Non-commutative polynomial optimization and the variational RDM method

Antonio Acín[1] Artur Garcia[1]
Miguel Navascués[2] Stefano Pironio[3]

[1]ICFO, Barcelona
[2]Imperial College, London
[3] GAP, Geneva

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Outlook

RDM method:
N-representability of the 2-RDM $\rightarrow$ positivity constraints.
$\Rightarrow$ Semidefinite programming can be used to compute electronic energy of atoms and molecules.

This talk: The SDP-based RDM method is a special case of a more general and abstract approach (not motivated by N-representability).

- We have introduced a method to solve *non-commutative polynomial optimization* problems.
- Computing the energy of a system of N electrons is an instance of these optimization problems.
- When applying our method to this particular instance, we recover the RDM method.

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Variational approach

Introduce finite set of R basis functions (orbitals)

$$\phi_1(\mathbf{r}), \phi_2(\mathbf{r}), \ldots, \phi_R(\mathbf{r})$$

and expand the N-electron wave-function $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ as

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_{j_1 \ldots j_N} c_{j_1 \ldots j_N} \, \phi_{j_1}(\mathbf{r}_1) \ldots \phi_{j_N}(\mathbf{r}_N) \, .$$

The corresponding Hamiltonian is

$$H = \sum_{ij} H_{ij} a_i^\dagger a_j + \sum_{ijkl} H_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

where a_i, $a_i^\dagger$ are the annihilation and creation operators associated to orbital ϕ_i.

Energy is determined by the 2-RDM

$$
\begin{aligned}
E = \langle H \rangle &= \sum_{ij} H_{ij} \langle a_i^\dagger a_j \rangle + \sum_{ijkl} H_{ijkl} \langle a_i^\dagger a_j^\dagger a_k a_l \rangle \\
&= \sum_{ij} H_{ij}\, {}^1D_{ij} + \sum_{ijkl} H_{ijkl}\, {}^2D_{ijkl}
\end{aligned}
$$

where ${}^1D$ and ${}^2D$ are the one-particule and two-particule reduced density matrices defined by

$$ {}^1D_{ij} = \langle a_i^\dagger a_j \rangle $$

$$ {}^2D_{ijkl} = \langle a_i^\dagger a_j^\dagger a_k a_l \rangle $$

Note that ${}^1D_{ij} = (N-1) \sum_k {}^2D_{ikkj}$.

N-representability problem

Ground state energy:

$$E_g = \min_{{}^2D} \left\{ \sum_{ij} H_{ij}\, {}^1D_{ij} + \sum_{ijkl} H_{ijkl}\, {}^2D_{ijkl} \right\}$$

N-representability problem

Ground state energy:

$$E_g = \min_{^2D} \left\{ \sum_{ij} H_{ij} \, {}^1D_{ij} + \sum_{ijkl} H_{ijkl} \, {}^2D_{ijkl} \right\}$$

Problem: this yields an energy far lower than the exact ones because not every 2-particule density matrix ${}^2D$ originates from a N-particle wavefunction $|\psi\rangle$.

We must impose N-representability conditions on ${}^2D$

Necessary N-representability conditions

1. Positivity conditions [Coleman 63, Garrod and Percus 64]:
   - ${}^1D \succeq 0$, ${}^1Q \succeq 0$, where

$$\begin{aligned} {}^1D_{ij} &= \langle a_i^\dagger a_j \rangle \\ {}^1Q_{ij} &= \langle a_i a_j^\dagger \rangle \end{aligned}$$

   - *D, Q, G conditions*: ${}^2D \succeq 0$, ${}^2Q \succeq 0$, ${}^2G \succeq 0$, where

$$\begin{aligned} {}^2D_{ijkl} &= \langle a_i^\dagger a_j^\dagger a_k a_l \rangle \\ {}^2Q_{ijkl} &= \langle a_i a_j a_k^\dagger a_l^\dagger \rangle \\ {}^2G_{ijkl} &= \langle a_i^\dagger a_j a_k^\dagger a_l \rangle \end{aligned}$$

2. Linear conditions that relate all these matrices to ${}^2D$
   For instance:

$${}^1Q_{ij} = \delta_{ij} - {}^1D_{ij} = (N-1)\sum_k {}^2D_{ikkj}$$

$${}^2Q_{ijkl} = \delta_{jk}\,{}^1D_{il} - {}^2D_{ikjl}$$

Ground-state energy from semidefinite programming

Minimization of

$$E = \sum_{ij} H_{ij}\, {}^1D_{ij} + \sum_{ijkl} H_{ijkl}\, {}^2D_{ijkl}$$

subject to the previous positivity and linear constraints is a typical instance of semidefinite programming.

