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

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

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 $CS_+^n$

- 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 $CP^n$

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

- Clearly: $CP^n \subseteq CS_+^n \subseteq \text{cl}(CS_+^n) \subseteq S_+^n \cap \mathbb{R}_+^{n \times n} =: DNN^n$

Is the cone $CS_+^n$ closed?
Strict inclusions $\mathcal{CP}^n \subseteq \mathcal{CS}^n_+ \subseteq \mathcal{DNN}^n$

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

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

$$A = \begin{pmatrix} 1 & a & b & b & a \\ a & 1 & a & b & b \\ b & a & 1 & a & b \\ b & b & a & 1 & a \\ a & b & b & a & 1 \end{pmatrix}$$

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 $\sqrt{A} \succeq 0$:

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

$\blacktriangleright$ [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 $\text{cl}(\mathcal{CS}^n_+)$

Moreover, $A = \begin{pmatrix} 4 & 2 & 0 & 0 & 2 \\ 2 & 4 & 2 & 0 & 0 \\ 0 & 2 & 4 & 3 & 0 \\ 0 & 0 & 3 & 4 & 2 \\ 2 & 0 & 0 & 2 & 4 \end{pmatrix} \not\in \text{cl}(\mathcal{CS}^5_+) !$

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 $\mathcal{M}_U$ such that $\text{cl}(\mathcal{CS}^n_+)$ consists of all matrices $A$ having a Gram factorization by positive elements in $\mathcal{M}_U$

(using tracial ultraproducts of matrix algebras)

New cone $\mathcal{CS}^n_{+C^*}$: all matrices having a Gram representation by positive elements in some $C^*$-algebra with trace. Then $A \not\in \mathcal{CS}^n_{+C^*}$, $\mathcal{CS}^n_{+C^*}$ is closed, and

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

Equality $\text{cl}(\mathcal{CS}_+^n) = \mathcal{CS}^n_{+C^*}$ under Connes’ embedding conjecture
SDP outer approximations of $\mathcal{CS}^n_+$

Assume $A \in \mathcal{CS}^n_+$: $A = (\text{Tr}(X_iX_j))$ for some $X_1, \ldots, X_n \in S^d_+$

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

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

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

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

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

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

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

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

$\mathcal{CS}^n_+ \subseteq \mathcal{F}_{t+1} \subseteq \mathcal{F}_t, \quad \mathcal{CS}^n_+ \subseteq \text{cl}(\mathcal{CS}^n_+) \subseteq \mathcal{CS}^n_+^{C^*} \subseteq \bigcap_{t \geq 1} \mathcal{F}_t$

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

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

Noncommutative analogue of outer approximations of $\mathcal{CP}^n$ [Nie’14]
Quantum graph coloring
Classical coloring number

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

\[ \sum_{i \in [k]} x_u^i = 1 \quad \forall u \in V(G) \]

\[ x_u^i x_v^i = 0 \quad \forall i \in [k] \quad \forall uv \in E(G) \]

\[ x_u^i x_u^j = 0 \quad \forall i \neq j \in [k], \forall u \in V(G) \]
Quantum coloring number

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

\[ \chi_q(G) = \min k \in \mathbb{N} \text{ s.t. } \exists d \in \mathbb{N} \exists X^i_u \in S^d_+ \text{ for } u \in V(G), i \in [k] \]
\[ \sum_{i\in[k]} X^i_u = I \quad \forall u \in V(G) \]
\[ X^i_u X^i_v = 0 \quad \forall i \in [k], \forall uv \in E(G) \]
\[ X^i_u X^j_u = 0 \quad \forall i \neq j \in [k], \forall u \in V(G) \]

\[ \chi_q(G) \leq \chi(G) \]

[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

  $\begin{align*}
  i = j & \quad \text{if } u = v \\
  i \neq j & \quad \text{if } uv \in E
  \end{align*}$

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 $\{A_u^i\}_{i \in [k]}$: $A_u^i \in \mathcal{H}_+^d$, $\sum_{i \in [k]} A_u^i = I$

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

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

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

- 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 $\chi_q(G) \leq 3$ 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

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

\[
\sum_{i \in [k]} X^i_u = \sum_{j \in [k]} X^j_v \ (\neq 0) \quad (u, v \in V) \quad \text{(Q1)}
\]

\[
X^i_u X^j_v = 0 \ (i \neq j \in [k], u \in V), \quad X^i_u X^i_v = 0 \ (i \in [k], uv \in E) \quad \text{(Q2)}
\]

