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 

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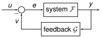
What do I need it for?

- 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?

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

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Example

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

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Problem

Calculating p_{min} is in general NP-hard ☹

- Find a way to make it easier $\rightarrow$ approximation
- Involves sums of squares and semidefinite programs ☺

What is a semidefinite program?

$$\boxed{\begin{aligned} &\max \ \langle C, X \rangle \\ &\text{s.t. } \langle A_j, X \rangle = b_j, \quad j = 1, \ldots, m \\ &\qquad X \succeq 0 \end{aligned}}$$

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$\leftarrow$ linear function

- Optimization of a linear function

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$\leftarrow$ affine space

- Optimization of a linear function over an affine space

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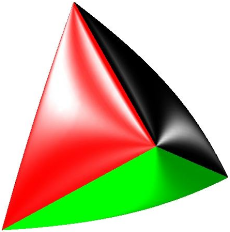

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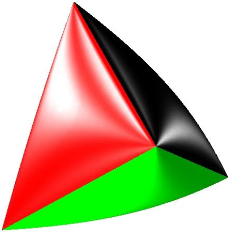

poly in $\log(1/\varepsilon)$
for precision ε

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

NC polynomial optimization

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

- Model NC polynomials
  - Polynomials in noncommuting variables $\underline{X} = (X_1, \ldots, X_n)$
  - Like usual polynomials, only difference $X_1 X_2 \neq X_2 X_1$ EAT$\neq$TEA

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- Evaluation in symmetric matrices
  - $p = 1 + 2X_1^2 + X_2X_1 - X_1X_2,$
  - $\underline{A} = (A_1, A_2) \in (\mathcal{S}\mathbb{R}^{s\times s})^2$

$$\left.\begin{array}{l} p = 1 + 2X_1^2 + X_2X_1 - X_1X_2, \\ \underline{A} = (A_1, A_2) \in (\mathcal{S}\mathbb{R}^{s\times s})^2 \end{array}\right\} p(\underline{A}) = \mathbf{1}_s + 2A_1^2 + A_2A_1 - A_1A_2$$

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- NC polynomial optimization

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

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

We can add polynomial constraints like $g(\underline{A}) \succeq 0$ to define a region where we want to optimize p

Where is the SDP?

- We can reformulate our nc optimization problem

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

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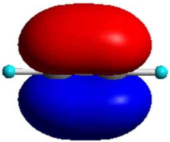
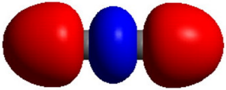
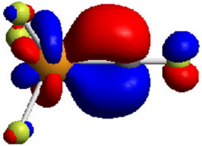
But first, let's look at applications
of nc polynomial optimization

Compute ground state energy of atoms

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

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

Application: Quantum Chemistry

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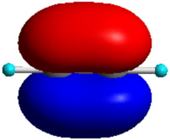
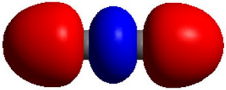
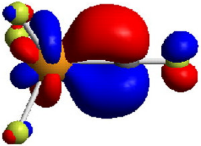
\qquad
\begin{aligned} & \leftarrow \langle \varphi, p(a, a^\dagger)\varphi \rangle \\ & \leftarrow \|\varphi\| = 1 \\ & \left.\begin{aligned} & \\ & \\ & \end{aligned}\right] \text{additional constraints} \end{aligned}$$

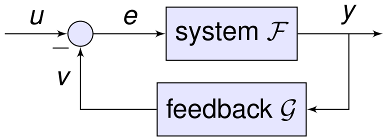






Application: Systems Control

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



Math. System

$$\dot{\vec{x}}(t) = \mathcal{A}\vec{x}(t) + \mathcal{B}\vec{u},$$
$$\vec{y}(t) = \mathcal{C}\vec{x}(t)$$

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

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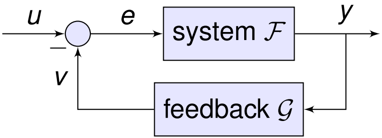

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NC polynomial with matrix coefficients

Lyapunov 1892

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

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

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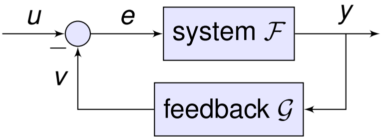

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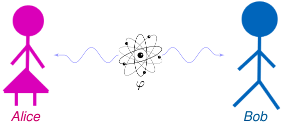
- Lyapunov's idea can be extended to our problem: Riccati equations
- Optimization problem is first a feasibility problem
- Can be refined by optimizing a specific singular value
- For a uniform strategy to get $\mathcal{G}$ we have to work free of dimensions

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



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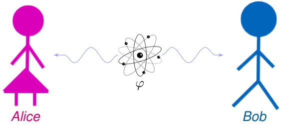

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- Correlations between A and B: Joint probabilities $P(i,j) = \langle \varphi, E_i E_j \varphi \rangle$
- Violation of Bell inqualities
  - Linear combination of (joint) probabilities
  - Get inequalities by considering classical random variables
  - Want to find violations using quantum setup

$$
\boxed{\begin{aligned}
\max_{(E,\varphi)} \ & \Big\langle \varphi, \sum_{i,j} c_{ij} E_i E_j \varphi \Big\rangle \\
\text{s.t.} \ & \|\varphi\| = 1 \\
& E_i E_j = \delta_{ij} \text{ for } i,j \in M_k \\
& \sum_{i \in M_k} E_i = 1 \\
& [E_i, E_j] = 0 \text{ for } i \in A, j \in B
\end{aligned}}
\qquad
\begin{aligned}
& \leftarrow \langle \varphi, p(\underline{E}) \varphi \rangle \\
& \leftarrow \|\varphi\| = 1 \\
& \left.\right] \text{measurement} \\
& \left.\right] A/B \text{ separated}
\end{aligned}
$$