Completely positive semidefinite matrices: conic approximations and matrix factorization ranks

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Objective

- New matrix cone $\mathcal{CS}_+^n$: **completely positive semidefinite matrices**
  Noncommutative analogue of $\mathcal{CP}^n$: **completely positive matrices**

- Motivation: conic optimization approach for quantum information
  - **quantum graph coloring**
  - **quantum correlations**

- (Noncommutative) polynomial optimization: common approach for (quantum) graph coloring and for **matrix factorization ranks:**
  - symmetric rks: $\text{cpsd-rank}(A)$ for $A \in \mathcal{CS}_+^n$, $\text{cp-rank}(A)$ for $A \in \mathcal{CP}^n$
  - asymmetric analogues: $\text{psd-rank}(A)$, $\text{rank}_+(A)$ for A nonnegative

- Based on joint works with
  Sabine Burgdorf, Sander Gribling, David de Laat, Teresa Piovesan

Completely positive semidefinite matrices

Completely positive semidefinite matrices

- A matrix $A \in \mathcal{S}^n$ is completely positive semidefinite (cpsd) if A has a Gram factorization by **positive semidefinite matrices** $X_1., \ldots, X_n \in \mathcal{S}^d_+$ of **arbitrary size** $d \geq 1$:

$$A_{ij} = \langle X_i, X_j \rangle \;\; (= \mathrm{Tr}(X_i X_j)) \;\; \forall i, j \in [n]$$

  The **smallest** such d is $\text{cpsd-rank}(A)$ [back to it later]

  The cpsd matrices form a convex cone

  $\rightsquigarrow$ the completely positive semidefinite cone $\mathcal{CS}^n_+$

- If X_i are **diagonal psd matrices** (equivalently, replace X_i by **nonnegative vectors** $x_i \in \mathbb{R}^d_+$), then A is completely positive

  $\rightsquigarrow$ the completely positive cone $\mathcal{CP}^n$

  The smallest such d is $\text{cp-rank}(A)$ [back to it later]

- Clearly: $\mathcal{CP}^n \subseteq \mathcal{CS}^n_+ \subseteq \text{cl}(\mathcal{CS}^n_+) \subseteq \mathcal{S}^n_+ \cap \mathbb{R}^{n \times n}_+ =: \mathcal{DNN}^n$

  Is the cone $\mathcal{CS}^n_+$ **closed**?

Strict inclusions $\mathcal{CP}^n \subseteq \mathcal{CS}_+^n \subseteq \mathcal{DNN}^n$

- $\mathcal{CP}^n = \mathcal{CS}_+^n = \mathcal{DNN}^n$ if $n \leq 4$; but **strict inclusions** if $n \geq 5$

- [Fawzi-Gouveia-Parrilo-Robinson-Thomas'15] $A \in \mathcal{CS}_+^5 \setminus \mathcal{CP}^5$ for

$$A = \begin{pmatrix} 1 & a & b & b & a \\ a & 1 & a & b & b \\ b & a & 1 & a & b \\ b & b & a & 1 & a \\ a & b & b & a & 1 \end{pmatrix} \quad \text{with } a = \cos^2\left(\frac{2\pi}{5}\right), \; b = \cos^2\left(\frac{4\pi}{5}\right)$$

$A \in \mathcal{CS}_+^5$ because $\sqrt{A} \succeq 0$:

$$\sqrt{A} = \text{Gram}(u_1, \ldots, u_5) \implies A = \text{Gram}(u_1 u_1^T, \ldots, u_5 u_5^T)$$

- [L-Piovesan 2015] $A = \begin{pmatrix} 4 & 2 & 0 & 0 & 2 \\ 2 & 4 & 2 & 0 & 0 \\ 0 & 2 & 4 & 3 & 0 \\ 0 & 0 & 3 & 4 & 2 \\ 2 & 0 & 0 & 2 & 4 \end{pmatrix} \in \mathcal{DNN}^5 \setminus \mathcal{CS}_+^5$

because A is supported by a cycle: $A \in \mathcal{CS}_+^n \iff A \in \mathcal{CP}^n$

On the closure $\mathrm{cl}(\mathcal{CS}_+^n)$

Moreover, $A = \begin{pmatrix} 4 & 2 & 0 & 0 & 2 \\ 2 & 4 & 2 & 0 & 0 \\ 0 & 2 & 4 & 3 & 0 \\ 0 & 0 & 3 & 4 & 2 \\ 2 & 0 & 0 & 2 & 4 \end{pmatrix} \notin \mathrm{cl}(\mathcal{CS}_+^5)$!

Because [Frenkel-Weiner 2014] show that A **does not have** a Gram representation by **positive elements in any C^*-algebra $\mathcal{A}$ with trace** ...

