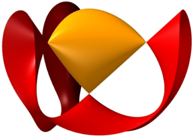
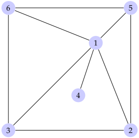
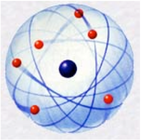
Large-scale noncommutative optimization & applications to quantum information

Victor Magron, MAC Team

Workshop Technologies Quantiques, LAAS
10 March 2021

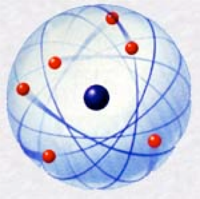




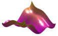


General idea

Verification/analysis of quantum systems



. . . CAST AS CERTIFIED OPTIMIZATION ⇝ SOLVE **OFFLINE**

Input: linear (LP)  semidefinite (SDP)  polynomial 

Output: value + **certificate**

Motivation: entanglement

Entanglement in quantum mechanics
$\rightarrow$ **upper bounds** for violation levels of Bell inequalities

Conditional probabilities $p(i, j)$ generated by Alice & Bob after performing measurements on a shared entangled state

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$p(i, j) = \mathbf{v} x_i y_j \mathbf{v}$ for unit $\mathbf{v}$ & self-adjoint (projection) x_i, y_j
Finding violation $\rightarrow$ solving a **maximal** eigenvalue problem!

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[Pozas et al 19] extension $\rightarrow$ identify correlations not attainable in entanglement-swapping scenario (quantum teleportation)

quantum physics operators x_i, y_j satisfy causal constraints:

$$\operatorname{trace}(x_1 x_2 y_1 y_2) - \operatorname{trace}(x_1 x_2) \operatorname{trace}(y_1 y_2) = 0.$$

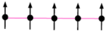
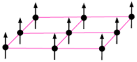
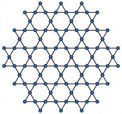
Motivation: condensed matter

Ground-state energy $\Leftrightarrow$ minimal eigenvalue of an Hamiltonian

$$H = \sum_{\langle i,j \rangle} \left(x_i \, x_j + y_i \, y_j + z_i \, z_j \right)$$

spin states (x_i, y_i, z_i), constraints

Lattices: 1D 2D Kagome

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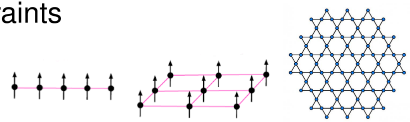

First neighbors interactions : $H = \sum_{i=1}^{n} x_i x_{i+1} + y_i y_{i+1} + z_i z_{i+1}$

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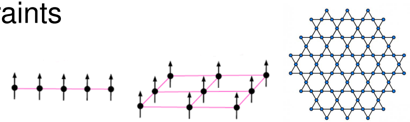

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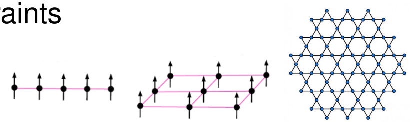

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Existing ± efficient techniques: quantum Monte Carlo & variational algorithms ⇒ **upper bounds** on minimal energy

Noncommutative (NC) Polynomials

Polynomials in symmetric **matrix** variables x_i, y_j

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$\mathbf{I}_{3322}$ Bell inequality:

$$f = x_1(y_1 + y_2 + y_3) + x_2(y_1 + y_2 - y_3) + x_3(y_1 - y_2) - x_1 - 2y_1 - y_2$$

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MINIMAL EIGENVALUE OPTIMIZATION

$$\lambda_{\min} = \inf \{\langle f(x, y)\mathbf{v}, \mathbf{v}\rangle : (x, y) \in \mathbf{K}, \|\mathbf{v}\| = 1\}$$

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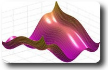
Sums of squares hierarchies

NP-hard NON CONVEX Problem $f^\star = \inf f(\mathbf{x})$

Theory



INFINITE LP $\Leftarrow$ with

$$\begin{aligned} \sup \quad & \lambda \\ \text{with} \quad & f - \lambda \geqslant 0 \end{aligned}$$

Sums of squares hierarchies

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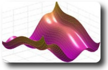
Practice



with $f - \lambda =$ **sum of squares**

CONVEX $\Leftarrow$ **fixed** degree

HIERARCHY of **CONVEX** (semidefinite) **PROBLEMS** $\uparrow f^*$
[Lasserre/Parrilo 01]
[Navascués-Pironio-Acín 08] for NC problems

✗ degree d & n vars $\Longrightarrow n^{2d}$ variables

✓ Relaxations $\Longrightarrow$ **certified lower bounds**

What can you do with hierarchies?

