Algorithmic Conversion of Polynomial Optimization Problems of Noncommuting Variables to Semidefinite Programming Relaxations

Sparsity and Scalability

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Outline

Problem Statement

We are interested in finding the global minimum p^* of a polynomial $p(x)$:

$$\mathbb{P}_K \mapsto p^* := \min_{x \in K} p(x), \quad (1)$$

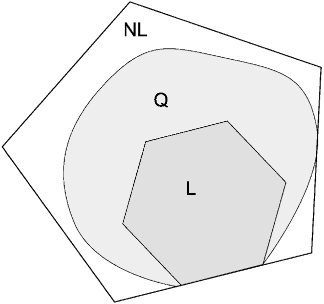
where K is a not necessarily convex set defined by polynomial inequalities $g_i(x) \geq 0, i = 1, \ldots, r$.

Bounding Quantum Correlations

$$\max_{E,\phi} \langle \phi, \sum_{ij} c_{ij} E_i E_j \phi \rangle$$

subject to

$$\begin{aligned} ||\phi|| &= 1 \\ E_i E_j &= \delta_{ij} E_i \qquad \forall i, j \\ \sum_i E_i &= 1 \\ [E_i, E_j] &= 0 \qquad \forall i, j. \end{aligned}$$



Navascués, M.; Pironio, S. & Acín, A. Bounding the set of quantum correlations. *Physical Review Letters*, 2007, 98, 1040.

Ground-state Energy

$$\min\langle\phi, H\phi\rangle$$

$$H_{\text{free}} = \sum_{<rs>} \left[c_r^\dagger c_s + c_s^\dagger c_r - \gamma(c_r^\dagger c_s^\dagger + c_s c_r)\right] - 2\lambda \sum_r c_r^\dagger c_r, \quad (2)$$

where $< rs >$ goes through nearest neighbour pairs in the lattice. The fermionic operators are subject to the following constraints:

$$\begin{aligned} \{c_r, c_s^\dagger\} &= \delta_{rs} I_r \\ \{c_r, c_s\} &= 0. \end{aligned}$$

Corboz, P.; Evenbly, G.; Verstraete, F. & Vidal, G. Simulation of interacting fermions with entanglement renormalization. *Physics Review A*, 2010, 81, 010303.

Detection of Multipartite Entanglement

- Partitions: $s = \{AB|C, AC|B, BC|A\}$.
- $P(abc|xyz)$ is biseparable iff it equals to $\sum_s \mathrm{tr}[M^s_{a|x} \otimes M^s_{b|y} \otimes M^s_{c|z}\rho^s]$,
- Where measurement operators for an isolated party commute: $[M^{AB|C}_{c|z}, M^{AB|C}_{c'|z'}]$.
- Bancal, J.-D.; Gisin, N.; Liang, Y.-C. & Pironio, S. Device-Independent Witnesses of Genuine Multipartite Entanglement. *Physics Review Letters*, 2011, 106, 250404.

Mutually Unbiased Bases

Mutually unbiased bases in Hilbert space $\mathbb{C}^d$ are two orthonormal bases $\{|e_1\rangle, \ldots, |e_d\rangle\}$ and $\{|f_1\rangle, \ldots, |f_d\rangle\}$ such that $|\langle e_j|f_k\rangle|^2 = \frac{1}{d}, \quad \forall j, k \in \{1, \ldots, d\}$.

Translating it to a noncommutative optimization problem:

1. $\Pi_i^x = (\Pi_i^x)^*$;
2. $\Pi_i^x \Pi_j^x = \delta_{ij} \Pi_i^x$;
3. $\sum_{i=1}^d \Pi_i^x = \mathbb{I}$;
4. $\Pi_i^x \Pi_j^{x'} \Pi_i^x = \frac{1}{d} \Pi_i^x$, for $x \neq x'$;
5. $[\Pi_i^x O_1 \Pi_i^x, \Pi_i^x O_2 \Pi_i^x] = 0$, for any x, i, and any pair of monomials O_1 and O_2 of $\{\Pi_i^x\}$ of length three.

Words and Involution

- Given n noncommuting variables, words are sequences of letters of $x = (x_1, x_2, \ldots, x_n)$ and $x^* = (x_1^*, x_2^*, \ldots, x_n^*)$.
- E.g., $w = x_1 x_2^*$.
- Involution: similar to a complex conjugation on sequences of letters.
- A polynomial is a linear combination of words $p = \sum_w p_w w$.
- Hermitian moment matrix.
- Hermitian variables.
- Versus commutative case.

The Target SDP

We replace the optimization problem (1) by the following SDP:

$$\begin{aligned} \min_{y} \quad & \sum_w p_w y_w \\ \text{s.t.} \quad & M(y) \succeq 0, \\ & M(g_i y) \succeq 0, i = 1, \ldots, r. \end{aligned} \tag{3}$$

- A truncated Hankel matrix.