... while [Burgdorf-L-Piovesan 2015] construct a C^*-**algebra with trace** $\mathcal{M}_\mathcal{U}$ such that $\mathrm{cl}(\mathcal{CS}_+^n)$ consists of all matrices A having a Gram factorization by positive elements in $\mathcal{M}_\mathcal{U}$

(using tracial ultraproducts of matrix algebras)

New cone $\mathcal{CS}_{+C^*}^n$: all matrices having a Gram representation by positive elements in **some** C^***-algebra with trace**. Then $A \notin \mathcal{CS}_{+C^*}^n$, $\mathcal{CS}_{+C^*}^n$ is closed, and

$$\mathcal{CS}_+^n \subseteq \mathrm{cl}(\mathcal{CS}_+^n) \subseteq \mathcal{CS}_{+C^*}^n \subsetneq \mathcal{DNN}^n$$

Equality $\mathrm{cl}(\mathcal{CS}_+^n) = \mathcal{CS}_{+C^*}^n$ under **Connes' embedding conjecture**

SDP outer approximations of $\mathcal{CS}_+^n$

Assume $A \in \mathcal{CS}_+^n$: $\quad A = (\mathrm{Tr}(X_iX_j))$ for some $X_1, \ldots, X_n \in \mathcal{S}_+^d$

Define the **trace evaluation** at $\mathbf{X} = (X_1, \ldots, X_n)$:

$L : \mathbb{R}\langle x_1, \ldots, x_n \rangle \to \mathbb{R} \qquad p \mapsto L(p) = \mathrm{Tr}(p(X_1, \ldots, X_n))$

(1) L is *tracial*: $\quad L(pq) = L(qp) \quad \forall p, q \in \mathbb{R}\langle \mathbf{x} \rangle$

(2) L is *symmetric*: $\quad L(p^*) = L(p) \quad \forall p \in \mathbb{R}\langle \mathbf{x} \rangle$

(3) L is *positive*: $\quad L(p^*p) \geq 0 \quad \forall p \in \mathbb{R}\langle \mathbf{x} \rangle$

(4) *localizing constraint:* $\quad L(p^*x_ip) \geq 0 \quad \forall p \in \mathbb{R}\langle \mathbf{x} \rangle$

(5) $A = (L(x_ix_j))$

$\mathcal{F}_t$ = matrices $A \in \mathcal{S}^n$ for which there exists $L \in \mathbb{R}\langle \mathbf{x} \rangle_{2t}^*$ satisfying (1)-(5)

$$\mathcal{CS}_+^n \subseteq \mathcal{F}_{t+1} \subseteq \mathcal{F}_t, \qquad \mathcal{CS}_+^n \subseteq \mathrm{cl}(\mathcal{CS}_+^n) \subseteq \mathcal{CS}_{+C^*}^n \subseteq \bigcap_{t \geq 1} \mathcal{F}_t$$

$\mathcal{F}_t$ is the solution set of a **semidefinite program:**

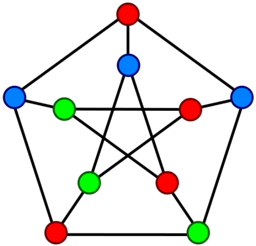
(3) $M_t(L) = (L(u^*v))_{u,v \in \langle \mathbf{x} \rangle_t} \succeq 0$, $\quad$ (4) $(L(u^*x_iv))_{u,v \in \langle \mathbf{x} \rangle_{t-1}} \succeq 0$

Noncommutative analogue of outer approximations of $\mathcal{CP}^n$ [Nie'14]

Quantum graph coloring

Classical coloring number

$\chi(G)$ = minimum number of colors needed for a proper coloring of $V(G)$



$$\chi(\mathsf{G}) = \min\ \mathsf{k} \in \mathbb{N} \text{ s.t. } \quad \exists\ \mathsf{x}_\mathsf{u}^\mathsf{i} \in \{0,1\} \ \text{ for }\ \mathsf{u} \in \mathsf{V(G)},\ \mathsf{i} \in [\mathsf{k}]$$

$$\textstyle\sum_{\mathsf{i}\in[\mathsf{k}]} \mathsf{x}_\mathsf{u}^\mathsf{i} = 1 \quad \forall \mathsf{u} \in \mathsf{V(G)}$$

$$\mathsf{x}_\mathsf{u}^\mathsf{i}\mathsf{x}_\mathsf{v}^\mathsf{i} = 0 \quad \forall i \in [k]\ \forall\, \mathsf{uv} \in \mathsf{E(G)}$$

$$\mathsf{x}_\mathsf{u}^\mathsf{i}\mathsf{x}_\mathsf{u}^\mathsf{j} = 0 \quad \forall\, \mathsf{i} \neq \mathsf{j} \in [k],\ \forall \mathsf{u} \in \mathsf{V(G)}$$

