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Polynomial optimization in non-commuting variables

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Polynomial optimization problems arise across many sciences, e.g. in control theory, operations research, combinatorics and, computer science. However, very simple instances of polynomial optimization problems are known to be NP hard, thus approximation techniques based on sums of squares concepts taken from real algebraic geometry and inspired by moment theory from probability and functional analysis were developed. We focus on polynomial optimization problems in matrix variables, since many applied problems, e.g. in quantum chemistry, or in quantum information theory naturally involve polynomials in matrix variables.

Background

Polynomial Optimization

Let $p, g_i \in \mathbb{R}[x_1, \dots, x_n]$ be polynomials. We want to optimmize p over the semialgebraic set

$$K = \{a \in \mathbb{R}^n \mid g_i(a) \geq 0, i \in I\}$$

Polynomial optimization is NP-hard

$$p_{min} = \min p(a) \text{ s.t. } a \in K$$
$$= \max \lambda \text{ s.t. } p - \lambda \geq 0 \text{ on } K$$

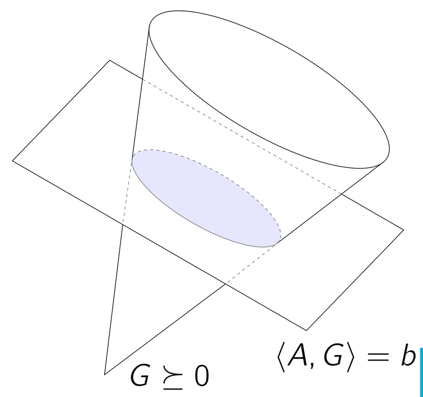
Challenge: Certify positivity over the set K.

Semidefinite Programming

Let C, A_i be matrices and b_i be real vectors. An SDP is of the following form

$$\max \langle C, G\rangle \text{ s.t. } \langle A_i, G\rangle = b_i, i \in I$$
$$G \succeq 0$$

SDPs essentially solvable in polynomial time, implemented e.g. in SeDuMi, SDPT3, or Mosek.



SOS Approximation

$$p_{sos} = \max \lambda \text{ s.t. } p - \lambda \text{ sos}$$

sos: $\sum_i f_i^2 + \sum_j g_j \sum_k h_k^2$

Fact 1: $p_{sos} \leq p_{min}$

Fact 2: This is de facto an SDP via Gram matrices:

$$f^2 = [x]^T G [x]$$

with $G \succeq 0$ and $[x]$ a vector of all monomials of degree $\leq \deg f$.

Fact 3: For compact K, Positivstellensätze & degree bounds imply an approximation hierarchy p_t converging monotonically to p_{min}.

We consider now polynomials $p \in \mathbb{R}\langle X_1, \dots, X_n\rangle$, where the X_i are noncommuting variables (i.e. EAT≠TEA) with an involution $*$ fixing the variables (i.e. $X_i^* = X_i$ and $a^* = a$ for $a \in \mathbb{R}$). Let $\mathcal{S}^n$ be the set of all $n-$tuples A consisiting of symmetric matrices A_i of arbitrary but similar size. We can then evaluate a polynomial p in A simply by replacing X_i with A_i.
To get a polynomial optimization problem we need to definie when a polynomial is considered to be positive. There are two natural options: positivity by eigenvalue and positivity by trace.

Positivity by eigenvalue

Optmization Problem

Def.: p is matrix-positive if $p(A) \succeq 0$ for all $A \in \mathcal{S}^n$.

Let $p, g_i \in \mathbb{R}\langle X_1, \dots, X_n\rangle$ be symmetric polynomials. We want to optimmize p over

$$K = \{A \in \mathcal{S}^n \mid g_i(A) \succeq 0\}.$$

Optimization Problem:

$$p_{min} = \max \lambda \text{ s.t. } p - \lambda \succeq 0 \text{ on } K$$
$$= \min \langle \varphi, p(A)\varphi\rangle \text{ s.t. } A \in K, \|\varphi\| = 1$$

This is still NP-hard!

SOS Approximation

$$p_{sos} = \max \lambda \text{ s.t. } p - \lambda \text{ sos}$$

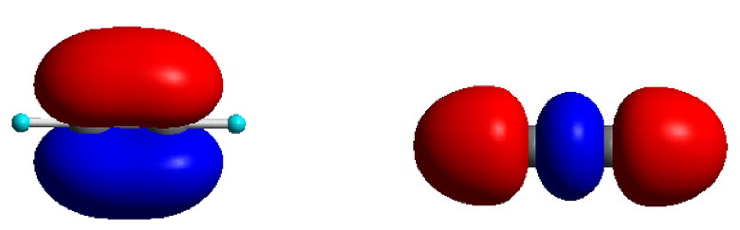
with sos: $\sum_i f_i^* f_i + \sum_{j,k} h_{jk}^* g_j h_{jk}$

Fact 1, 2 & 3 also hold in this case!

Application: Ground state energy

We have a molecule of N electrons which can occupy M orbitals. Each orbital is associated with creation/anihilation operators $a_i^\dagger, a_i$, and its pairwise interaction is described via $h_{ijkl} \in \mathbb{R}$

$$\min_{(a, a^\dagger, \varphi)} \left\langle \varphi, \sum_{ijkl} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \varphi \right\rangle$$
$$\text{s.t. } \|\varphi\| = 1$$
$$\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0$$
$$\{a_i^\dagger, a_j\} = \delta_{ij}$$
$$\Big(\sum_i a_i^\dagger a_i - N\Big)\varphi = 0$$



Positivity by trace

Optmization Problem

Def.: p is trace-positive if $\mathrm{Tr}(p(A)) \geq 0$ for all $A \in \mathcal{S}^n$.