Set \( A := \text{Gram}(X^i_u) \). Then: \( X^i_u X^j_v = 0 \iff \text{Tr}(X^i_u X^j_v) = 0 = A_{ui,vj} \)

Then: \( \chi_q(G) = \min k \quad \text{s.t. } \exists A \in CS_{nk}^+ \text{ satisfying:} \)

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

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

Theorem (L-Piovesan 2015)

- Replacing \( CS_+ \) by the cone \( CP \), we get \( \chi(G) \)
- Replacing \( CS_+ \) by the cone \( DNN \), get the theta number \( \vartheta^+(\overline{G}) \)
- Hence: \( \vartheta^+(\overline{G}) \leq \chi_q(G) \) \quad \text{[Mancinska-Roberson 2015]}
SDP relaxations for coloring

If \((X^i_u)\) 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
   
   \[
   1 - \sum_{i=1}^{k} x^i_u \ (u \in V), \ x^i_u x^j_u \ (i \neq j, u \in V), \ x^i_u x^i_v \ (uv \in E, i \in [k])
   \]

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

\[
\xi^{nc}_t(G) = \min k \text{ such that } \exists L \in \mathbb{R}\langle x\rangle^{*}_{2t} \text{ satisfying (1)-(3)}
\]

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

\[
\xi^{nc}_t(G) \leq \chi_q(G) \quad \xi^c_t(G) \leq \chi(G)
\]

- For \(t = 1\) get the theta number: \(\xi^{nc}_1(G) = \xi^c_1(G) = \vartheta^+(\overline{G})\) [Gvozdenović-L 2008]
- \(\xi^c_t(G) = \chi(G) \forall t \geq n\) [Gribling-de Laat-L 2017]
- \(\xi^{nc}_{t_0}(G) = \chi_{C^*}(G) \leq \chi_q(G) \forall t \geq t_0\) [Ortiz-Paulsen 2016]

\(\chi_{C^*}(G)\) = allow solutions \(X^i_u \in A\) for any \(C^*\)-algebra \(A\) with trace
Quantum correlations

\[ C_q(n, k) = \text{quantum correlations} \quad p = (p(i, j|u, v)) := (\langle \psi, A^i_u \otimes B^j_v \psi \rangle), \]
with \( d \in \mathbb{N}, A^i_u, B^j_v \in \mathcal{H}^d_+ \) with \( \sum_i A^i_u = \sum_j B^j_v = I, \psi \in \mathbb{C}^d \otimes \mathbb{C}^d \) unit

Theorem (Sikora-Varvitsiotis 2015)

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

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

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

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 \( \implies \mathcal{CS}^N_+ \) is not closed for large \( N \) (\( \geq 1942 \))
Matrix factorization ranks
Four matrix factorization ranks

**Symmetric** factorizations:

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

Applications: probability, entanglement dimension in quantum information

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

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

Applications: (quantum) communication complexity, extended formulations of polytopes
rank\(_+\), psd-rank\(_R\) and extended formulations

[\textbf{Slack matrix}: \( S = (b_i - a_i^T v)_{v,i} \) if \( P = \text{conv}(V) = \{ x : a_i^T x \leq b_i \ \forall i \} \)]

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

Smallest \( k \) s.t. \( P \) is \textbf{projection of affine section} of \( S_+^k \) is \( \text{psd-rank}_R(S) \)

[Rothvoss’14] The matching polytope of \( K_n \) has \textbf{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 $\text{cpsd-rank}$ exists in terms of matrix size!

$\text{rank}_{+}$, $\text{psd-rank}$, $\text{cp-rank}$ are computable; is $\text{cpsd-rank}$ computable?