Quantum coloring number

$$\chi(G) = \min\ k \in \mathbb{N} \text{ s.t. } \quad \exists\, x_u^i \in \{0,1\} \text{ for } u \in V(G),\ i \in [k]$$
$$\textstyle\sum_{i\in[k]} x_u^i = 1 \quad \forall\, u \in V(G)$$
$$x_u^i x_v^i = 0 \quad \forall i \in [k],\ \forall\, uv \in E(G)$$
$$x_u^i x_u^j = 0 \quad \forall\, i \neq j \in [k],\ \forall\, u \in V(G)$$

$$\chi_q(G) = \min\ k \in \mathbb{N} \text{ s.t. } \quad \exists\, d \in \mathbb{N}\ \ \exists\, X_u^i \in \mathcal{S}_+^d \text{ for } u \in V(G),\ i \in [k]$$
$$\textstyle\sum_{i\in[k]} X_u^i = I \quad \forall\, u \in V(G)$$
$$X_u^i X_v^i = 0 \quad \forall i \in [k],\ \forall\, uv \in E(G)$$
$$X_u^i X_u^j = 0 \quad \forall\, i \neq j \in [k],\ \forall\, u \in V(G)$$

$$\chi_q(G) \leq \chi(G)$$

[Cameron, Newman, Montanaro, Severini, Winter: On the quantum chromatic number of a graph, Electronic J. Combinatorics, 2007]

Motivation: non-local coloring game

Two players: Alice and Bob, want to convince a referee that they **can color a given graph** $G = (V, E)$ **with** k **colors**

Agree on strategy before the start, **no communication** during the game

- The referee chooses a pair of vertices $(u, v) \in V^2$ with prob. $\pi(u, v)$
- The referee sends vertex u to Alice and vertex v to Bob
- Alice answers color $i \in [k]$, Bob answers color $j \in [k]$, *using some strategy they have chosen before the start of the game*
- Alice & Bob **win the game** when $\begin{cases} i = j & \text{if } u = v \\ i \neq j & \text{if } uv \in E \end{cases}$

When using a **classical strategy**, the minimum number of colors needed to always win the game is the **classical coloring number** $\chi(G)$

Quantum strategy for the coloring game

- $\forall u \in V$ Alice has POVM $\{A_u^i\}_{i\in[k]}$: $\quad A_u^i \in \mathcal{H}_+^d, \ \sum_{i\in[k]} A_u^i = I$

- $\forall v \in V$ Bob has POVM $\{B_v^j\}_{j\in[k]}$: $\quad B_v^j \in \mathcal{H}_+^d, \ \sum_{j\in[k]} B_v^j = I$

- Alice and Bob share an **entangled state** $\Psi \in \mathbb{C}^d \otimes \mathbb{C}^d$ (unit vector)

- **Probability of answer** (i,j): $\quad p(i,j|u,v) := \langle \Psi, A_u^i \otimes B_v^j \ \Psi \rangle$

- Alice and Bob **win the game** if they *never give a wrong answer* :
  $p(i,j|u,v) = 0$ if $(u = v \ \& \ i \neq j)$ or $(uv \in E \ \& \ i = j)$

- **Theorem:** [Cameron et al. 2007] The minimum number of colors for which there is a quantum winning strategy is equal to $\chi_q(G)$

Classical and quantum coloring numbers

- $\chi_q(G) \leq \chi(G)$
- $\exists$ G for which $\chi_q(G) = 3 < \chi(G) = 4$ [Fukawa et al. 2011]
- The separation $\chi_q < \chi$ is **exponential** for Hadamard graphs G_n:
  $n = 4k$, with vertices $x \in \{0,1\}^n$, edges (x, y) if $d_H(x, y) = n/2$
  $\chi(G_n) \geq (1 + \epsilon)^n$ [Frankl-Rödl'87]
  $\chi_q(G_n) = n$ [Avis et al.'06][Mancinska-Roberson'16]
- Deciding whether $\chi_{\mathrm{q}}(G) \leq 3$ is NP-hard [Ji 2013]
- **Approach:** Model $\chi_q(G)$ as conic optimization problem using the cone of completely positive semidefinite matrices

