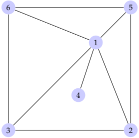
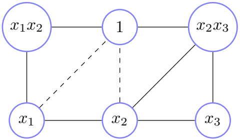
Sparsity in Polynomial Optimization

Victor Magron (LAAS CNRS)

Aromath seminar
13 November 2022



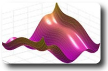




Dense polynomial optimization

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

Theory

(Primal)		(Dual)
$\inf \int f \, d\mu$		$\sup \; b$
with μ proba $\Rightarrow$	**INFINITE-DIM**	$\Leftarrow$ with $f - b \geqslant 0$

Dense polynomial optimization

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

Practice

(Primal **Relaxation**)

moments $\int \mathbf{x}^\alpha \, d\mu$

(Dual **Strengthening**)

$f - b =$ **sum of squares**

finite number $\Rightarrow$ **FINITE-DIM** $\Leftarrow$ **fixed** degree

[Lasserre '01] HIERARCHY of **CONVEX PROBLEMS** $\uparrow f_{\min}$
Based on representing positive polynomials [Putinar '93]

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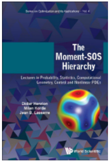

Attracted a lot of attention in optimization, applied mathematics, quantum computing, engineering, theoretical computer science

Sparse polynomial optimization

Structure exploitation with "SPARSE" cost f and constraints

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Correlative sparsity: few variable products in f

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$\rightsquigarrow f = x_1 x_2 + x_2 x_3 + \cdots + x_{99} x_{100}$

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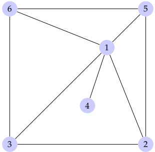

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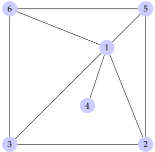
Term sparsity: few terms in f



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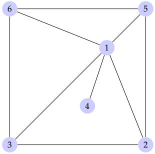

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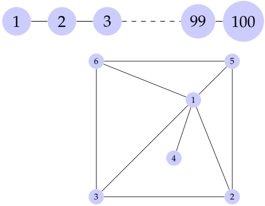

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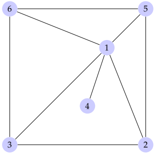

Ideal sparsity: constraints

$\rightsquigarrow x_1 x_2 = x_2 x_3 = 0$

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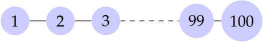

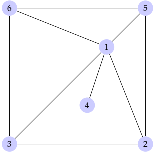

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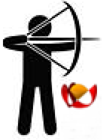
PERFORMANCE  VS  ACCURACY

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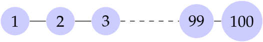

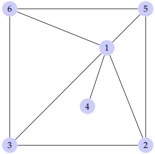

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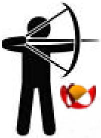
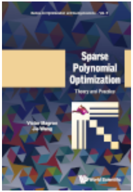
PERFORMANCE  VS  ACCURACY

Tons of applications: computer arithmetic, deep learning, entanglement, optimal power-flow, analysis of dynamical systems, matrix ranks



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Everywhere!

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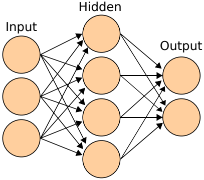
Deep learning

$\rightsquigarrow$ robustness, computer vision



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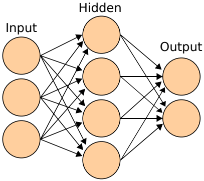
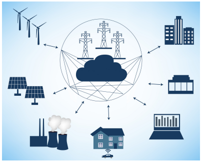


Power systems
⇝ AC optimal power-flow, stability



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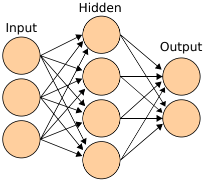

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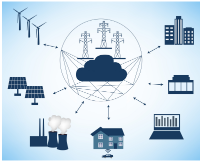
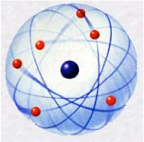


Quantum Systems
$\rightsquigarrow$ condensed matter, entanglement



Moment-SOS hierarchies

Correlative sparsity

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Ideal sparsity

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Moment-SOS hierarchies: an example

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

Semialgebraic set $\mathbf{X} = \{\mathbf{x} \in \mathbb{R}^n : g_j(\mathbf{x}) \geqslant 0\}$