Modeling Power

$$f = x^2 - 2xy + 3y^2 - 2x^2y + 2x^2y^2 - 2yz + 6z^2 + 18y^2z - 54yz^2 + 142y^2z^2$$

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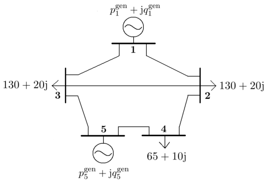
💡 f = sum of squares $\Rightarrow \inf f \geqslant 0$

💡 LARGE-SCALE **Polynomial Optimization**

Optimal Powerflow $n \simeq \mathbf{10^3}$ [Josz et al 16]

$<1\%$ optimal solution [Magron & Wang 21]

Roundoff Error $n \simeq \mathbf{10^2}$ [Magron et al 17]



Contribution: modeling & scalability

Modeling

Symmetric NC variables x, y & sums of product traces

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💡 minimal eigenvalue/trace

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SCALABILITY

Large-scale sparse NC problems with $n = 10^2 - 10^3$ variables

Software libraries NCTSSOS $\Rightarrow$ condensed matter

Extensive use of HPC cluster PFCALUL at LAAS

Noncommutative (NC) Polynomials

Contribution: modeling & scalability

Sparse Polynomial Optimization

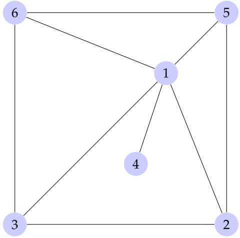
Ongoing collaborations

Sparse Polynomial Optimization [Waki, Lasserre 06]

- Correlative (variable) sparsity

$$f = x_2 x_5 + x_3 x_6 - x_2 x_3 - x_5 x_6 + x_1(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6)$$

Chordal graph G



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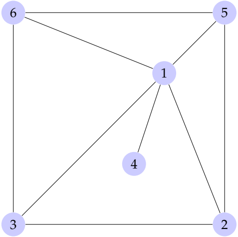


$C_1 = \{1, 4\}$

$C_2 = \{1, 2, 3, 5\}$

$C_3 = \{1, 3, 5, 6\}$

Dense: 210 variables

Sparse: 115 variables

1. Maximal cliques C_k
2. Average size $\kappa \rightsquigarrow \kappa^{2d}$ variables

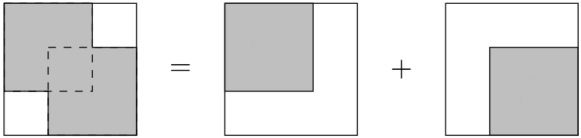
Sparse Polynomial Optimization [Waki, Lasserre 06]

Theorem [Griewank-Toint 84]

Chordal graph G with maximal cliques C_1, C_2

$Q_G \succcurlyeq 0$ with nonzero entries at edges of G

$\Longrightarrow$ $Q_G = {P_{C_1}}^T Q_1 P_{C_1} + {P_{C_2}}^T Q_2 P_{C_2}$ with $Q_k \succcurlyeq 0$ indexed by C_k



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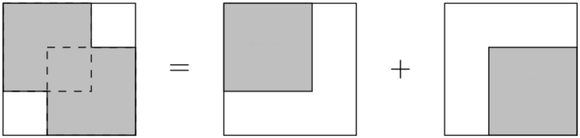

Sparse $f = f_1 + f_2$ where f_k involves **only** variables in C_k

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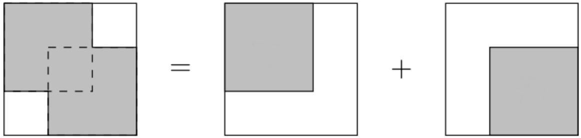

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Theorem: Sparse sums of squares [Waki 06]

f sum of squares + chordal graph G with cliques C_k

$\Longrightarrow \ \boxed{f = \sigma_1 + \sigma_2}$ with σ_k sum of squares involving vars in C_k

Sparse Examples

Generalized Rosenbrock function:

$$f = 1 + \sum_{i=1}^{n-1} \left(100(x_{i+1} - x_i^2)^2 + (1 - x_{i+1})^2\right)$$

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Exploiting term sparsity [Magron-Wang 20-21]

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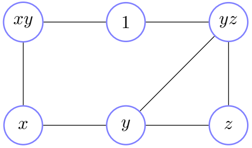
💡 **Term** sparsity pattern graph G