Conic formulation for quantum graph coloring

$$\chi_q(G) = \min\ k \ \text{ s.t. } \exists\ X_u^i \succeq 0\ (u \in V, i \in [k]) \ \text{ satisfying:}$$

$$\textstyle\sum_{i\in[k]} X_u^i = \sum_{j\in[k]} X_v^j\ (\neq 0) \qquad (u, v \in V) \qquad \text{(Q1)}$$

$$X_u^i X_u^j = 0\ \ (i \neq j \in [k], u \in V), \quad X_u^i X_v^i = 0\ \ (i \in [k], uv \in E) \qquad \text{(Q2)}$$

Set $A := \mathrm{Gram}(X_u^i)$. Then: $X_u^i X_v^j = 0 \iff \mathrm{Tr}(X_u^i X_v^j) = 0 = A_{ui,vj}$

Then: $\chi_q(G) = \min\ k \ \text{ s.t. } \exists\ A \in \mathcal{CS}_+^{nk}$ satisfying:

$$\textstyle\sum_{i,j\in[k]} A_{ui,vj} = 1\ \ (u, v \in V), \qquad \text{(C1)}$$

$$A_{ui,uj} = 0\ (i \neq j \in [k], u \in V), \quad A_{ui,vi} = 0\ (i \in [k], uv \in E). \qquad \text{(C2)}$$

Theorem (L-Piovesan 2015)

- *Replacing* $\mathcal{CS}_+$ *by the cone* $\mathcal{CP}$, *we get* $\chi(G)$
- *Replacing* $\mathcal{CS}_+$ *by the cone* $\mathcal{DNN}$, *get the* **theta number** $\vartheta^+(\overline{G})$
- *Hence:* $\vartheta_+(\overline{G}) \leq \chi_q(G)$ *[Mancinska-Roberson 2015]*

SDP relaxations for coloring

If (X_u^i) is solution to $\chi_q(G) = k$, its normalized trace evaluation satisfies

(1) $L(1) = 1$

(2) L is symmetric, tracial, positive (on Hermitian squares)

(3) $L = 0$ on the ideal generated by

$$1 - \sum_{i=1}^k x_u^i \ (u \in V), \quad x_u^i x_u^j \ (i \neq j, u \in V), \quad x_u^i x_v^i \ (uv \in E, i \in [k])$$

Restricting to the truncated polynomial space $\mathbb{R}\langle \mathbf{x} \rangle_{2t}$, get the parameters:

$$\xi_t^{nc}(G) \ = \ \min k \ \text{ such that } \ \exists L \in \mathbb{R}\langle \mathbf{x} \rangle_{2t}^* \ \text{ satisfying (1)-(3)}$$

$$\xi_t^{c}(G) \ = \ \min k \ \text{ such that } \ \exists L \in \mathbb{R}[\mathbf{x}]_{2t}^* \ \text{ satisfying (1)-(3)}$$

$$\xi_t^{nc}(G) \leq \chi_q(G) \qquad \xi_t^{c}(G) \leq \chi(G)$$

- For $t = 1$ get the theta number: $\xi_1^{nc}(G) = \xi_1^{c}(G) = \vartheta^+(\overline{G})$
- $\xi_t^{c}(G) = \chi(G) \ \ \forall t \geq n$ [Gvozdenović-L 2008]
- $\xi_{t_0}^{nc}(G) = \chi_{C^*}(G) \ \leq \ \chi_q(G) \ \ \forall t \geq t_0$ [Gribling-de Laat-L 2017]

  $\chi_{C^*}(G)$= allow solutions $X_u^i \in \mathcal{A}$ for any C^*-algebra $\mathcal{A}$ with trace [Ortiz-Paulsen 2016]

Quantum correlations

$C_q(n,k)$ = **quantum correlations** $p = (p(i,j|u,v)) := (\langle \Psi, A_u^i \otimes B_v^j \Psi \rangle)$,
with $d \in \mathbb{N}$, $A_u^i, B_v^j \in \mathcal{H}^d{}_+$ with $\sum_i A_u^i = \sum_j B_v^j = I$, $\Psi \in \mathbb{C}^d \otimes \mathbb{C}^d$ unit

Theorem (Sikora-Varvitsiotis 2015)

$C_q(n,k)$ *is* the projection of an affine section *of* $\mathcal{CS}_+^{2nk}$:

$$p = (p(i,j|u,v)) \rightsquigarrow A_p = (p(i,j|u,v))_{(i,u),(j,v) \in [k] \times V}$$

$$p \in C_q(n,k) \iff \exists M = \begin{pmatrix} ? & A_p \\ A_p^{\mathsf{T}} & ? \end{pmatrix} \in \mathcal{CS}_+^{2nk}$$ *satisfying additional affine conditions*

Theorem (Gribling-de Laat-L 2017)

