Semidefinite optimization for polynomials in noncommuting variables

Networks & Optimization
Algorithm & Complexity

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What is it and why should I care?

What are we up to?
- Generalize *polynomial optimization* over scalar variables
- Want to optimize polynomials evaluated in matrices $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

What do we need?
- Polynomials in *noncommuting variables* $EAT \neq TEA$
- Approximation technique using *semidefinite programs*
What is it and why should I care?

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What do I need it for?
- Applications in quantum physics
  - quantum chemistry: ground state electronic energy of atoms
  - quantum theory: upper bounds for violation of Bell inequalities
  - quantum information: multi prover games/quantum correlation
- Application in systems control
  - Systematic strategy to compute stabilizing feedback for closed loop systems
What is polynomial optimization?

- $p \in \mathbb{R}[x]$ polynomial
- Find

$$p_{\text{min}} = \min_{a \in \mathbb{R}^n} p(a)$$
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$$p_{\min} = \min_{a \in \mathbb{R}^n} p(a)$$

We can add polynomial constraints like $g(a) \geq 0$ to define a region where we want to optimize $p$.

Example

A matrix $M$ is copositive if $p_{\min} \geq 0$ for $p = \sum_{i,j} M_{ij} x_i^2 x_j^2$. 
What is polynomial optimization?

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Example

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Problem

Calculating \( p_{\min} \) is in general NP-hard 😞

- Find a way to make it easier → approximation
- Involves sums of squares and semidefinite programs 😊
What is a semidefinite program?

\[
\begin{align*}
\text{max } & \langle C, X \rangle \\
\text{s.t. } & \langle A_j, X \rangle = b_j, \quad j = 1, \ldots, m \\
& X \succeq 0
\end{align*}
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\[\text{← linear function}\]

- Optimization of a linear function
What is a semidefinite program?

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- Optimization of a linear function over an affine space
What is a semidefinite program?

<table>
<thead>
<tr>
<th>max $\langle C, X \rangle$</th>
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</thead>
<tbody>
<tr>
<td>s.t. $\langle A_j, X \rangle = b_j$, $j = 1, \ldots, m$</td>
</tr>
<tr>
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</tr>
</tbody>
</table>

$\leftarrow$ psd matrix

- Optimization of a **linear function** over an **affine space** intersected with the set of **positive semidefinite matrices**:
What is a semidefinite program?

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\[
\left\{ \text{spectrahedron} \right\}
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- Optimization of a \textbf{linear function} over an \textbf{affine space} intersected with the set of \textbf{positive semidefinite matrices}: a \textbf{spectrahedron}
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- Optimization of a linear function over an affine space intersected with the set of positive semidefinite matrices: a spectrahedron

poly in \( \log(1/\varepsilon) \) for precision \( \varepsilon \)

- Essentially solvable in polynomial time using interior point algorithms, e.g. SeDuMi, SDPT3, SDPA, Mosek,...
NC polynomial optimization

Idea: Replace $a$ with $a_i \in \mathbb{R}$ by $A$ with $A_i$ symmetric matrices

- Model NC polynomials
  - Polynomials in noncommuting variables $\underline{X} = (X_1, \ldots, X_n)$
  - Like usual polynomials, only difference $X_1X_2 \neq X_2X_1$ \(\text{EAT} \neq \text{TEA}\)
NC polynomial optimization

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- **Evaluation in symmetric matrices**
  - $p = 1 + 2X_1^2 + X_2 X_1 - X_1 X_2,$
  - $A = (A_1, A_2) \in (\mathbb{S}_s)^2$

\[
p(A) = 1 + 2A_1^2 + A_2 A_1 - A_1 A_2
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NC polynomial optimization

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- **Evaluation in symmetric matrices**
  - $p = 1 + 2X_1^2 + X_2 X_1 - X_1 X_2,$
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- **NC polynomial optimization**

$$p_{min} = \min_{(\varphi, A)} \{ \langle \varphi, p(A) \varphi \rangle \mid \| \varphi \| = 1 \}$$

- $p_{min}$ is the smallest eigenvalue $p(A)$ can attain over all $A$

We can add polynomial constraints like $g(A) \succeq 0$ to define a region where we want to optimize $p$
Where is the SDP?

