Non-commutative polynomial optimization in quantum physics

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Computational aspects of commutative and noncommutative positive polynomials 8th European Congress of Mathematics, Portoroz, 21 June 2021



Polynomial optimization problems

$$\overline{p} = \min_{x_1, \dots, x_n} p(x_1, \dots, x_n)$$

s.t. $q_j(x_1, \dots, x_n) \ge 0$

where
$$x = (x_1, \dots, x_n) \in \mathbb{R}^n$$

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Convergence can be proven using Putinar's result on Positivstellensatz.

Non-commutative polynomial optimization

$$\overline{p} = \min_{|\psi\rangle, X_1, \dots, X_n} \langle \psi | P(X_1, \dots, X_n) | \psi \rangle$$

s.t. $Q_j(X_1, \dots, X_n) \ge 0$

where $X_1, ..., X_n$ are now non-commuting bounded operators, of arbitrary dimension, and P and Q_j are Hermitian polynomial operators of bounded degree $\leq d$.

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M. Navascués. S. Pironio, AA, Phys. Rev. Lett. 98, 010401 (2007); New J. Phys. 10 (7), 073013 (2008).

S. Pironio, M. Navascués, AA, SIAM J. Optim. 20, 2157 (2010).



We consider the set of monomials of a given degree $\leq k$ on the previous operators, where each monomial is defined by a vector of indices α . The degree of the monomial is $|\alpha| = k$.

Example:

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We consider maps from this set to complex numbers: $\Lambda(Y_{\alpha}) = y_{\alpha} \in C$



For a given sequence, we define the moment matrix M_k of degree k as

$$\begin{pmatrix} M_k \end{pmatrix}_{\alpha,\beta} = \Lambda \begin{pmatrix} X_{\overline{\alpha}} X_{\beta} \end{pmatrix}$$

$$M_1 = \begin{pmatrix} 1 & y_1 & y_2 & y_{\overline{1}} & y_{\overline{2}} \\ y_{\overline{1}} & y_{\overline{1}1} & y_{\overline{12}} & y_{\overline{11}} & y_{\overline{12}} \\ y_{\overline{2}} & y_{\overline{2}1} & y_{\overline{2}2} & y_{\overline{2}\overline{1}} & y_{\overline{2}2} \\ y_1 & y_{11} & y_{12} & y_{1\overline{1}} & y_{1\overline{2}} \\ y_2 & y_{21} & y_{22} & y_{2\overline{1}} & y_{2\overline{2}} \end{pmatrix}$$



For a given sequence, we define the moment matrix M_k of degree k as

$$(M_k)_{\alpha,\beta} = \Lambda (X_{\overline{\alpha}} X_{\beta})$$

$$|\alpha|, |\beta| \le k$$

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For a polynomial $P(X) = \sum p_{\delta} X_{\delta}$ the localizing matrix $L_{P,k}$ of degree k is defined as

$$\begin{aligned} \left(L_{P,k}\right)_{\alpha,\beta} &= \sum p_{\delta} \Lambda \left(X_{\overline{\alpha}} X_{\delta} X_{\beta}\right) \\ & \left|\alpha\right|, \left|\beta\right| \leq k \end{aligned}$$



Every specific choice of operators X_i and state ψ defines a map Λ :

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Proof:

$$\langle v | L_{P,k} | v \rangle = \sum_{\alpha,\beta} v_{\alpha}^{*} (L_{P,k})_{\alpha,\beta} v_{\beta} = \sum_{\alpha,\beta} v_{\alpha}^{*} \sum_{\delta} p_{\delta} \Lambda (X_{\overline{\alpha}} X_{\delta} X_{\beta}) v_{\beta} =$$

$$\sum_{\alpha,\beta} v_{\alpha}^{*} \sum_{\delta} p_{\delta} \langle \psi | X_{\overline{\alpha}} X_{\delta} X_{\beta} | \psi \rangle v_{\beta} = \langle \psi | \left(\sum_{\alpha} v_{\alpha}^{*} X_{\overline{\alpha}} \right) \left(\sum_{\delta} p_{\delta} X_{\delta} \right) \left(\sum_{\beta} v_{\beta} X_{\beta} \right) | \psi \rangle \ge 0$$



$$\overline{p} = \min \left\langle \psi \left| P(X_1, \dots, X_n) \right| \psi \right\rangle$$

s.t. $Q_j(X_1, \dots, X_n) \ge 0$



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Relaxation of order k:

$$p^{(k)} = \min \sum p_{\delta} y_{\delta}$$

s.t. $M_k \ge 0, L_{Q_j, k - \deg(Q_j)/2} \ge 0$



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Clearly:

$$p^{(1)} \le p^{(2)} \le \dots \le \overline{p}$$



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Positivity domain:

$$S_Q = \{ (X_1, ..., X_n) \text{ s.t. } Q_j (X_1, ..., X_n) \ge 0 \}$$



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$$M_{Q} = \left\{ P \text{ s.t. } P = \sum_{i} F_{i}^{*} F_{i} + \sum_{i,j} G_{i,j}^{*} Q_{j} G_{i,j} \right\}$$