For **synchronous** *correlations:* $p(i,j|u,u) = 0$ *whenever* $i \neq j$

$p \in C_q(n,k) \iff A_p \in \mathcal{CS}_+^{nk}$

The **smallest dimension** d *realizing* p *is equal to* $\text{cpsd-rank}(A_p)$

Theorem (Slofstra 2017)

$C_q(n,k)$ *is* **not closed** $\Longrightarrow$ $\mathcal{CS}_+^N$ *is* **not closed** *for large* N *(*≥ 1942*)*

Matrix factorization ranks

Four matrix factorization ranks

Symmetric factorizations:

- $A \in \mathcal{CP}^n$ if $A = (x_i^\mathsf{T} x_j)$ for nonnegative $x_i \in \mathbb{R}^d_+$
  Smallest such $d = \mathrm{cp\text{-}rank}(A)$
- $A \in \mathcal{CS}^n_+$ if $A = (\mathrm{Tr}(X_i X_j))$ for $X_i \in \mathcal{H}^d_+$ or $\mathcal{S}^d_+$
  Smallest such $d = \mathrm{cpsd\text{-}rank}_{\mathbb{K}}(A)$ with $\mathbb{K} = \mathbb{C}$ or $\mathbb{R}$

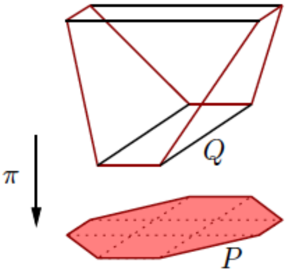
Applications: probability, entanglement dimension in quantum information

Asymmetric factorizations for $A \in \mathbb{R}^{m \times n}_+$:

- $A = (x_i^\mathsf{T} y_j)$ for nonnegative $x_i, y_j \in \mathbb{R}^d_+$
  Smallest such $d = \mathrm{rank}_+(A)$: nonnegative rank
- $A = (\mathrm{Tr}(X_i Y_j))$ for $X_i, Y_j \in \mathcal{H}^d_+$ or $\mathcal{S}^d_+$
  Smallest such $d = \mathrm{psd\text{-}rank}_{\mathbb{K}}(A)$ with $\mathbb{K} = \mathbb{C}$ or $\mathbb{R}$

Applications: (quantum) communication complexity, extended formulations of polytopes

rank_+, $\mathrm{psd\text{-}rank}_{\mathbb{R}}$ and extended formulations



[Yannakakis 1991]

Slack matrix: $S = (b_i - a_i^\mathsf{T} v)_{v,i}$ if $P = \mathrm{conv}(V) = \{x : a_i^\mathsf{T} x \le b_i \ \forall i\}$

Smallest k s.t. P is **projection of affine section** of $\mathbb{R}_+^k$ is $\mathrm{rank}_+(S)$

Smallest k s.t. P is **projection of affine section** of $\mathcal{S}_+^k$ is $\mathrm{psd\text{-}rank}_{\mathbb{R}}(S)$

[Rothvoss'14] The matching polytope of K_n has **no polynomial size LP extended formulation**: smallest $k = 2^{\Omega(n)}$

Basic upper bounds

- For $A \in \mathbb{R}_+^{m\times n}$: $\text{psd-rank}(A) \leq \text{rank}_+(A) \leq \min\{m, n\}$
- For $A \in \mathcal{CP}^n$: $\text{cp-rank}(A) \leq \binom{n+1}{2}$
- For $A \in \mathcal{CS}_+^n$: $\text{cpsd-rank}_{\mathbb{C}}(A) \leq \text{cpsd-rank}_{\mathbb{R}}(A) \leq ?$

  No upper bound on cpsd-rank **exists in terms of matrix size!**

rank_+, psd-rank, cp-rank are computable; is cpsd-rank computable?

[Vavasis 2009] rank_+ is NP-complete

Theorem (G-dL-L 2016, Prakash-Sikora-Varvitsiotis-Wei 2016)

Construct $A_n \in \mathcal{CS}_+^n$ *with* **exponential** $\text{cpsd-rank}_{\mathbb{C}}(A_n) = 2^{\Omega(\sqrt{n})}$

Example (G-dL-L 2016)

$A_n = \begin{pmatrix} nI_n & J_n \\ J_n & nI_n \end{pmatrix} \in \mathcal{CP}^{2n}$ has **quadratic separation** for cp and cpsd rks:

- $\text{cp-rank}(A_n) = n^2$, $\text{cpsd-rank}_{\mathbb{C}}(A_n) = n$
- $\text{cpsd-rank}_{\mathbb{R}}(A_n) = n \iff \exists$ real Hadamard matrix of order n

What about lower bounds?