Let $p, g_i \in \mathbb{R}\langle X_1, \dots, X_n\rangle$ be symmetric polynomials. We want to optimmize p over

$$K = \{A \in \mathcal{S}^n \mid g_i(A) \succeq 0\}$$

Optimization Problem

$$p_{min} = \max \lambda \text{ s.t. } \mathrm{Tr}(p - \lambda) \geq 0 \text{ on } K$$
$$= \min \mathrm{Tr}(p(A)) \text{ s.t. } A \in K$$

This is still NP-hard!

SOS Approximation

$$p_{sos} = \max \lambda \text{ s.t. } p - \lambda \text{ sos}$$

with sos: $\sum_i f_i^* f_i + \sum_{j,k} h_{jk}^* g_j h_{jk} + \sum_i [q_i, r_i]$

Fact 1, 2 & 3 also hold in this case!

Application: Completely psd cone

A matrix $A \in M_n(\mathbb{R})$ is called completely psd if it has a symmetric psd factorization, i.e., there exist $B_i \succeq 0$ s.t.

$$A_{ij} = \mathrm{Tr}(B_i B_j)$$

for all $i, j \in [n]$. The set of all those matrices is the convex cone $\mathcal{CS}_+^n$.
This cone is the matrix analog of the completely positive cone, i.e., the cone of matrices which have a Gram representation using vectors in the nonnegative orthant.
It is thus closely related to symmetric psd lifts of polyhedra. In other words, can one reformulate a Linear Program with plenty of nodes as a Semidefinite Program of higher dimension with fewer conditions.
If we optimize over the dual cone of $\mathcal{CS}_+$ instead of $\mathcal{CS}_+$ itself, we optimize over all noncommutative polynomials p of the form $p = \sum_{i,j} p_{ij} X_i^2 X_j^2$ which are trace-positive.

Application: Quantum Correlations

Entanglement is a striking feature of quantum mechanics which creates (bipartite) correlations which cannot be obtained classically. There are two descriptions of the set of bipartite quantum correlations:

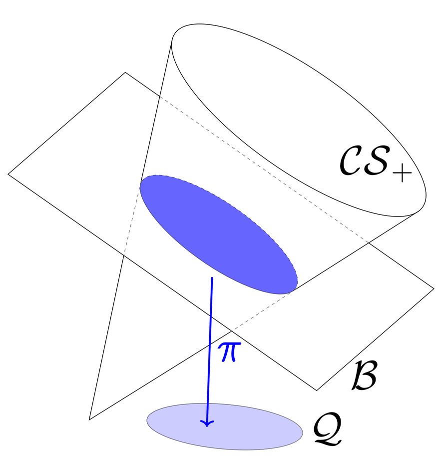
$\mathcal{Q} = \{p_{ab,xy} = \varphi^T(E_x^a \otimes F_y^b)\varphi \mid E_x^a, F_y^b \text{ POVM}, \|\varphi\| = 1\}$ and

$\mathcal{Q} = \{p_{ab,xy} = \varphi^T(E_x^a F_y^b)\varphi \mid E_x^a, F_y^b \text{ POVM}, \|\varphi\| = 1, [E_x^a, F_y^b] = 0\}$,

where x, y are the input parameters and a, b is the output. A POVM is a set $\{E_a\}_a$ of psd operators whith $\sum_a E_a = 1$.

If we allow only finite dimensional operators as POVMs, both descriptions coincide.

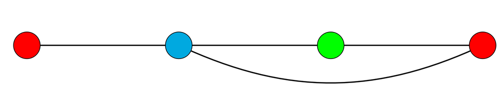
Most concrete examples of quantum correlations are in $\mathcal{Q}$.



$\mathcal{Q} = \pi(\mathcal{CS}_+ \cap \mathcal{B})$.

Optimizing over $\mathcal{Q}$ can thus be reformulated to optimize over $\mathcal{CS}_+$.

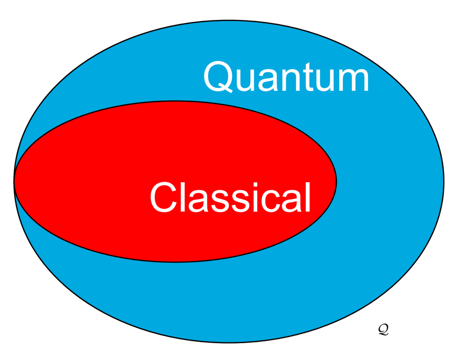
This has been done for quantum graph parameters, e.g. the quantum chromatic numer.



Most bounds on quantum correlations are based on $\mathcal{Q}_c$. Optimization over $\mathcal{Q}_c$ can be reformulated as polynomial optimization problem using matrix-positivity.

Example: Bell inequalities

$$\max_{(E,\varphi)} \left\langle \varphi, \sum_{i,j} c_{ij} E_i E_j \varphi \right\rangle$$
$$\text{s.t. } \|\varphi\| = 1$$
$$E_i E_j = \delta_{ij} \text{ for some } i, j$$
$$\sum_{i \in M_k} E_i = 1$$
$$[E_i, E_j] = 0 \text{ for } i \in A, j \in B$$



Reference: *Optimization of Polynomials in Non-Commuting Variables, Sabine Burgdorf, I. Klep, J. Povh, Springer Briefs in Mathematics, ISBN 978-3-319-33338-0*

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