This minimization problem can be solved exactly.

It provides a lower-bound on the ground-state energy.

Higher-order constraints

A whole hierarchy of additional SDP constraints can be added to increase accuracy *[Erdahl, Jin 00], [Mazziotti, Erdahl 01]*.

E.g.: Positivity conditions on the 3-RDMs:

$$
\begin{aligned}
{}^3D_{ijklmn} &= \langle a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n \rangle \\
{}^3E_{ijklmn} &= \langle a_i^\dagger a_j^\dagger a_k a_l^\dagger a_m a_n \rangle \\
{}^3F_{ijklmn} &= \langle a_i^\dagger a_j a_k a_l^\dagger a_m^\dagger a_n \rangle \\
{}^3Q_{ijklmn} &= \langle a_i a_j a_k a_l^\dagger a_m^\dagger a_n^\dagger \rangle
\end{aligned}
$$

Why are all these matrices positive?

- All previous matrices are of the form

$$\begin{aligned} M_{ij} &= \langle \Psi | C_i^\dagger C_j | \Psi \rangle \\ &= \langle v_i | v_j \rangle \end{aligned}$$

 where $|v_i\rangle = C_i|\Psi\rangle$.

 For instance: ${}^2G_{ijkl} = \langle a_i^\dagger a_j a_k^\dagger a_l \rangle = \langle \Psi | C_{ji}^\dagger C_{kl} | \Psi \rangle$
 with $C_{kl} = a_k^\dagger a_l$.

- M is positive semidefinite if and only if $M_{ij} = \langle v_i | v_j \rangle$.

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Non-commutative polynomial optimization

Let $X = \{X_1, \ldots, X_n\}$ be n variables that we view as operators acting on some unspecified Hilbert space H.

Let $p(X), q(X), r(X)$ be polynomials in X.
E.g.: $p(X) = X_1 + 3X_1X_2 - 4X_4X_2$.

We want to solve

$$\begin{array}{cl} \min\limits_{H,X,|\Psi\rangle} & \langle\Psi|p(X)|\Psi\rangle \\ \text{s.t.} & q(X) = 0 \\ & r(X)|\Psi\rangle = 0 \end{array}$$

Note: H is not fixed in advance, $\dim(H)$ is not bounded.

Why *non-commutative* optimization?

If we add the commutativity constraints $X_i X_j + X_j X_i = 0$, the scalar representation $X_i = x_i \in \mathbb{R}$ is always a solution.

The optimization problem is then equivalent to a standard polynomial optimization over $\mathbb{R}^n$

$$\begin{array}{ll} \min\limits_{x \in \mathbb{R}^n} & p(x) \\ \text{s.t.} & q(x) = 0 \\ & r(x) = 0 \end{array}$$

Solving NCPO through semidefinite programming

In arXiv:0903.4368, we introduce a sequence of relaxations R_i that provide lower-bounds on the global solution of the original NCPO problem.

Each of these relaxations R_i is a semidefinite program.

In the limit $R_i \to R_\infty$, the lower-bounds converge to the global solution of NCPO.

Notation

Monomials

- Given the n operators $X_1, \ldots, X_n$,
  a monomial X_α of degree k is a product of k operators X_i:

$$X_\alpha = X_{\alpha_1} X_{\alpha_2} \ldots X_{\alpha_k}$$

- We denote the identity operator I as the monomial $X_0 = I$.
- The product of two monomials $X_\alpha X_\beta$ is itself a monomial that we denote $X_{\alpha\beta} = X_\alpha X_\beta$.

Polynomials

A polynomial $p(X)$ is a linear combination of monomials

$$p(X) = \sum_\alpha p_\alpha X_\alpha$$

Construction of the relaxation of degree k

- Consider the set of all vectors of the form

$$\{X_\alpha|\Psi\rangle\} = \{|\Psi\rangle, X_i|\Psi\rangle, X_iX_j|\Psi\rangle, \ldots, (X_{i_1}\ldots X_{i_k})|\Psi\rangle\}$$

where X_α is at most of degree k.