- [Fawzi-Parrilo 2016] defines lower bounds $\tau_+(\cdot)$ for rank_+, and $\tau_{cp}(\cdot)$ for $\mathrm{cp\text{-}rank}$, based on their **atomic definition:**

$$\mathrm{rank}_+(A) = \min\ d \ \text{ s.t. } A = u_1 v_1^\mathsf{T} + \ldots + u_d v_d^\mathsf{T} \ \text{ with } u_i, v_i \in \mathbb{R}^n_+$$

$$\mathrm{cp\text{-}rank}(A) = \min\ d \ \text{ s.t. } A = u_1 u_1^\mathsf{T} + \ldots + u_d u_d^\mathsf{T} \ \text{ with } u_i \in \mathbb{R}^n_+$$

$$\tau_+(A) = \min \alpha \ \text{ s.t. } A \in \alpha \cdot \mathrm{conv}(R \in \mathbb{R}^{m\times n} : 0 \le R \le A, \mathrm{rank}(R) \le 1)$$

$$\tau_{cp}(A) = \min \alpha \ \text{ s.t. } A \in \alpha\cdot\mathrm{conv}(R \in \mathcal{S}^n : 0 \le R \le A, \mathrm{rank}(R) \le 1, R \preceq A)$$

- [FP 2016] also defines tractable SDP relaxations $\tau_+^{sos}(\cdot)$ and $\tau_{cp}^{sos}(\cdot)$:

$$\tau_+^{sos}(A) \le \tau_+(A) \le \mathrm{rank}_+(A), \quad \mathrm{rank}(A) \le \tau_{cp}^{sos}(A) \le \tau_{cp}(A) \le \mathrm{cp\text{-}rank}(A)$$

- Combinatorial lower bound: **Boolean rank** $\mathrm{rank}_B(A) \le \mathrm{rank}_+(A)$

$\mathrm{rank}_B(A) = \chi(RG(A))$: coloring number of the 'rectangle graph' $RG(A)$

$$\tau_+(A) \ge \chi_f(RG(A)), \qquad \tau_+^{sos}(A) \ge \vartheta(\overline{RG(A)})$$

[Fiorini & al. 2015] shows **no polynomial LP extended formulations** exist for TSP, correlation, cut, stable set polytopes

No atomic definition exists for psd-rank and cpsd-rank ...

... using **(nc) polynomial optimization** we get a common framework which applies to *all four* factorization ranks [G-dL-L 2017]

Commutative polynomial optimization [Lasserre, Parrilo 2000–]
Noncommutative: eigenvalue opt. [Pironio, Navascués, Acín 2010–]
Noncommutative: tracial opt. [Burgdorf, Cafuta, Klep, Povh 2012–]

$$f_*^c = \inf f(x) \text{ s.t. } x \in \mathbb{R}^n, g(x) \geq 0 \ (g \in S)$$

$$f_*^{nc} = \inf \mathrm{Tr}(f(\mathbf{X})) \text{ s.t. } d \in \mathbb{N}, \ \mathbf{X} \in (\mathcal{S}^d)^n, \ g(\mathbf{X}) \succeq 0 \ (g \in S)$$

$$f_{C^*}^{nc} = \inf \tau(f(\mathbf{X})) \text{ s.t. } \mathcal{A} \ C^*\text{-algebra}, \mathbf{X} \in \mathcal{A}^n, \ g(\mathbf{X}) \succeq 0 \ (g \in S)$$

$$f_{C^*}^{nc} \leq f_*^{nc} \leq f_*^c$$

• SDP lower bounds: $\min L(f)$ s.t. $L \in \mathbb{R}\langle \mathbf{x} \rangle_{2t}$ or $L \in \mathbb{R}[\mathbf{x}]_{2t}$ s.t. ....
Asymptotic convergence: $f_t^{nc} \longrightarrow f_{C^*}^{nc}$, $f_t^c \longrightarrow f_*^c$ as $t \to \infty$

• Equality: $f_t^{nc} = f_*^{nc}$, $f_t^c = f_*^c$ if order t bound has **flat** optimal solution

For matrix factorization ranks: same framework, but now minimizing $L(1)$

Polynomial optimization approach for cpsd-rank

Assume $\mathbf{X} = (X_1, \ldots, X_n) \in (\mathcal{H}_+^d)^n$ is a Gram factorization of $A \in \mathcal{CS}_+^n$

The (real part of the) trace evaluation L at $\mathbf{X}$ satisfies:

(0) $L(1) = d$

(1) $A = (L(x_i x_j))$

(2) L is symmetric, tracial, positive

(3) $L(p^*(\sqrt{A_{ii}} x_i - x_i^2)p) \geq 0 \;\; \forall p$ [localizing constraints]