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

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Hierarchy of SDP relaxations:

$$\lambda_d := \sup_{\lambda} \Big\{ \lambda : f - \lambda \in \mathcal{M}(\mathbf{X})_d \Big\}$$

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

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Correlative sparsity

Term sparsity

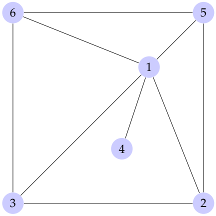
Ideal sparsity

Correlative sparsity

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

$x_2x_5 + x_3x_6 - x_2x_3 - x_5x_6 + x_1(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6)$

Chordal graph after adding edge $(3, 5)$



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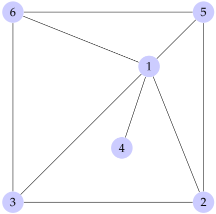


Chordal graph after adding edge $(3,5)$

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

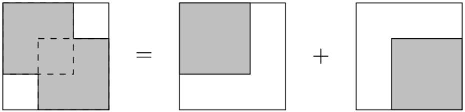
Correlative sparsity

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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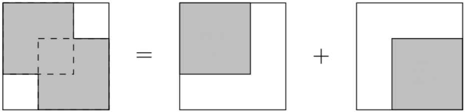

Sparse $f = f_1 + f_2$ where f_k involves **only** variables in I_k

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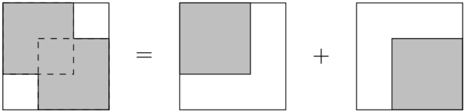


Sparse $f = f_1 + f_2$ where f_k involves **only** variables in I_k

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

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

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

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

Application to robustness of neural networks

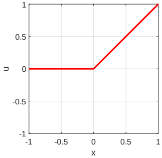
[SIAM News March '21]

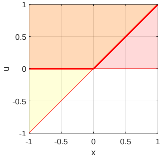
"Yet DL has an Achilles' heel. Current implementations can be highly unstable, meaning that a certain small perturbation to the input of a trained neural network can cause substantial change in its output. This phenomenon is both a nuisance and a major concern for the safety and robustness of DL-based systems in critical applications—like healthcare—where reliable computations are essential"

Application to robustness of neural networks

$$\mathbf{x}_0 \in \mathbb{R}^p \longrightarrow \mathbf{z}_0 \in \mathbb{R}^p \longrightarrow \mathbf{z}_1 \in \mathbb{R}^{p_1} \longrightarrow \cdots \longrightarrow \mathbf{z}_m \in \mathbb{R}^{p_m} \quad \mathbf{z}_i = \mathbf{A}_i \mathrm{ReLU}(\mathbf{z}_{i-1}) + \mathbf{b}_i$$

ReLU (left) & its "semialgebraicity" (right)





$$u = \max\{x, 0\} \qquad\qquad u(u - x) = 0, u \geq x, u \geq 0$$

Application to robustness of neural networks

"Direct" certification of a classifier with 1 hidden layer

$$\max_{\mathbf{x},\mathbf{z}} \quad (\mathbf{C}^{i,:} - \mathbf{C}^{k,:})\mathbf{z}$$

$$\text{s.t.} \quad \begin{cases} \mathbf{z} = \mathrm{ReLU}(\mathbf{A}\mathbf{x} + \mathbf{b}) \\ ||\mathbf{x} - \mathbf{x}_0|| \leq \epsilon \end{cases}$$

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Monotone equilibrium networks [Winston Kolter ’20]

$$\mathbf{z} = \mathrm{ReLU}(\mathbf{A}\mathbf{x} + \mathbf{b}) \to \mathbf{z} = \mathrm{ReLU}(\mathbf{W}\mathbf{z} + \mathbf{A}\mathbf{x} + \mathbf{b})$$

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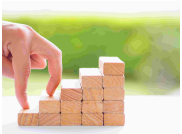
- "Indirect" with Lipschitz constant/ellipsoid approximation

- Go between 1ST & 2ND stair in SPARSE hierarchy



Trained $(784, 500)$ network

MNIST classifier [Raghunathan et al. '18]

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PERFORMANCE  VS  ACCURACY

Extension to noncommutative optimization

Self-adjoint noncommutative (NC) variables $x = (x_1, \ldots, x_n)$

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Theorem: Sparse NC Positivstellensatz [Klep Magron Povh '21]