Pironio, S.; Navascués, M. & Acín, A. Convergent relaxations of polynomial optimization problems with noncommuting variables. *SIAM Journal on Optimization*, SIAM, 2010, 20, 2157–2180.

The Complexity of Translation

- Generating the moment and localizing matrices is not a trivial task.
- The number of words – the monomial basis – grows exponentially in the order of relaxation.
- The number of elements in the moment matrix is the square of that.

Commutative Examples

- SparsePOP
  - Approximative, up to 1,000 variables in optimal cases.
- Gloptipoly 3.
- Philipp Rostalski's convex algebraic geometry package.

Supporting Libraries

- Efficient noncommutative symbolic operations
  - Undocumented and dying feature in Yalmip (Matlab).
  - SymPy and its quantum physics extension.
  - SymbolicC++.
  - NCAlgebra in Mathematica.
  - Singular, GAP, etc.

The Kinds of SDPs

- Equality constraints
  - Solving the equalities is less efficient.
- Structural Sparsity
- Sparsity in the generated SDP

Reduce the Monomial Basis

- We often encounter equality constraints of the following form:
  - $a + b = 0$, where a and b are monomials.
- Remove a from the monomial basis, and substitute it with $-b$ when encountered.

Toy Example: Polynomial Optimization

Consider the following polynomial optimization problem:

$$\min_{x\in\mathbb{R}^2} 2x_1x_2$$

such that

$$-x_2^2 + x_2 + 0.5 \geq 0$$

$$x_1^2 - x_1 = 0.$$

Toy Example: Corresponding SDP

$$\min_y 2y_{12}$$

such that

$$\left[\begin{array}{c|cc|ccc} 1 & y_1 & y_2 & y_{11} & y_{12} & y_{22} \\ \hline y_1 & y_{11} & y_{12} & y_{111} & y_{112} & y_{122} \\ y_2 & y_{12} & y_{22} & y_{112} & y_{122} & y_{222} \\ \hline y_{11} & y_{111} & y_{112} & y_{1111} & y_{1112} & y_{1122} \\ y_{12} & y_{112} & y_{122} & y_{1112} & y_{1122} & y_{1222} \\ y_{22} & y_{122} & y_{222} & y_{1122} & y_{1222} & y_{2222} \end{array}\right] \succeq 0$$

$$\left[\begin{array}{c|cc} -y_{22}+y_2+0.5 & -y_{122}+y_{12}+0.5y_1 & -y_{222}+y_{22}+0.5y_2 \\ \hline -y_{122}+y_{12}+0.5y_1 & -y_{1122}+y_{112}+0.5y_{11} & -y_{1222}+y_{122}+0.5y_{12} \\ -y_{222}+y_{22}+0.5y_2 & -y_{1222}+y_{122}+0.5y_{12} & -y_{2222}+y_{222}+0.5y_{22} \end{array}\right] \succeq 0.$$

$$\left[\begin{array}{c|cc} y_{11}-y_1 & y_{111}-y_{11} & y_{112}-y_{12} \\ \hline y_{111}-y_{11} & y_{1111}-y_{111} & y_{1112}-y_{112} \\ y_{112}-y_{12} & y_{1112}-y_{112} & y_{1122}-y_{122} \end{array}\right] = 0.$$

Toy Example: Reduced SDP

$$\min_{y} 2y_{12}$$

such that

$$\left[\begin{array}{c|cc|cc} 1 & y_1 & y_2 & y_{12} & y_{22} \\ \hline y_1 & y_1 & y_{12} & y_{12} & y_{122} \\ y_2 & y_{12} & y_{22} & y_{122} & y_{222} \\ \hline y_{12} & y_{12} & y_{122} & y_{122} & y_{1222} \\ y_{22} & y_{122} & y_{222} & y_{1222} & y_{2222} \end{array}\right] \succeq 0$$

$$\left[\begin{array}{c|cc} -y_{22}+y_2+0.5 & -y_{122}+y_{12}+0.5y_1 & -y_{222}+y_{22}+0.5y_2 \\ \hline -y_{122}+y_{12}+0.5y_1 & -y_{122}+y_{12}+0.5y_1 & -y_{1222}+y_{122}+0.5y_{12} \\ -y_{222}+y_{22}+0.5y_2 & -y_{1222}+y_{122}+0.5y_{12} & -y_{2222}+y_{222}+0.5y_{22} \end{array}\right] \succeq 0.$$

Fast Monomial Substitution

- Noncommutative symbolic libraries come with substitution routines.
- They are prepared for all eventualities.
- We know what monomials look like.
- Substitution routine can be tuned accordingly.

Ground-state Energy

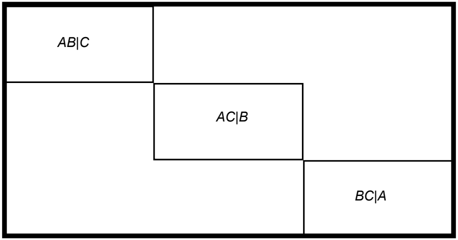
The constraints are simple:

$$\begin{aligned} \{c_r, c_s^\dagger\} &= \delta_{rs} I_r \\ \{c_r, c_s\} &= 0. \end{aligned}$$

- Most of these are monomial substitutions.
- The number of actual equalities is linear.