Quadratic module:



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 $M_{\mathcal{Q}}$ is Archimedean if

$$\exists C \text{ s.t. } C - X_1^* X_1 - \ldots - X_n^* X_n \in M_Q$$



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If S_Q is bounded, we can make M_Q Archimedean by choosing a large enough C and adding to the set of polynomial constraints the condition:

$$C-X_1^*X_1-\ldots-X_n^*X_n$$

If M_Q is Archimedean: $\lim_{k \to \infty} p^{(k)} = \overline{p}$

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Convergence can be established at a finite step whenever the optimal solution y_k for relaxation of order k is such that:

$$\operatorname{rank}(M_k) = \operatorname{rank}(M_{k-\max(d_i)})$$



Consider the problem:

$$\lambda^{(k)} = \max_{\lambda, B_i, C_{ij}} \lambda$$

s.t. $P(X_1, \dots, X_n) - \lambda = \sum_i B_i^* B_i + \sum_{i,j} C_{i,j}^* Q_j C_{i,j}$
 $\max_i \operatorname{deg}(B_i) \le k, \max_i \operatorname{deg}(C_{i,j}) \le k - d_i$



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This problem can be cast in a sdp form, and proven to be the dual of step k before.

$$\lambda^{(k)} \le p^{(k)} \le \overline{p}$$



 $P(X_1,...,X_n) - (\overline{p} - \varepsilon)$ is positive in S_Q for any $\varepsilon > 0$.



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Helton and McCullough Positivellensatz

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This defines a feasible point for the previous problem, so one has:

$$\overline{p} - \varepsilon \leq \lambda^{(k)} \leq p^{(k)} \leq \overline{p} \quad \forall \varepsilon > 0$$



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 $[X_i, X_j] = 0 \; \forall i, j$





$$\overline{p} = \min \left\langle \psi \middle| P(X_1, \dots, X_n) \middle| \psi \right\rangle \qquad \overline{p} = \min p(x_1, \dots, x_n)$$

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s.t. $X_i^2 - X_i = 0$
$$p^{(1)} = \overline{p} \quad \text{Easy!}$$

$$\overline{p} = \min p(x_1, \dots, x_n)$$

s.t. $x_i^2 - x_i = 0$
NP-hard



Why do we care about this?



Quantum physics

The postulates of quantum theory:



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1. A complex Hilbert space of dimension d is associated to any physical system. The state of the system is specified by a normalised ray in this space, $|\psi\rangle \in \mathbb{C}^d$ such that $\langle \psi | \psi \rangle = 1$.



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- 4. When combining two systems, A and B, with corresponding Hilbert spaces \mathbb{C}^{d_A} and \mathbb{C}^{d_B} , the Hilbert space of the joint system is the tensor product of the two spaces.



Statistics in quantum experiments





Statistics in quantum experiments



Quantum physics is a natural source of problems involving polynomials of operators.



Characterization of Quantum Correlations

Navascués, Pironio, Acin, PRL 2007, NJP 2009



















Example







$$p(ab|xy) = \begin{pmatrix} p(+1,+1|0,0) & p(+1,-1|0,0) & p(-1,+1|0,0) & p(-1,-1|0,0) \\ p(+1,+1|0,1) & p(+1,-1|0,1) & p(-1,+1|0,1) & p(-1,-1|0,1) \\ p(+1,+1|1,0) & p(+1,-1|1,0) & p(-1,+1|1,0) & p(-1,-1|1,0) \\ p(+1,+1|1,1) & p(+1,-1|1,1) & p(-1,+1|1,1) & p(-1,-1|1,1) \end{pmatrix}$$





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$$p_A(+1|0) = p(+1, +1|00) + p(+1, -1|00) = \frac{1}{2}$$



No-signalling correlations: correlations compatible with the no-signalling principle, i.e. the impossibility of instantaneous communication.

$$\sum_{a_{k+1},...,a_N} p(a_1,...,a_N | x_1,...,x_N) = p(a_1,...,a_k | x_1,...,x_k)$$



 $p_A(+1|0) = p(+1,+1|00) + p(+1,-1|00) = \frac{1}{2} = p(+1,+1|01) + p(+1,-1|01)$



Classical correlations: correlations established by classical means.

$$p(a_1,\ldots,a_N|x_1,\ldots,x_N) = \sum_{\lambda} p(\lambda) D(a_1|x_1,\lambda) \ldots D(a_N|x_N,\lambda)$$

These are the standard "EPR" correlations. Independently of fundamental issues, these are the correlations achievable by classical resources. Bell inequalities define the limits on these correlations.



