Exploiting Correlative and Term Sparsity in Noncommutative Polynomial Optimization

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Joint work with Igor Klep, Janez Povh and Jie Wang

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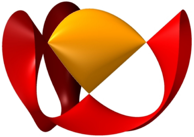

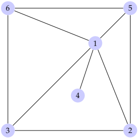

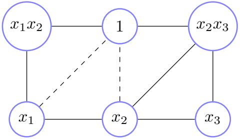

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Symmetric noncommutative variables $\underline{x} = (x_1, \ldots, x_n)$

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with $x_1 x_2 \neq x_2 x_1$, **involution** $(x_1 x_2)^\star = x_2 x_1$

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sums of hermitian squares (SOHS): $f^\star f$ hermitian square

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$S \subset \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ $\quad X_j \in$ finite von Neumann algebra

Constraints: $\mathcal{D}_S = \{ \underline{X} = (X_1, \ldots, X_n) : s(\underline{X}) \succcurlyeq 0, \quad \forall s \in S \}$

Motivation: quantum information

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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[Werner '89] Werner witnesses to separate pure/entangled states

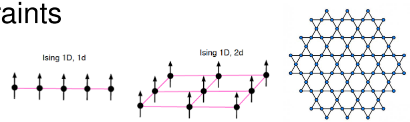
Motivation: condensed matter

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

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

spin states (x_i, y_i, z_i), constraints

Lattices: 1D 2D Kagome



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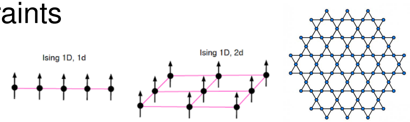

First neighbors interactions : $f = \sum_{i=1}^{n} x_i x_{i+1} + y_i y_{i+1} + z_i z_{i+1}$

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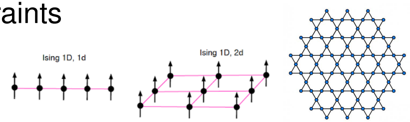

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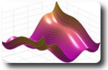
Existing $\pm$ efficient techniques: quantum Monte Carlo & variational algorithms $\Rightarrow$ **upper bounds** on minimal energy

Fighting the scalability issue

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

Theory



$$\sup \quad \lambda$$

INFINITE LP $\Leftarrow$ with $\quad f - \lambda \geqslant 0$

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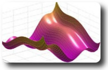
Practice



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

FINITE SDP $\Leftarrow$ **fixed** degree

HIERARCHY of **CONVEX** (semidefinite) **PROBLEMS** $\uparrow f_{\min}$

[Lasserre '01]

[Navascués Pironio Acín '08] for NC problems

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

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

Moment-sums of squares hierarchies

Correlative sparsity

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Commutative Polynomial Optimization

NP hard General Problem: $f_{\min} := \min_{\mathbf{x} \in \mathcal{D}_S} f(\mathbf{x})$

Semialgebraic set $\mathcal{D}_S = \{\mathbf{x} \in \mathbb{R}^n : s_j(\mathbf{x}) \geqslant 0\}$

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$$\overbrace{x_1 x_2}^{f} =$$

$$-\frac{1}{8} + \overbrace{\frac{1}{2}\left(x_1 + x_2 - \frac{1}{2}\right)^2}^{\sigma_0} + \overbrace{\frac{1}{2}}^{\sigma_1} \overbrace{x_1(1-x_1)}^{s_1} + \overbrace{\frac{1}{2}}^{\sigma_2} \overbrace{x_2(1-x_2)}^{s_2}$$

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Quadratic module: $\mathcal{M}(S)_d = \left\{ \sigma_0 + \sum_j \sigma_j s_j, \ \deg \sigma_j \, s_j \leqslant 2d \right\}$

Hierarchies for Polynomial Optimization

Hierarchy of SDP relaxations:

$$\lambda_d := \sup_{\lambda} \left\{ \lambda : f - \lambda \in \mathcal{M}(S)_d \right\}$$

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Can be computed with SDP solvers (`CSDP`, `SDPA`, `MOSEK`)

"No Free Lunch" Rule: $\binom{n+2r}{n}$ SDP variables

Eigenvalue optimization

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Theorem: NC Putinar's Psatz [Helton-McCullough 02]

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$f - \lambda \mathbf{1} = \sum_i h_i^\star h_i + \sum_j \sum_i t_{ji}^\star s_j t_{ji}$ with h_i, t_{ji} of **bounded** degrees

Trace optimization

$$\mathrm{tr}_{\min} = \inf\{\mathrm{tr}(f(\underline{X})) : \underline{X} \in \mathcal{D}_S\}$$

$$= \sup \quad m$$

$$\text{s.t.} \quad \mathrm{tr}(f(\underline{X}) - m) \geqslant 0\,, \quad \forall \underline{X} \in \mathcal{D}_S$$

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$\mathrm{tr}_{\min}^{\mathrm{II}_1}$ = minimal trace over the union of type $-\,\mathrm{II}_1$ vN algebras