- We can reformulate our nc optimization problem

\[
p_{\min} = \min_{(\varphi, A)} \{ \langle \varphi, p(A)\varphi \rangle \mid \|\varphi\| = 1 \}\]

using nc sums of squares

- This will turn out to be a semidefinite program
Where is the SDP?

- We can reformulate our nc optimization problem

\[ p_{\min} = \min_{(\varphi, A)} \{ \langle \varphi, p(A)\varphi \rangle \mid \| \varphi \| = 1 \} \]

using nc sums of squares

- This will turn out to be a semidefinite program

But first, let’s look at applications of nc polynomial optimization
Application: Quantum Chemistry

Compute ground state energy of atoms

- Molecule of \( N \) electrons that can occupy \( M \) orbitals
- Each orbital associated with creation/annihilation operators \( a_i^\dagger, a_i \)
- Pairwise interaction described by \( h_{ijkl} \)

\[
\min_{(a,a^\dagger,\varphi)} \langle \varphi, \sum_{ijkl} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \varphi \rangle \\
\text{s.t.} \quad \|\varphi\| = 1 \\
\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0 \\
\{a_i^\dagger, a_j\} = \delta_{ij} \\
\left( \sum_i a_i^\dagger a_i - N \right) \varphi = 0
\]
Application: Quantum Chemistry

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- Each orbital associated with creation/annihilation operators $a_i^\dagger$, $a_i$
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\{a_i^\dagger, a_j\} = \delta_{ij} \\
(\sum_i a_i^\dagger a_i - N) \varphi = 0
\end{align*}$$

$\left\langle \varphi, p(a, a^\dagger) \varphi \right\rangle$
$\left\|\varphi\right\| = 1$
additional constraints
Application: Systems Control

- Linear closed loop system with unknown feedback $\mathcal{G}$

Math. System
\[
\dot{x}(t) = Ax(t) + Bu, \\
y(t) = Cx(t)
\]

- Goal Find $\mathcal{G}$ which stabilizes the system
Application: Systems Control

- Linear closed loop system with unknown feedback $G$

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\dot{x}(t) &= Ax(t) + Bu, \\
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- Goal: Find $G$ which stabilizes the system

Lyapunov\textsuperscript{1892}

A system $\dot{x}(t) = Ax(t)$ is stable if there is a $P \succeq 0$ with $A^tP + PA < 0$

- Lyapunov’s idea can be extended to our problem: Riccati equations
Application: Systems Control

- Linear closed loop system with unknown feedback $\mathcal{G}$

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\begin{align*}
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\end{align*}
$$

- **Goal** Find $\mathcal{G}$ which stabilizes the system

Lyapunov\textsuperscript{1892}

A system $\dot{x}(t) = Ax(t)$ is stable if there is a $P \succeq 0$ with $A^TP + PA \prec 0$

- Lyapunov's idea can be extended to our problem: Riccati equations

- Optimization problem is first a feasibility problem

- Can be refined by optimizing a specific singular value

- For a uniform strategy to get $\mathcal{G}$ we have to work free of dimensions
Application: Quantum Correlations

- Two separated systems $A = M_1 \cup \cdots \cup M_n$ and $B = M_{n+1} \cup \cdots \cup M_N$
- Measurements of $M_i$ described by operators $E_i$ performed on a joint quantum state $\varphi$
- Correlations between $A$ and $B$: Joint probabilities $P(i, j) = \langle \varphi, E_i E_j \varphi \rangle$
Application: Quantum Correlations

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- Measurements of \( M_i \) described by operators \( E_i \) performed on a joint quantum state \( \varphi \)

- Correlations between \( A \) and \( B \): Joint probabilities \( P(i,j) = \langle \varphi, E_i E_j \varphi \rangle \)

- Violation of Bell inequalities
  - Linear combination of (joint) probabilities
  - Get inequalities by considering classical random variables
  - Want to find violations using quantum setup

\[
\begin{align*}
\max_{(E,\varphi)} & \langle \varphi, \sum_{i,j} c_{ij} E_i E_j \varphi \rangle \\
\text{s.t.} & \quad \| \varphi \| = 1 \\
& \quad E_i E_j = \delta_{ij} \text{ for } i, j \in M_k \\
& \quad \sum_{i \in M_k} E_i = 1 \\
& \quad [E_i, E_j] = 0 \text{ for } i \in A, j \in B
\end{align*}
\]