[Vavasis 2009] $\text{rank}_{+}$ 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 $\text{cp}$ and $\text{cpsd}$ 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 $\text{rank}_+$, and $\tau_{cp}(\cdot)$ for cp-rank, based on their **atomic definition**:
  \[
  \text{rank}_+(A) = \min d \text{ s.t. } A = u_1 v_1^T + \ldots + u_d v_d^T \text{ with } u_i, v_i \in \mathbb{R}_+^n
  \]
  \[
  \text{cp-rank}(A) = \min d \text{ s.t. } A = u_1 u_1^T + \ldots + u_d u_d^T \text{ with } u_i \in \mathbb{R}_+^n
  \]
  \[
  \tau_+(A) = \min \alpha \text{ s.t. } A \in \alpha \cdot \text{conv}(R \in \mathbb{R}^{m \times n} : 0 \leq R \leq A, \text{rank}(R) \leq 1)
  \]
  \[
  \tau_{cp}(A) = \min \alpha \text{ s.t. } A \in \alpha \cdot \text{conv}(R \in S^n : 0 \leq R \leq A, \text{rank}(R) \leq 1, R \preceq A)
  \]

- [FP 2016] also defines tractable SDP relaxations $\tau^{sos}_+(\cdot)$ and $\tau^{sos}_{cp}(\cdot)$:
  \[
  \tau^{sos}_+(A) \leq \tau_+(A) \leq \text{rank}_+(A), \quad \text{rank}(A) \leq \tau^{sos}_{cp}(A) \leq \tau_{cp}(A) \leq \text{cp-rank}(A)
  \]

- Combinatorial lower bound: **Boolean rank** $\text{rank}_B(A) \leq \text{rank}_+(A)$
  \[
  \text{rank}_B(A) = \chi(RG(A)) : \text{coloring number of the 'rectangle graph' } RG(A)
  \]
  \[
  \tau_+(A) \geq \chi_f(RG(A)), \quad \tau^{sos}_+(A) \geq \vartheta(RG(A))
  \]

[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–]

\[
f^c_\ast = \inf f(x) \text{ s.t. } x \in \mathbb{R}^n, g(x) \geq 0 \ (g \in S)
\]

\[
f^{nc}_\ast = \inf \text{Tr}(f(X)) \text{ s.t. } d \in \mathbb{N}, X \in (S^d)^n, g(X) \succeq 0 \ (g \in S)
\]

\[
f^{nc}_{C^\ast} = \inf \tau(f(X)) \text{ s.t. } \mathcal{A} \ C^\ast\text{-algebra}, X \in \mathcal{A}^n, g(X) \succeq 0 \ (g \in S)
\]

\[
f^{nc}_{C^\ast} \leq f^{nc}_\ast \leq f^c_\ast
\]

• SDP lower bounds: \( \min L(f) \) s.t. \( L \in \mathbb{R}\langle x \rangle_{2t} \) or \( L \in \mathbb{R}[x]_{2t} \) s.t. ....

Asymptotic convergence: \( f^{nc}_t \longrightarrow f^{nc}_{C^\ast}, \ f^c_t \longrightarrow f^c_\ast \) as \( t \rightarrow \infty \)

• Equality: \( f^{nc}_t = f^{nc}_\ast, \ f^c_t = f^c_\ast \) if order \( t \) bound has flat optimal solution

For matrix factorization ranks: same framework, but now minimizing \( L(1) \)
Polynomial optimization approach for \textit{cpsd-rank}

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

The (real part of the) trace evaluation $L$ at $X$ satisfies:

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

(2) $L$ is symmetric, tracial, positive

(3) $L(p^* (\sqrt{A_{ii}} x_i - x_i^2) p) \geq 0 \ \forall p$ \hspace{1cm} [localizing constraints]
(3) holds: $A_{ii} = \text{Tr}(X_i^2) \implies \sqrt{A_{ii}} X_i - X_i^2 \succeq 0$

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

$$\xi_{c_{psd}}^{t}(A) = \min L(1) \text{ s.t. } L \in \mathbb{R}\langle x \rangle_{2t}^* \text{ satisfies (1)-(3)}$$

$$\xi_{c_{psd}}^{*}(A) : \text{ add to } \xi_{c_{psd}}^{\infty} \text{ the constraint rank } M(L) < \infty$$

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

$$\xi_{c_{psd}}^{1}(A) \leq \ldots \leq \xi_{c_{psd}}^{t}(A) \leq \ldots \leq \xi_{c_{psd}}^{\infty}(A) \leq \xi_{c_{psd}}^{*}(A) \leq \text{cpsd-rank}_\mathbb{C}(A)$$
Properties of the bounds $\xi_t^{cpsd}$