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Converging hierarchy with cyclic quadratic modules:

💡 replace "$\mathrm{tr}(f - m) \geqslant 0$ on $\mathcal{D}_S^{\mathrm{II}_1}$" by $f - m\mathbf{1} \in \mathcal{M}^{\mathrm{cyc}}(S)_d$

$\mathcal{M}^{\mathrm{cyc}}(S)_d$ = polynomials with same trace as some from $\mathcal{M}(S)_d$

Moment-sums of squares hierarchies

Correlative sparsity

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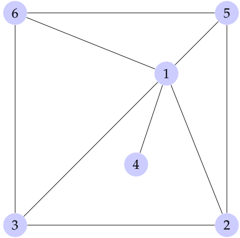
💡 Exploit few links between **variables** [Lasserre, Waki et al. '06]

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

Chordal graph G



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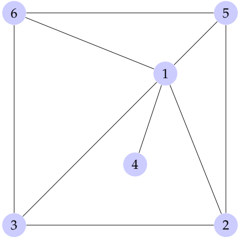


Chordal graph G

maximal cliques I_k

Average size $\kappa \rightsquigarrow \kappa^{2d}$ vars

$I_1 = \{1, 4\}$
$I_2 = \{1, 2, 3, 5\}$
$I_3 = \{1, 3, 5, 6\}$

Dense SDP: 210 vars

Sparse SDP: 115 vars

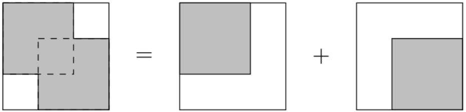
Correlative sparsity

Theorem [Griewank Toint '84]

Chordal graph G with maximal cliques I_1, I_2

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

$\Longrightarrow \; Q_G = {P_1}^T Q_1 P_1 + {P_2}^T Q_2 P_2$ with $Q_k \succcurlyeq 0$ indexed by I_k



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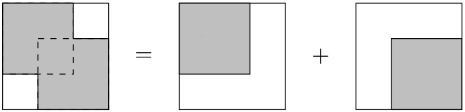

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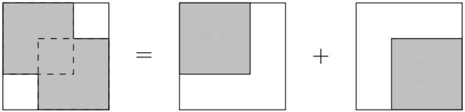

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Theorem: Sparse Putinar's representation [Lasserre '06]

$f > 0$ on $\{\mathbf{x} : s_j(\mathbf{x}) \geqslant 0\}$
chordal graph G with cliques I_k $\Longrightarrow$
ball constraints for each $\mathbf{x}(I_k)$

$$\boxed{f = \sigma_{01} + \sigma_{02} + \sum_j \sigma_j s_j}$$

SOS σ_{0k} "sees" vars in I_k
σ_j "sees" vars from s_j

Correlative sparsity

symmetric noncommutative (NC) variables $\underline{x} = (x_1, \ldots, x_n)$

Theorem [Helton-McCullough 02]

$f \succcurlyeq 0 \Leftrightarrow f \in \Sigma$ (all positive polynomials are sums of squares)

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BAD NEWS: there is **no** sparse analog! [Klep Magron Povh '21]

sparse $f \in \Sigma \not\Rightarrow f$ is a sparse SOS

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GOOD NEWS: there is an NC analog of the sparse Putinar's representation! Based on GNS construction & **amalgamation** [Blackadar '78, Voiculescu '85]

Correlative sparsity

symmetric noncommutative (NC) variables $\underline{x} = (x_1, \ldots, x_n)$

Theorem [Helton-McCullough 02]

$f \succcurlyeq 0 \Leftrightarrow f \in \Sigma$ (all positive polynomials are sums of squares)

BAD NEWS: there is **no** sparse analog! [Klep Magron Povh '21]

sparse $f \in \Sigma \not\Rightarrow f$ is a sparse SOS Take $f = (x_1 + x_2 + x_3)^2$

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Theorem [Klep Magron Povh '21]

$f \succ 0$ on $\{\underline{x} : s_j(\underline{x}) \succcurlyeq 0\}$

chordal graph G with cliques I_k $\Longrightarrow$

ball constraints for each $\mathbf{x}(I_k)$

$$f = \sum_{k,i} s_{ki}^{\star} s_{ki} + \sum_{j,i} t_{ji}^{\star} s_j t_{ji}$$

s_{ki} "sees" vars in I_k

t_{ji} "sees" vars from s_j

Correlative sparsity

$\mathbf{I}_{3322}$ Bell inequality (entanglement in quantum information)

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

Maximal violation levels $\rightarrow$ **upper bounds** on $\lambda_{\max}$ of f on $\{(x, y) : x_i^2 = x_i, y_j^2 = y_j, x_i y_j = y_j x_i\}$

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d	sparse	dense [Pál-Vértesi 18]
2	0.2550008	0.2509397

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3’		0.250854 (1 day)

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d	sparse	dense [Pál-Vértesi 18]
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4	0.2508917	