Then the matrix ${}^kM$ with entries

$${}^kM_{\alpha\beta} = \langle\Psi|X_\alpha^\dagger X_\beta|\Psi\rangle$$

is positive definite: ${}^kM \succeq 0$.

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  is positive definite: ${}^kM \succeq 0$.

- The objective function

$$\begin{aligned}\langle\Psi|p(X)|\Psi\rangle &= \sum_\alpha p_\alpha\langle\Psi|X_\alpha|\Psi\rangle \\ &= \sum_\alpha p_\alpha\langle\Psi|X_0^\dagger X_\alpha|\Psi\rangle = \sum_\alpha p_\alpha\, {}^kM_{0\alpha}\end{aligned}$$

  is a linear function of the entries of ${}^kM$

Construction of the relaxation of degree k

- The conditions $q(X) = 0$ and $r(X)|\Psi\rangle = 0$ induce linear constraints on ${}^kM$:

$$q(X) = \sum_\nu q_\nu X_\nu = 0 \quad \Rightarrow \quad \sum_\nu q_\nu \langle\Psi|X_\alpha^\dagger X_\nu X_\beta|\Psi\rangle = 0 \quad \forall\alpha,\beta$$

$$\sum_\nu q_\nu \langle\Psi|X_\alpha^\dagger X_{\nu\beta}|\Psi\rangle = 0 \quad \forall\alpha,\beta$$

$$\sum_\nu q_\nu\, {}^kM_{\alpha,\nu\beta} = 0 \quad \forall\alpha,\beta$$

$$r(X)|\Psi\rangle = \sum_\nu r_\nu X_\nu|\Psi\rangle = 0 \quad \Rightarrow \quad \sum_\nu r_\nu \langle\Psi|X_\alpha^\dagger X_\nu|\Psi\rangle = 0 \quad \forall\alpha$$

$$\sum_\nu r_\nu\, {}^kM_{\alpha,\nu} = 0 \quad \forall\alpha$$

Relaxation of degree k

We define the relaxation R_k of degree k as the following SDP:

$$\begin{array}{ll} \min\limits_{{}^kM} & \sum_\alpha p_\alpha \, {}^kM_{0\alpha} \\ \text{s.t.} & {}^kM \succeq 0 \\ & \sum_\nu q_\nu \, {}^kM_{\alpha,\nu\beta} = 0 \quad \forall \alpha, \beta \\ & \sum_\nu r_\nu \, {}^kM_{\alpha,\nu} = 0 \quad \forall \alpha \end{array}$$

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Let p_k be the solution of R_k
and $p_\star$ be the solution of the original NCPO problem, then

$$p_k \leq p_{k+1} \leq \ldots \leq p_\star$$

Results

- If $q(X) = 0$ implies that $\|X_i\|_2 \leq C$:

$$\lim_{k \to \infty} p_k = p_\star$$

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$$\lim_{k\to\infty} p_k = p_\star$$

- In practice, we observe very often that R_2, R_3, or R_4 already yield the optimal solution $p_\star$

- Stopping criterion: if $\operatorname{rank} {}^kM = \operatorname{rank}^{k-1}\left({}^kM\right)$:
  - $p_k = p_\star$
  - the optimal $|\Psi\rangle$ and X live
    in a Hilbert space H of $\dim(H) = \operatorname{rank} {}^kM$.
  - We have a procedure to reconstruct the optimal $|\Psi\rangle$ and X.

Method is related to other mathematical techniques

- $$\begin{array}{ll} \min\limits_{H,X,|\Psi\rangle} & \langle\Psi|p(X)|\Psi\rangle \\ \text{s.t.} & q(X) = 0 \\ & X_iX_j - X_jX_i = 0 \end{array} \quad \Leftrightarrow \quad \begin{array}{ll} \min\limits_{x\in\mathbb{R}^n} & p(x) \\ \text{s.t.} & q(x) = 0 \end{array}$$

  $\rightarrow$ Recover the SDP method for scalar polynomial optimization of *[Parrilo 00, Lasserre 01]*.

- Dual formulation of the SDP relaxations linked to the theory of SOS decompositions of positive polynomials *[Putinar 93, Helton and McCullough 04]*.