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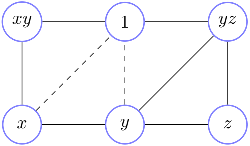
Term sparsity pattern graph G

Chordal extension



Replace Q by Q_G with nonzero entries at edges of G

$\rightsquigarrow$ 6 + 9 = 15 “unknown” entries in Q_G

I_{3322} Bell Inequality

→ **upper bounds** on $\lambda_{\max}$ of f on $\mathbf{K}$

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level	sparse	dense [Pál-Vértesi 18]
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3'		0.2508754

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$\mathbf{I}_{3322}$ Bell inequality

$$f = x_1(y_1 + y_2 + y_3) + x_2(y_1 + y_2 - y_3) + x_3(y_1 - y_2) - x_1 - 2y_1 - y_2$$

$\mathbf{K} = \{(x, y) : x_i^2 = x_i, y_j^2 = y_j, x_i y_j = y_j x_i\}$

💡 $C_k \rightarrow \{x_1, x_2, x_3, y_k\}$

level	sparse	dense [Pál-Vértesi 18]
2	0.2550008	0.2509397
3	0.2511592	0.2508756
3’		0.250854
4	0.2508917	

I_{3322} Bell Inequality

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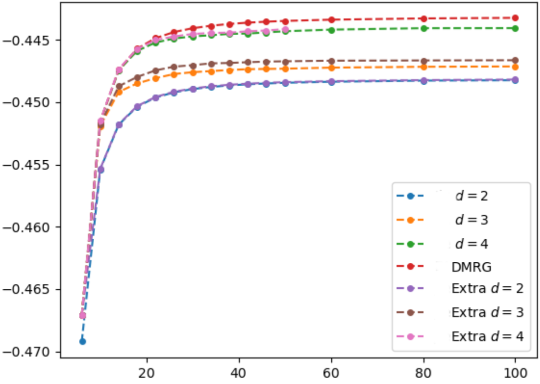
6	0.2508753977180	!!!!!

An example from condensed matter

Hamiltonian ground-state energy 1D lattice 



Dense $d = 4$, $n = 10^2 \Rightarrow 10^{19}$ variables (solvers handle $\simeq 10^4$)

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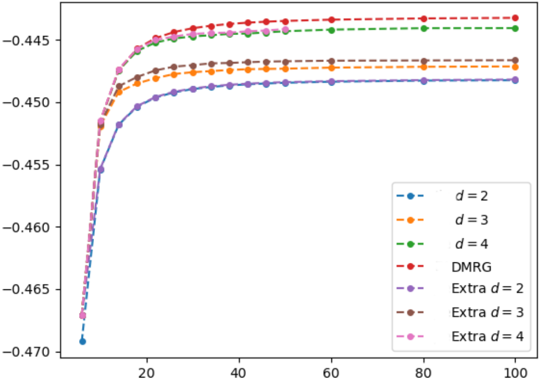

Dense $d = 4$, $n = 10^2 \Rightarrow 10^{19}$ variables (solvers handle $\simeq 10^4$)

Sparse solved in $\simeq$ 1 hour on PFCALCUL at LAAS

Conclusion and Perspectives

EFFICIENT tool, new applications of correlative/term sparsity

- **Symmetric** noncommutative problems?
- **Sparsity** for trace polynomials $\rightsquigarrow$ Werner witnesses

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EFFICIENT tool, new applications of correlative/term sparsity

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APPLICATIONS IN QUANTUM PHYSICS

- Quantum games: number of mutually unbiased bases in dim 6, OPEN FOR SEVERAL DECADES! 💡 **symmetric**
- Ground state energy of hamiltonians 💡 **symmetric** & **sparse**
- Inflation for quantum correlations 💡 **symmetric** & **sparse**
- Werner witnesses 💡 **symmetric** & **sparse**

Ongoing collaborations

PROJECT: MODELING AND SCALABILITY

LAAS MAC D. Henrion, M. Korda & J.-B. Lasserre
IRSAMC, LPT I. Nechita
IMT S. Belinschi

ICFO, Barcelona Acín's group (submitted proposal at Institut Quantique Occitan)
U. Ljubljana I. Klep & J. Povh (PHC funding)
U. Krakow F. Huber

Mini-symposium accepted with I. Klep *Computational aspects of commutative and noncommutative positive polynomials* at EUROPEAN CONGRESS OF MATHEMATICIANS

Thank you for your attention!

https://homepages.laas.fr/vmagron

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