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

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

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

- **$\xi_*^{cpsd}(A)$**

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

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

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

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

- **Can strengthen the bounds** by adding constraints on $L$:
  1. $L(p^*(v^T Av - (\sum_i v_i x_i)^2)p) \geq 0$ for all $v \in \mathbb{R}^n$ [v-constraints]
  2. $L(pg p^* g') \geq 0$ for $g, g'$ are localizing for $A$ [Berta et al.'16]
  3. $L(px_i x_j) = 0$ if $A_{ij} = 0$ [zeros propagate]
  4. $L(p(\sum_i v_i x_i)) = 0$ for all $v \in \ker A$
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 $X = \text{Diag}(1, 1, 0, 0, 0)$ and its cyclic shifts
then $X/\sqrt{2}$ is a factorization of $A$

▶ $L = \frac{1}{2}L_X$ is feasible for $\xi_{\text{cpsd}}^*(A)$, with value $L(1) = 5/2$

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

▶ But $\xi_{2,\nu}(A) = 5 \implies \text{cpsd-rank}(A) = 5$

with the $\nu$-constraints for $\nu = (1, -1, 1, -1, 1)$ and its cyclic shifts
Lower bounds for cp-rank

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

(4) $L(p^2(A_{ij} - x_ix_j)) \geq 0$
(5) $L(u) \geq 0$, $L(u(A_{ij} - x_ix_j)) \geq 0$ for $u$ monomial
(6) $A^\otimes l - (L(u^*v))_{u,v \in \langle x \rangle = l} \geq 0$ for $2 \leq l \leq t$

Comparison to the bounds $\tau_{\text{sos}}^{\text{cp}}$ and $\tau_{\text{cp}}$ of [Fawzi-Parrilo'16]:

- $\xi_{cp}^{\text{cp}}(A) \geq \tau_{\text{sos}}^{\text{cp}}(A)$
- $\tau_{cp}(A) = \xi_{*}^{\text{cp}}(A)$
- $\tau_{cp}(A)$ 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 $a, b \geq 0$

- $\xi_{\text{cp}}(A) \geq pq$
- $\xi_{2}^{\text{cp}}(A) = 6$ is tight for $(p, q) = (2, 3)$, since $\text{cp-rank}(A) = 6$
- but $\tau_{\text{cp}}^{\text{sos}} < 6$ for nonzero $(a, b) \in [0, 1]^2$, equal to 5 on large region
Lower bounds for rank$_+$ and psd-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 $\tau_+(A) = \xi_+(A)$ directly as asymptotic limit of the SDP bounds

**Example for rank$_+$:** [Fawzi-Parrilo’16]

\[
S_{a,b} = \begin{pmatrix}
1 - a & 1 + a & 1 + a & 1 - a \\
1 + a & 1 - a & 1 - a & 1 + a \\
1 - b & 1 - b & 1 + b & 1 + b \\
1 + b & 1 + b & 1 - b & 1 - b
\end{pmatrix}
\]

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. $R \subseteq T \subseteq P \iff \text{rank}_+(S_{a,b}) = 3$
\[ \text{rank}_+(S_{a,b}) = 3 \iff (1 + a)(1 + b) \leq 2 \quad \text{(in dark blue region)} \]

- \( \text{rank}_+(S_{a,b}) = 4: \quad \text{outside dark blue region} \)
- \( \tau^sos_+(S_{a,b}) > 3: \quad \text{in yellow region} \)
- \( \xi^+_2(S_{a,b}) > 3: \quad \text{in green \\& yellow regions} \)
Small example for psd-rank

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

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

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:

<table>
<thead>
<tr>
<th>commutative</th>
<th>(tracial) noncommutative</th>
</tr>
</thead>
<tbody>
<tr>
<td>copositive cone $\mathcal{CP}^n$</td>
<td>completely positive semidefinite cone $\mathcal{CS}_+^n$</td>
</tr>
<tr>
<td>classical coloring $\chi(G)$</td>
<td>quantum coloring $\chi_q(G)$</td>
</tr>
<tr>
<td>cp-rank, rank$_+$</td>
<td>cpsd-rank$<em>\mathbb{C}$, psd-rank$</em>\mathbb{C}$</td>
</tr>
</tbody>
</table>

- 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: cpsd-rank$_\mathbb{R}$, psd-rank$_\mathbb{R}$?

- Structure of the cone $\mathcal{CS}_+^n$? little known already for small $n \geq 5$...