Contents

Electronic energy as NCPO

The ground-state energy of N e$^-$ that can occupy R orbitals is the solution to the following NCPO with operator variables $\{a_1, \ldots, a_r, a_1^\dagger, \ldots, a_r^\dagger\}$

$$\begin{array}{ll} \min & \sum_{ij} H_{ij} \langle \Psi | a_i^\dagger a_j | \Psi \rangle + \sum_{ijkl} H_{ijkl} \langle \Psi | a_i^\dagger a_j^\dagger a_k a_l | \Psi \rangle \\ \text{s.t.} & \{a_i, a_j\} = 0 \\ & \{a_i^\dagger, a_j^\dagger\} = 0 \\ & \{a_i^\dagger, a_j\} - \delta_{ij} = 0 \\ & \sum_i \left(a_i^\dagger a_i - N \right) |\Psi\rangle = 0 \end{array}$$

Example: relaxation of degree 2

Remember: matrix ${}^{k}M$ is built as overlap matrix of set of vectors $\{X_\alpha|\Psi\rangle\}$ where X_α is at most of degree k.

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In our case ${}^{2}M$ is thus built on set of vectors

$$\{|\Psi\rangle, a_i|\Psi\rangle, a_i^\dagger|\Psi\rangle, a_i a_j|\Psi\rangle, a_i^\dagger a_j^\dagger|\Psi\rangle, a_i^\dagger a_j|\Psi\rangle, a_i a_j^\dagger|\Psi\rangle\}$$

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General property

It is sufficient to consider set of vectors $\{X_\alpha|\Psi\rangle\}$ that are linearly independent under the constraints $q(X) = 0$, $r(X)|\Psi\rangle = 0$

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General property

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Thus since $a_i^\dagger a_j + a_j a_i^\dagger - \delta_{ij} = 0$ and $\sum_i \left(a_i^\dagger a_i - N\right)|\Psi\rangle = 0$, it is sufficient to consider set

$$\{a_i|\Psi\rangle, a_i^\dagger|\Psi\rangle, a_i a_j|\Psi\rangle, a_i^\dagger a_j^\dagger|\Psi\rangle, a_i^\dagger a_j|\Psi\rangle\}$$

Example: relaxation of degree 2

$$
{}^2M = \begin{array}{c|ccccc}
 & a_i\rangle & a_i^\dagger\rangle & a_i a_j\rangle & a_i^\dagger a_j^\dagger\rangle & a_i^\dagger a_j\rangle \\
\hline
\langle a_k^\dagger & \langle a_k^\dagger a_i\rangle & \langle a_k^\dagger a_i^\dagger\rangle & \langle a_k^\dagger a_i a_j\rangle & \langle a_k^\dagger a_i^\dagger a_j^\dagger\rangle & \langle a_k^\dagger a_i^\dagger a_j\rangle \\
\langle a_k & & \langle a_k a_i^\dagger\rangle & \langle a_k a_i a_j\rangle & \langle a_k a_i^\dagger a_j^\dagger\rangle & \langle a_j a_i^\dagger a_j\rangle \\
\langle a_k^\dagger a_l^\dagger & & & \langle a_k^\dagger a_l^\dagger a_i a_j\rangle & \langle a_k^\dagger a_l^\dagger a_i^\dagger a_j^\dagger\rangle & \langle a_k^\dagger a_l^\dagger a_i^\dagger a_j\rangle \\
\langle a_k a_l & & & & \langle a_k a_l a_l^\dagger a_i^\dagger a_j^\dagger\rangle & \langle a_k a_l a_i^\dagger a_j\rangle \\
\langle a_k^\dagger a_l & & & & & \langle a_k^\dagger a_l a_i^\dagger a_j\rangle
\end{array}
$$

Example: relaxation of degree 2

Linear constraints on ${}^kM$ which follow from

- the conditions $q(X) = \sum_\nu q_\nu X_\nu = 0$:

$$\sum_\nu q_\nu \langle X_\alpha^\dagger X_\nu X_\beta \rangle = 0 \quad \forall \alpha, \beta$$

  For instance: $q(X) = \{a_i^\dagger, a_j\} - \delta_{ij}$, $X_\alpha = a_k^\dagger$, $X_\beta = a_l$

$$\Rightarrow \langle a_k^\dagger a_i^\dagger a_j a_l \rangle + \langle a_k^\dagger a_j a_i^\dagger a_l \rangle - \delta_{ij} \langle a_k^\dagger a_l \rangle = 0$$

- and the conditions $r(X)|\Psi\rangle = \sum_\nu r_\nu X_\nu |\Psi\rangle = 0$:

$$\sum_\nu q_\nu \langle X_\alpha^\dagger X_\nu \rangle = 0 \quad \forall \alpha$$