(3) holds: $A_{ii} = \mathrm{Tr}(X_i^2) \Longrightarrow \sqrt{A_{ii}} X_i - X_i^2 \succeq 0$

Define the parameters for $t \in \mathbb{N} \cup \{\infty\}$

$$\xi_t^{cpsd}(A) = \min \; L(1) \;\; \text{s.t.} \;\; L \in \mathbb{R}\langle \mathbf{x} \rangle_{2t}^* \text{ satisfies (1)-(3)}$$

$$\xi_*^{cpsd}(A): \;\; \text{add to } \xi_\infty^{cpsd} \text{ the constraint } \mathrm{rank}\, M(L) < \infty$$

$$\text{moment matrix:} \;\; M(L) = (L(u^* v))_{u,v \in \langle \mathbf{x} \rangle}$$

$$\xi_1^{cpsd}(A) \leq \ldots \leq \xi_t^{cpsd}(A) \leq \ldots \leq \xi_\infty^{cpsd}(A) \leq \xi_*^{cpsd}(A) \leq \text{cpsd-rank}_{\mathbb{C}}(A)$$

Properties of the bounds ξ_t^{cpsd}

$$\xi_1^{cpsd}(A) \leq \ldots \leq \xi_t^{cpsd}(A) \leq \ldots \leq \xi_\infty^{cpsd}(A) \leq \xi_*^{cpsd}(A) \leq \text{cpsd-rank}_{\mathbb{C}}(A)$$

- **Asymptotic convergence**: $\xi_t^{cpsd}(A) \to \xi_\infty^{cpsd}(A)$ as $t \to \infty$

  $\xi_\infty^{cpsd}(A) = \min\ \alpha$ s.t. $A = \alpha\ (\tau(X_iX_j))$ for some C^*-algebra $(\mathcal{A}, \tau)$ and $\mathbf{X} \in \mathcal{A}^n$ with $\sqrt{A_{ii}}X_i - X_i^2 \succeq 0\ \forall i$

- $\xi_*^{cpsd}(A) = \min \alpha$ s.t. ... $\mathcal{A}$ **finite dimensional** ...

  $= \min L(1)$ s.t. L **conic combination of trace evaluations** at $\mathbf{X}$ ...

- **Finite convergence**: $\xi_t^{cpsd}(A) = \xi_*^{cpsd}(A)$ if $\xi_t^{cpsd}(A)$ has an optimal solution L which is **flat**: $\mathrm{rank} M_t(L) = \mathrm{rank} M_{t-1}(L)$

- $\xi_1^{cpsd}(A) \geq \frac{(\sum_i \sqrt{A_{ii}})^2}{\sum_{i,j} A_{ij}}$ [analytic bound of Prakash et al.'16]

- Can **strengthen the bounds** by adding constraints on L:
  1. $L(p^*(v^\mathsf{T}Av - (\sum_i v_ix_i)^2)p) \geq 0$ for all $v \in \mathbb{R}^n$ [v-constraints]
  2. $L(pgp^*g') \geq 0$ for g, g' are localizing for A [Berta et al.'16]
  3. $L(px_ix_j) = 0$ if $A_{ij} = 0$ [zeros propagate]
  4. $L(p(\sum_i v_ix_i)) = 0$ for all $v \in \ker A$

Small example

Consider $A = \begin{pmatrix} 1 & 1/2 & 0 & 0 & 1/2 \\ 1/2 & 1 & 1/2 & 0 & 0 \\ 0 & 1/2 & 1 & 1/2 & 0 \\ 0 & 0 & 1/2 & 1 & 1/2 \\ 1/2 & 0 & 0 & 1/2 & 1 \end{pmatrix}$

- $\text{cpsd-rank}(A) \leq 5$

  because if $\mathbf{X} = \text{Diag}(1,1,0,0,0)$ and its cyclic shifts
  then $\mathbf{X}/\sqrt{2}$ is a factorization of A

- $L = \frac{1}{2} L_{\mathbf{X}}$ is feasible for $\xi_*^{cpsd}(A)$, with value $L(1) = 5/2$

  Hence $\xi_*^{cpsd}(A) \leq 5/2$, in fact $\xi_2^{cpsd}(A) = \xi_*^{cpsd}(A) = 5/2$

- But $\xi_{2,V}^{cpsd}(A) = 5 \implies \text{cpsd-rank}(A) = 5$
  with the v-constraints for $v = (1,-1,1,-1,1)$ and its cyclic shifts

Lower bounds for cp-rank

Same approach: Minimize $L(1)$ for $L \in \mathbb{R}[\mathbf{x}]_{2t}$ (commutative)
satisfying (1)-(3): $L(p^2) \geq 0$, $L(p^2(\sqrt{A_{ii}}x_i - x_i^2)) \geq 0$, $A = (L(x_i x_j))$
and

