_j)=0 \text{ for } i\neq j \\ & \varsigma(a_ib_jc_k)=0 \text{ for } |\{i,j,k\}|\leq 2 \end{cases}$$

- SDP with $r=3$ yields 4.46 (few seconds)
- SDP with $r=4$ yields 4.38 (few hours)
- SDP with $r=5$ yields 4.37 (one week)

Bilocal Bell inequality

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Bilocal Bell inequality

$$
\begin{cases}
\sup & \frac{1}{3}\sum_{i\in\{1,2,3\}}(\varsigma(b_ic_i)-\varsigma(a_ib_i))-\sum_{\{i,j,k\}=\{1,2,3\}}\varsigma(a_ib_jc_k)\\
\text{s.t.} & \varsigma(a_1a_2a_3c_1c_2c_3)=\varsigma(a_1a_2a_3)\varsigma(c_1c_2c_3)\\
& \varsigma(a_i)=\varsigma(b_i)=\varsigma(c_i)=0 \text{ for } i\in\{1,2,3\}\\
& \varsigma(a_ib_j)=\varsigma(b_ic_j)=0 \text{ for } i\neq j\\
& \varsigma(a_ib_jc_k)=0 \text{ for } |\{i,j,k\}|\leq 2
\end{cases}
$$

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More applications

- Quantum uncertainty relation [Morán and Huber, 2024]
- Quantum code [Munné, Nemec, and Huber, 2024]
- Quantum causal compatibility problem [Ligthart, 2024]
- Quantum nonlocality [Renou, Xu, and Ligthart, 2024]

Software

- NCTSSOS: in Julia, based on JuMP

https://github.com/wangjie212/NCTSSOS

- Play with it if you have noncommutative/state polynomial optimization problems!

Take-home message

☞ Noncommutative polynomial optimization is a powerful tool for handling nonlinear expressions in operators arising in quantum information

☞ State polynomial optimization is a powerful tool for handling nonlinear expressions in both expectations and operators arising in quantum information

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Main references

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Thank You!

https://wangjie212.github.io/jiewang