Quantum correlations: correlations established by quantum means.

$$p(a_{1},...,a_{N} | x_{1},...,x_{N}) = \langle \Psi | M_{a_{1}}^{x_{1}} \otimes \cdots \otimes M_{a_{N}}^{x_{N}} | \Psi \rangle$$
$$\sum_{a_{i}} M_{a_{i}}^{x_{i}} = 1 \qquad M_{a_{i}'}^{x_{i}} M_{a_{i}}^{x_{i}} = \delta_{a_{i}a_{i}'} M_{a_{i}}^{x_{i}}$$

Everything is expressed in terms of operators (the quantum state and the measurement projectors) acting on a Hilbert space.









There exist correlations that cannot be explained by a classical model in which (deterministic) classical instructions specify the outcomes of the devices. These quantum correlations are known as **non-local** and they are detected by the violation of a Bell inequality.





 $C \subset Q \subset NS$

Tsirelson Popescu-Rohrlich



There exist correlations that are compatible with the no-signalling principle but cannot be obtained by performing local measurements on a quantum (entangled) state.

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Example: CHSH scenario





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CFO[®] Characterizing quantum correlations

Given p(a, b|x, y), does it have a quantum realization?

$$p(a,b|x,y) = \langle \Psi | M_a^x \otimes M_b^y | \Psi \rangle \qquad \sum_a M_a^x = 1$$
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Example:

$$p(a,b|0,0) = p(a,b|0,1) = p(a,b|1,0) = \frac{1}{8}(2+\sqrt{3},2-\sqrt{3},2-\sqrt{3},2+\sqrt{3})$$
$$p(a,b|1,1) = (0.245,0.255,0.255,0.245)$$

Previous work by Tsirelson



NPA hierarchy

Given a probability distribution p(a,b|x,y), we have defined a hierarchy consisting of a series of tests based on semi-definite programming techniques allowing the detection of supra-quantum correlations.



The hierarchy is asymptotically convergent.



NPA hierarchy



Every step in the hierarchy defines a convex set that is included in the previous step. Convergence is provably attained asymptotically.

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$$p(a,b|1,1) = (0.245,0.255,0.255,0.245)$$

Solution: it is not quantum, that is, there exists no quantum state of two particles and local measurements acting on them that produce these correlations.

The experimental observation of these correlations would imply the failure of quantum physics, as Bell violations did for classical physics.


Going beyond NPA



Ground-state energies

A standard problem in physics is to find the ground state energy of a systems of N particles whose interactions are described by a Hamiltonian operator H.



subject to some constraints



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If the problem can be cast as a non-commutative polynomial optimization, the previous hierarchy provides lower bounds. It complements the standard approach!



Classical spin systems

Classical spin problems:

$$\min_{\vec{\sigma}} H(\vec{\sigma}) = \sum_{i,j} J_{i,j} \sigma_i \sigma_j + \sum_i h_i \sigma_i$$

$$\begin{split} \min_{\vec{\sigma}} H(\vec{\sigma}) &= \sum_{i,j} J_{i,j} \sigma_i \sigma_j + \sum_i h_i \sigma_i \\ \text{such that:} \\ \sigma_i^2 - 1 &= 0 \text{ for all } i \end{split}$$

Commutative polynomial optimization:

$$E_1 \leq E_2 \leq \cdots \leq E_\infty \rightarrow E_g \leq E_a$$



Quantum spin systems

Quantum spin problems:

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such that:

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$$\left[\sigma_{j}^{\alpha}, \sigma_{k}^{\beta}\right] = 2i\delta_{jk}\epsilon_{\alpha\beta\gamma}\sigma_{k}^{\gamma}$$

Non-commutative polynomial optimization:

$$E_1 \leq E_2 \leq \cdots \leq E_\infty \to E_g \leq E_a$$



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See Jie Wang's talk.





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But even more intricate causation patterns could explain the correlations.



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Quantum causality

Bell's theorem: nonlocal correlations can be explained by a quantum causal model, but not by the classical counterpart.





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How is causality affected by quantum information?

See Alejandro Pozas-Kerstjens' talk.





CFO[®] Quantum information technologies



Quantum Computer



Quantum Simulator



Quantum Cryptography







Quantum certification



Is this a Quantum Computer?



Does this properly simulate a quantum system?



Is this quantum random?



Is this cryptographically secure?