$f = \sum_k f_k$, f_k depends on $x(I_k)$
$f > 0$ on $\{\mathbf{x} : g_j(\mathbf{x}) \geqslant 0\}$
chordal graph with cliques I_k
ball constraints for each $\mathbf{x}(I_k)$

$\Longrightarrow$

$$f = \sum_{k,i} (s_{ki}^\star s_{ki} + \sum_{j \in J_k} t_{ji}{}^\star g_j t_{ji})$$

s_{ki} "sees" vars in I_k
t_{ji} "sees" vars from g_j

Application to violation of Bell inequalities

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

$$f = a_1(b_1 + b_2 + b_3) + a_2(b_1 + b_2 - b_3) + a_3(b_1 - b_2) - a_1 - 2b_1 - b_2$$

Maximal violation levels → **upper bounds** on $\lambda_{\max}$ of f on $\{a, b : a_i^2 = a_i \quad b_i^2 = b_i \quad a_i b_j = b_j a_i\}$

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5	0.2508763	
6	0.25087539771 80	(1 hour)

PERFORMANCE  VS  ACCURACY

Application to violation of Bell inequalities

CLASSICAL WORLD

$$\psi^*(A_1 \otimes B_1 + A_1 \otimes B_2 + A_2 \otimes B_1 - A_2 \otimes B_2)\psi \leqslant 2$$

for separable states $\psi \in \mathbb{R}^k \otimes \mathbb{R}^k$ and self-adjoint matrices A_j, B_j satisfying $A_i^2 = B_j^2 = I$

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$\psi = \frac{1}{\sqrt{k}} \sum_{j=1}^k e_j \otimes e_j \in \mathbb{R}^k \otimes \mathbb{R}^k$

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$$2 \to 2\sqrt{2} = \operatorname{tr}_{\max}\{a_1 b_1 + a_1 b_2 + a_2 b_1 - a_2 b_2 : a_j^2 = b_j^2 = 1\}$$

Application to violation of Bell inequalities

COVARIANCES OF QUANTUM CORRELATIONS

$$\mathrm{cov}_{\psi}(X, Y) := \psi^*(X \otimes Y)\psi - \psi^*(X \otimes I)\psi \cdot \psi^*(I \otimes Y)\psi$$

Application to violation of Bell inequalities

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for separable states but ...

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💡 2nd sparse SDP gives 5 too . . . 10 times faster

Moment-SOS hierarchies

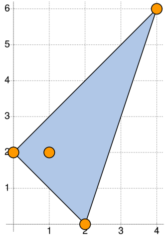
Correlative sparsity

Term sparsity

Ideal sparsity

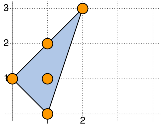
Term sparsity: unconstrained

$f = 4x_1^4x_2^6 + x_1^2 - x_1x_2^2 + x_2^2$
spt(f) = $\{(4,6),(2,0),(1,2),(0,2)\}$



Newton polytope $\mathscr{B} = \mathrm{conv}\,(\text{spt}(f))$

Squares in SOS decomposition $\subseteq \frac{\mathscr{B}}{2} \cap \mathbb{N}^n$
[Reznick '78]



$$f = \begin{pmatrix} x_1 & x_2 & x_1x_2 & x_1x_2^2 & x_1^2x_2^3 \end{pmatrix} \underbrace{Q}_{\succcurlyeq 0} \begin{pmatrix} x_1 \\ x_2 \\ x_1x_2 \\ x_1x_2^2 \\ x_1^2x_2^3 \end{pmatrix}$$

Term sparsity: unconstrained

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

COPS

$$f = x_1^2 - 2x_1x_2 + 3x_2^2 - 2x_1^2x_2 + 2x_1^2x_2^2 - 2x_2x_3 + 6x_3^2 + 9x_2^2x_3 - 45x_2x_3^2 + 142x_2^2x_3^2$$

[Reznick '78] → Newton polytope method

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

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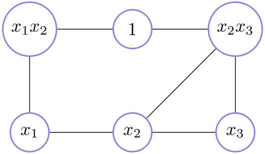
💡 **Term** sparsity pattern graph G



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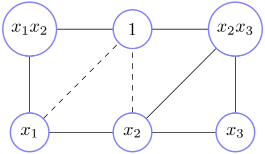
+ chordal extension G'



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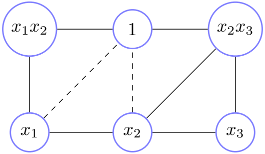