  For instance: $r(X) = \sum_i \left(a_i^\dagger a_j - N \right)$, $X_\alpha = a_k a_l$:

$$\Rightarrow \sum_i \langle a_k a_l a_i^\dagger a_i \rangle - N \langle a_k a_l \rangle = 0$$

Example: relaxation of degree 2

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{}^2M = \begin{array}{c|ccccc}
 & a_i\rangle & a_i^\dagger\rangle & a_i a_j\rangle & a_i^\dagger a_j^\dagger\rangle & a_i^\dagger a_j\rangle \\
\hline
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 & & & & &
\end{array}
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\hline
\langle a_k^\dagger & {}^1D & & & & \\
\langle a_k & & {}^1Q & & & \\
\langle a_k^\dagger a_l^\dagger & & & {}^2D & & \\
\langle a_k a_l & & & & {}^2Q & \\
\langle a_k^\dagger a_l & & & & & {}^2G \\
 & & & & &
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+ Linear relations between ${}^1D$, ${}^1Q$, ${}^2D$, ${}^2Q$, ${}^2G$

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 & & & & &
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$$

+ Linear relations between ${}^1D$, ${}^1Q$, ${}^2D$, ${}^2Q$, ${}^2G$

We recover the same SDP than in the RDM method

Electronic energy as NCPO

Similarly, relaxations of higher-degree of the problem

$$\begin{array}{ll} \min & \sum_{ij} H_{ij}\langle\Psi|a_i^\dagger a_j|\Psi\rangle + \sum_{ijkl} H_{ijkl}\langle\Psi|a_i^\dagger a_j^\dagger a_k a_l|\Psi\rangle \\ \text{s.t.} & \{a_i, a_j\} = 0 \\ & \{a_i^\dagger, a_j^\dagger\} = 0 \\ & \{a_i^\dagger, a_j\} - \delta_{ij} = 0 \\ & \sum_i \left(a_i^\dagger a_i - N\right)|\Psi\rangle = 0 \end{array}$$

correspond to implementing higher-order positivity N-representability constraints of the RDM method.

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correspond to implementing higher-order positivity N-representability constraints of the RDM method.

Note that here

$$p_2 \leq p_3 \leq \ldots p_N = p_\star$$

Contents

Quantum violation of Bell inequalities

Original motivation for our method *[PRL 07, NJP 08]*

$$
\begin{array}{ll}
\min & \sum_{abxy} c_{abxy} \langle \Psi | E_a^x E_b^y | \Psi \rangle \\
\text{s.t.} & E_a^x E_{a'}^x = \delta_{aa'} E_a^x \quad \text{and} \quad \sum_a E_a^x = I \\
 & E_b^y E_{b'}^y = \delta_{bb'} E_b^y \quad \text{and} \quad \sum_b E_b^y = I \\
 & [E_a^x, E_b^y] = 0
\end{array}
$$

The dimension of H is not bounded

Quantum violation of Bell inequalities

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 & [E_a^x, E_b^y] = 0
\end{array}$$

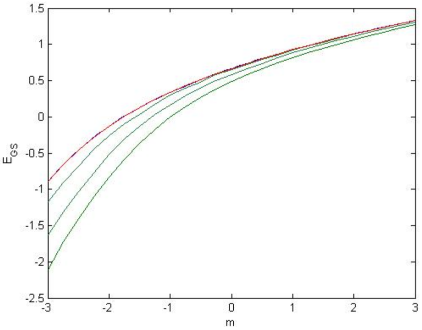
The dimension of H is not bounded

Has been applied to 241 Bell inequalities in *[Pal, Vertesi 08]*
Optimal solution obtained for 221 Bell inequalities
For the remaining 20 ones: gap between our LB and best known UB is of order 10^{-4}.

Other applications

- Security of device-independent cryptography ✓
- Continuous variable system ✓
  Particle in a double-well potential:

$$\begin{array}{ll} \min & \frac{p^2}{2} + \frac{x^2}{2} + mx^4 \\ \text{s.t.} & [x, p] = i \end{array}$$



- ...

Conclusion

Similar techniques than the ones in the SDP RDM method allow to solve a broad class of non-commutative polynomial optimization problems.

Interest of our method for solving NCPO:

- Flexible and works on different problems
- Yields lower-bounds
- Does not rely on symmetries (good for quantum chemistry)
- Allows to deal with infinite Hilbert space
  without truncating the Hilbert space