(4) $L(p^2(A_{ij} - x_i x_j)) \geq 0$

(5) $L(u) \geq 0$, $L(u(A_{ij} - x_i x_j)) \geq 0$ for u monomial

(6) $A^{\otimes l} - (L(u^* v))_{u,v \in \langle \mathbf{x} \rangle_{=l}} \succeq 0$ for $2 \leq l \leq t$

Comparison to the bounds τ_{cp}^{sos} and τ_{cp} of [Fawzi-Parrilo'16]:

- $\xi_2^{cp}(A) \geq \tau_{cp}^{sos}(A)$
- $\tau_{cp}(A) = \xi_*^{cp}(A)$
- $\tau_{cp}(A)$ is reached as asymptotic limit when using v-constraints for a dense subset of $\mathbb{S}^{n-1}$ instead of constraints (5)-(6)

Example: $A = \begin{pmatrix} (q+a)I_p & J_{p,q} \\ J_{q,p} & (p+b)I_q \end{pmatrix}$ for $a, b \geq 0$

- $\xi_2^{cp}(A) \geq pq$
- $\xi_2^{cp}(A) = 6$ is tight for $(p,q) = (2,3)$, since $\text{cp-rank}(A) = 6$ but $\tau_{cp}^{sos} < 6$ for nonzero $(a,b) \in [0,1]^2$, equal to 5 on large region

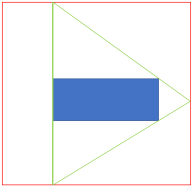
Lower bounds for rank_+ and $\mathrm{psd\text{-}rank}$

Same approach: as **no a priori bound** on the eigenvalues of the factors
... **rescale** the factors to get such bounds and thus localizing constraints
Get now $\tau_+(A) = \xi_\infty^+(A)$ directly as asymptotic limit of the SDP bounds

Example for rank_+: [Fawzi-Parrilo'16]

$$S_{a,b} = \begin{pmatrix} 1-a & 1+a & 1+a & 1-a \\ 1+a & 1-a & 1-a & 1+a \\ 1-b & 1-b & 1+b & 1+b \\ 1+b & 1+b & 1-b & 1-b \end{pmatrix} \quad \text{for } a, b \in [0,1]$$

slack matrix of nested rectangles: $R = [-a,a] \times [-b,b] \subseteq P = [-1,1]^2$



$\exists$ triangle T s.t. $R \subseteq T \subseteq P \iff \mathrm{rank}_+(S_{a,b}) = 3$

$$\mathrm{rank}_+(S_{a,b}) = 3 \iff (1+a)(1+b) \leq 2 \quad \text{(in dark blue region)}$$

$\mathrm{rank}_+(S_{a,b}) = 4$: outside dark blue region

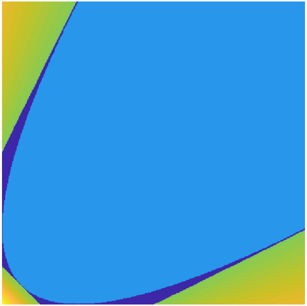
$\tau_+^{sos}(S_{a,b}) > 3$: in yellow region

$\xi_2^+(S_{a,b}) > 3$: in green & yellow regions

Small example for psd-rank

[Fawzi et al.'15] For $M_{b,c} = \begin{pmatrix} 1 & b & c \\ c & 1 & b \\ b & c & 1 \end{pmatrix}$

$$\text{psd-rank}_{\mathbb{R}}(M_{b,c}) \leq 2 \iff b^2 + c^2 + 1 \leq 2(b + c + bc)$$



$\text{psd-rank}(M_{b,c}) = 3$: outside light blue region

$\xi_2^{psd}(M_{b,c}) > 2$: in yellow region

Concluding remarks

- Polynomial optimization approach:

commutative	(tracial) noncommutative
copositive cone $\mathcal{CP}^n$	completely positive semidefinite cone $\mathcal{CS}_+^n$
classical coloring $\chi(G)$	quantum coloring $\chi_q(G)$
cp-rank, rank_+	$\text{cpsd-rank}_\mathbb{C}$, $\text{psd-rank}_\mathbb{C}$

- The approach extends to other quantum graph parameters
- Extension to nonnegative tensor rank [Fawzi-Parrilo 2016], nuclear norm of symmetric tensors [Nie 2016]
- How to tailor the bounds for **real** ranks: $\text{cpsd-rank}_\mathbb{R}$, $\text{psd-rank}_\mathbb{R}$?
- Structure of the cone $\mathcal{CS}_+^n$? little known already for small $n \geq 5$...