Replace Q by $Q_{G'}$ with nonzero entries at edges of G'

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

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Nodes V = monomials of degree $\leqslant d$

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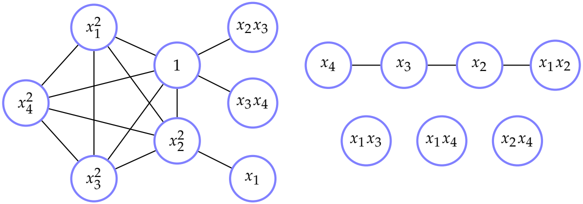
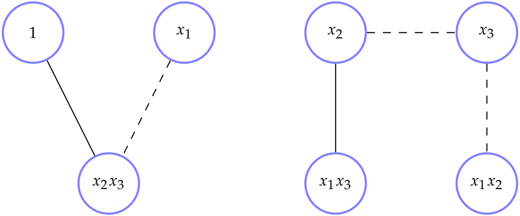
An example with $d = 2$
$f = x_1^4 + x_1 x_2^2 + x_2 x_3 + x_3^2 x_4^2$
$g_1 = 1 - x_1^2 - x_2^2 - x_3^2 \quad g_2 = 1 - x_3 x_4$



Term sparsity: support extension

$\alpha' + \beta' = \alpha + \beta$ and $(\alpha, \beta) \in E \Rightarrow (\alpha', \beta') \in E$



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Term sparsity: constrained

At step d of the hierarchy, tsp graph G has

Nodes V = monomials of degree $\leqslant d$
Edges E with

$$\{\alpha, \beta\} \in E \Leftrightarrow \alpha + \beta \in \operatorname{supp} f \bigcup \operatorname{supp} g_j \bigcup_{|\alpha| \leqslant d} 2\alpha$$

$\rightsquigarrow$ support extension $\rightsquigarrow$ chordal extension G'

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 $f_{\min}$, indexed by sparse order ℓ and relaxation order d

Term sparsity: convergence guarantees

Theorem [Lasserre Magron Wang '21]

The block structures converge to the one determined by the sign symmetries if the maximal chordal extension is used.

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Term sparsity blocks $(1 \quad x_1x_2^2 \quad x_1^2x_2^2) \quad (x_1x_2) \quad (x_1^2x_2)$

Term sparsity

CONVERGENCE GUARANTEES

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- handles Combo with correlative sparsity

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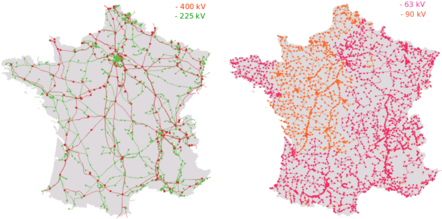
Application to AC optimal power-flow

Minimize active power injections of an alternating current transmission network under physical + operational constraints



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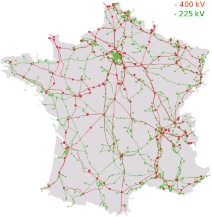

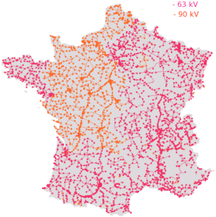

Artificial version of the control problem for electricity transmission network

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Network = Graph with buses N, *from* edges E, *to* edges E^R

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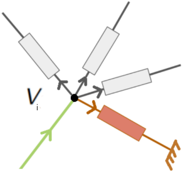

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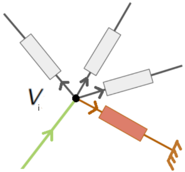

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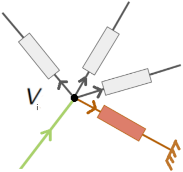

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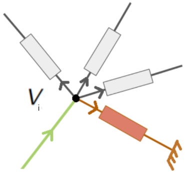

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$\rightsquigarrow$ leads to power-flow equations

Application to AC optimal power-flow

mb: maximal block size

gap: the optimality gap w.r.t. local optimal solution

n	m	CS ($d = 2$)			CS-TSSOS ($d = 2, \ell = 1$)		
		mb	time	gap	mb	time	gap
1112	4613	231	3114	0.85%	39	46.6	0.86%
		496	–	–	31	410	0.25%
4356	18257	378	–	–	27	934	0.51%
6698	29283	1326	–	–	76	1886	0.47%

Moment-SOS hierarchies

Correlative sparsity

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Ideal sparsity

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Theorem [Korda-Laurent-Magron-Steenkamp '22]