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6	0.250875397718 0	(1 hour)

PERFORMANCE  VS  ACCURACY

Term sparsity

[Postdoc Wang '19-21] ANR Tremplin-ERC

$$f = x_1^2 - x_1x_2 - x_2x_1 + 3x_2^2 - 2x_1x_2x_1 + 2x_1x_2^2x_1 - x_2x_3 - x_3x_2 + 6x_3^2 + 9x_2^2x_3 + 9x_3^2x_2 - 54x_3x_2x_3 + 142x_3x_2^2x_3$$

[Burgdorf Klep Povh '16] $\rightarrow$ Newton chip method

$$f = \begin{pmatrix} 1 & x_1 & x_2 & x_3 & x_2x_1 & x_3x_2 \end{pmatrix} \underbrace{Q}_{\succcurlyeq 0} \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ x_3 \\ x_1x_2 \\ x_2x_3 \end{pmatrix}$$

$\rightsquigarrow \frac{6\times 7}{2} = 28$ "unknown" entries in Q

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COPS

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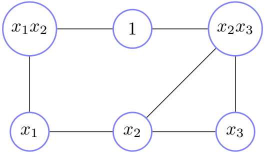
💡 **Term** sparsity pattern graph G



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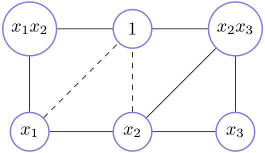
Term sparsity pattern graph G
+ chordal extension G'



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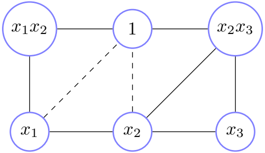

Replace Q by $Q_{G'}$ with nonzero entries at edges of G'

$\rightsquigarrow$ 6 + 9 = 15 "unknown" entries in $Q_{G'}$

Term sparsity

At step d of NC hierarchy, one considers vector $\mathbf{W}_d$ of words with length at most d

The tsp graph G has edges E with

$$\{u, v\} \in E \Leftrightarrow u^\star v \in \operatorname{supp}(f) \bigcup \cup_{s \in S} \operatorname{supp}(s) \bigcup \{w^\star w \mid w \in \mathbf{W}_d\}$$

$\rightsquigarrow$ support extension

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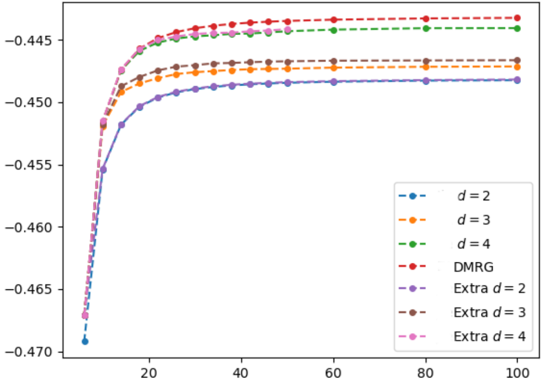
By iteratively performing support extension & chordal extension

$$G^{(1)} = G' \subseteq \cdots \subseteq G^{(\ell)} \subseteq G^{(\ell+1)} \subseteq \cdots$$

Two-level hierarchy of lower bounds for $\lambda_{\min}(f)$ on $\mathcal{D}_S^\infty$, indexed by sparse order ℓ and relaxation order d

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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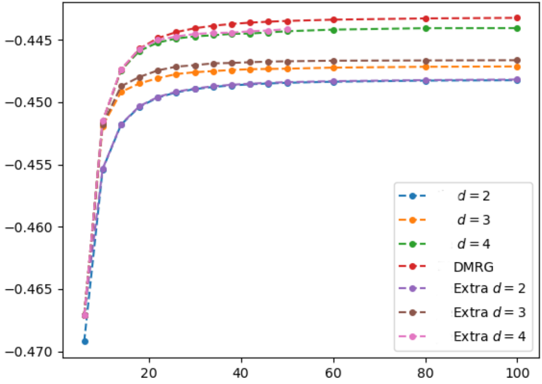

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Sparse solved in $\simeq$ 1 hour on the lab cluster

Conclusion and perspectives

SPARSITY EXPLOITING CONVERGING HIERARCHIES to minimize eigenvalue/trace

FAST IMPLEMENTATION IN JULIA: NCTSSOS

Combine correlative & term sparsity $\rightsquigarrow$ solves problems with 100-1000 variables

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💡 SYMMETRIC noncommutative problems?
Ground state energy of hamiltonians 💡 **symmetric** & **sparse**

Thank you for your attention!

`https://homepages.laas.fr/vmagron`

- Wang & Magron. Exploiting term sparsity in Noncommutative Polynomial Optimization. *Computational Optimization & Applications*, arxiv:2010.06956 NCTSSOS
- Klep, Magron & Povh. Sparse Noncommutative Polynomial Optimization. *Math Prog. A*, arxiv:1909.00569 NCSOStools