Multipartite Correlations

- $[M^{AB|C}_{c|z}, M^{AB|C}_{c'|z'}] = 0.$
- Notice the independence of algebras.
- Reduce the size of the moment matrix.



Mutually Unbiased Bases

- $[\Pi_i^x O_1 \Pi_i^x, \Pi_i^x O_2 \Pi_i^x] = 0$ implies over 34 billion constraints for $D = 6$, $K = 4$.
- Constant number of equalities: $\sum_{i=1}^{d} \Pi_i^x = \mathbb{I}$.
- The rest are all monomial substitutions.

We Cannot Change the Complexity

- We can make wise decisions in the implementation.
- SDP wrapper libraries will not generate sufficiently sparse SDPs: Yalmip, CvxOpt, PICOS.
- Re-implementation from symbolic manipulations.
- Choose your interpreter wisely: Pypy.

Memory Use

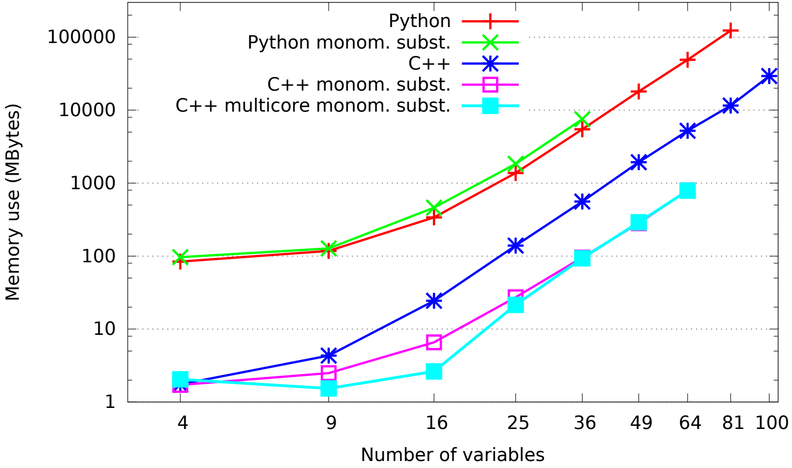


Figure : Memory use of different implementations (log log scale).

Running time

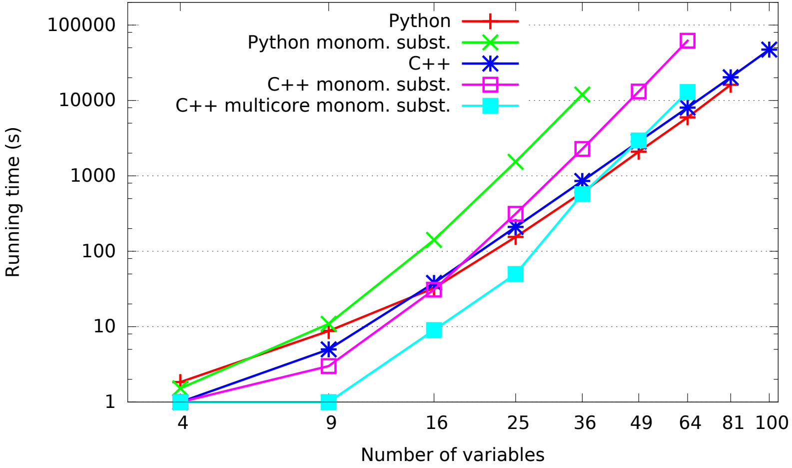


Figure : Running time of different implementations (log log scale).

Parallelization

- Not all programming languages parallelize easily.
- Internal symmetries of the moment matrix imply data dependencies.
- Race conditions exist.
- Only calculating the moment matrix is hard to parallelize.

Solving the SDPs

- Target solver: SDPA.
- Accepts sparse file format.
- Parallel and distributed.
- Accelerated by GPUs: Fujisawa, K.; Sato, H.; Matsuoka, S.; Endo, T.; Yamashita, M. & Nakata, M. High-performance general solver for extremely large-scale semidefinite programming problems. *Proceedings of SC-12, International Conference on High Performance Computing, Networking, Storage and Analysis*, 2012, 93:1–93:11.

Where the SDPs Go Wrong

- Generating the SPDs is not flawless.
- Toy example works.
- Calculating the ground-state energy of systems of harmonic oscillators works.
- Multipartite entanglement, MUBs, more involved Hamiltonians still have problems.

Summary

- http://arxiv.org/abs/1308.6029
- GitHub repositories: ncpol2sdpa, multipartite_entanglement, ncpol2sdpa-cpp.
- Problems in this domain imply sparse structures.
- Scalability to real-world problems: hundred noncommuting variables with quadratic numbers of constraints.
- Limitations apply.