Ideal-sparse hierarchies provide better bounds than the dense ones

ACCURACY

Application to matrix ranks

Given a symmetric nonnegative matrix A, find the smallest r s.t.

$$A = \sum_{\ell=1}^{r} a_\ell {a_\ell}^T \qquad \text{for } a_\ell \geqslant 0$$

r is called the completely positive rank

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$$K_A = \{ \mathbf{x} : \sqrt{A_{ii}} x_i - x_i \geqslant 0 \,, \quad A_{ij} - x_i x_j \geqslant 0 \ (i,j) \in E_A \,, \\ x_i x_j = 0 \ (i,j) \in \overline{E}_A \,, \quad A - \mathbf{x}\mathbf{x}^T \succcurlyeq 0 \}$$

Application to matrix ranks

Random instances, order 2

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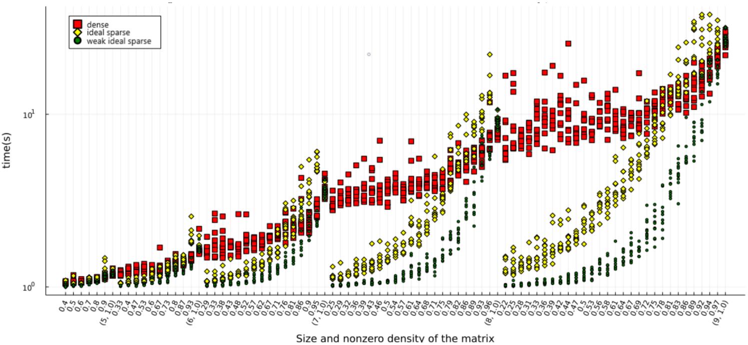

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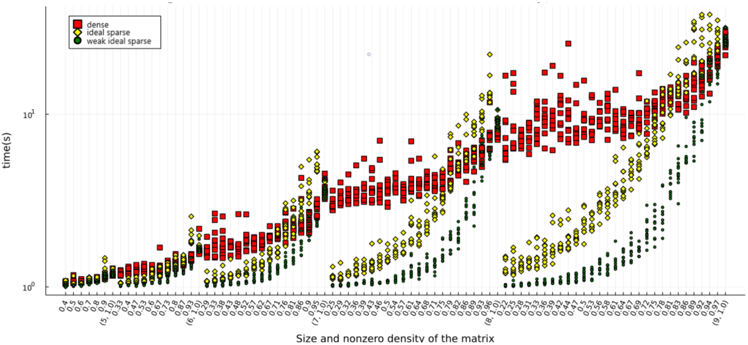

PERFORMANCE  AND  ACCURACY

Conclusion

SPARSITY EXPLOITING CONVERGING HIERARCHIES to minimize polynomials, eigenvalue/trace, joint spectral radius

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FAST IMPLEMENTATION IN JULIA: TSSOS, NCTSSOS, SparseJSR

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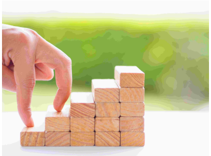
Combine correlative & term sparsity for problems with $n = 10^3$

Further topics

Correlative sparsity: convergence rate?



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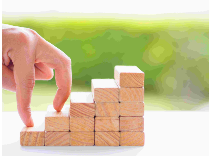

Correlative sparsity: convergence rate?

Term sparsity: (smart) solution extraction

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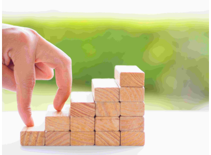

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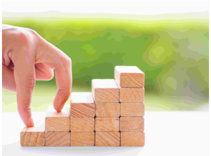

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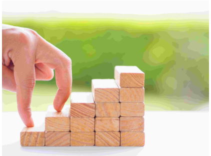

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💡 Tons of applications!

Take-away and advertisement

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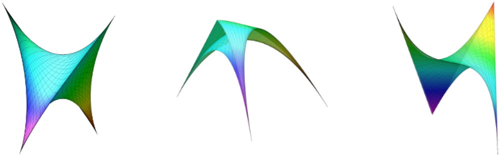
Complementary SYMMETRY exploiting framework on Thursday by Tobias



Thank you for your attention!

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

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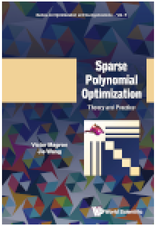

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