

Pairwise Completely Positive Matrices and Quantum Entanglement

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Completely Positive Matrices

Definition

A matrix $X \in M_n(\mathbb{R})$ is called **completely positive (CP)** if there exists some entrywise non-negative $B \in M_{n,m}(\mathbb{R})$ (with m arbitrary) such that

$$X = BB^T.$$

- Every CP matrix is positive semidefinite and entrywise non-negative.
- Converse holds if (and only if) $n \leq 4$.
- Determining complete positivity is NP-hard.
- Studied for decades, important in convex optimization.

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Pairwise Completely Positive Matrices

Definition

An ordered pair of matrices $(X, Y) \in M_n(\mathbb{C}) \times M_n(\mathbb{C})$ is called **pairwise completely positive (PCP)** if there exist matrices $A, B \in M_{n,m}(\mathbb{C})$ (with m arbitrary) such that

$$X = (A \odot B)(A \odot B)^* \quad \text{and} \quad Y = (A \odot \bar{A})(B \odot \bar{B})^*.$$

- Above, “ \odot ” is the Hadamard (entrywise) product.
- If (X, Y) is PCP then X is positive semidefinite and Y is entrywise non-negative.
- X is CP if and only if (X, X) is PCP (not quite trivial).

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Necessary Conditions

Showing (X, Y) is (not) PCP is hard. Let's develop one-sided tests!

Theorem (†)

If $(X, Y) \in M_n(\mathbb{C}) \times M_n(\mathbb{C})$ is PCP then:

- X is positive semidefinite.
- Y is real and entrywise non-negative.
- $x_{i,i} = y_{i,i}$ for all $1 \leq i \leq n$.
- $|x_{i,j}|^2 \leq y_{i,j}y_{j,i}$ for all $1 \leq i, j \leq n$.
- X is "more diagonal" than Y : $\|X\|_1 - \|X\|_{\text{tr}} \leq \|Y\|_1 - \|Y\|_{\text{tr}}$.

- $\|\cdot\|_{\text{tr}}$ is the trace norm, $\|\cdot\|_1$ is the entrywise 1-norm

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Answer in Small Dimensions

When $n = 2$, the first four necessary conditions of the previous theorem are actually sufficient as well:

Theorem

A pair $(X, Y) \in M_2(\mathbb{C}) \times M_2(\mathbb{C})$ is PCP if and only if conditions (a)–(d) of Theorem (†) hold.

- Analogous to $X \in M_4(\mathbb{R})$ being CP if and only if it is positive semidefinite and entrywise non-negative.
- The “if” direction fails for PCP matrices whenever $n \geq 3$:

$$X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad Y = \begin{bmatrix} 1 & 2 & 1/2 \\ 1/2 & 1 & 2 \\ 2 & 1/2 & 1 \end{bmatrix}.$$

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Sufficient Conditions

Let's develop a one-sided test in the other direction too. To do so, we need...

Definition

The *comparison matrix* of $X \in M_n(\mathbb{C})$ is the matrix

$$M(X) = \begin{bmatrix} |x_{1,1}| & -|x_{1,2}| & \cdots & -|x_{1,n}| \\ -|x_{2,1}| & |x_{2,2}| & \cdots & -|x_{2,n}| \\ \vdots & \vdots & \ddots & \vdots \\ -|x_{n,1}| & -|x_{n,2}| & \cdots & |x_{n,n}| \end{bmatrix}.$$

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Sufficient Conditions

We now recall a sufficient condition for complete positivity:

Theorem (Drew–Johnson–Loewy (1994))

If $X \in M_n(\mathbb{R})$ is positive semidefinite, entrywise non-negative, and such that $M(X)$ is positive semidefinite, then X is CP.

We have a natural generalization for PCP matrices:

Theorem

If $(X, Y) \in M_n(\mathbb{C}) \times M_n(\mathbb{C})$ satisfies conditions (a)–(d) of Theorem (†), and $M(X)$ is positive semidefinite, then (X, Y) is PCP.

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Separability and Entanglement

Definition

A matrix $Z \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ is called **separable** if there exist positive semidefinite $\{X_i\}, \{Y_i\} \in M_n(\mathbb{C})$ such that

$$Z = \sum_i X_i \otimes Y_i.$$

Otherwise, Z is called **entangled**.

- Separable matrices are positive semidefinite.
- Characterizing these matrices is one of the central problems in quantum information theory.
- Determining separability is NP-hard.

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Necessary Conditions for Separability

Again, we use one-sided tests. The most popular such test is based on the **partial transpose**, which is the linear map Γ on $M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ defined by

$$\Gamma(X \otimes Y) = X \otimes Y^T.$$

Theorem (Horodecki, Peres, Størmer, Woronowicz?)

If $Z \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ is separable then Z^Γ is positive semidefinite.

- If Z^Γ is positive semidefinite, we say that Z has **positive partial transpose (PPT)**.

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Connection with PCP Matrices

Let's establish the connection that makes this talk about PCP matrices make sense in a quantum information theory session.

- Given a pair $(X, Y) \in M_n(\mathbb{C}) \times M_n(\mathbb{C})$ with $x_{i,i} = y_{i,i}$ for all $1 \leq i \leq n$, we define $Z_{X,Y} \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ by

$$Z_{X,Y} = \sum_{i,j=1}^n x_{i,j} |i\rangle\langle j| \otimes |i\rangle\langle j| + \sum_{i \neq j=1}^n y_{i,j} |i\rangle\langle i| \otimes |j\rangle\langle j|.$$

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Connection with PCP Matrices

For example, if $n = 3$ then $Z_{X,Y}$ has the form (where \cdot means 0)...

$$Z_{X,Y} = \begin{bmatrix} x_{1,1} & \cdot & \cdot & \cdot & x_{1,2} & \cdot & \cdot & \cdot & x_{1,3} \\ \cdot & y_{1,2} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & y_{1,3} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & y_{2,1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ x_{2,1} & \cdot & \cdot & \cdot & x_{2,2} & \cdot & \cdot & \cdot & x_{2,3} \\ \cdot & \cdot & \cdot & \cdot & \cdot & y_{2,3} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & y_{3,1} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & y_{3,2} & \cdot \\ x_{3,1} & \cdot & \cdot & \cdot & x_{3,2} & \cdot & \cdot & \cdot & x_{3,3} \end{bmatrix} \cdot$$

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Connection with PCP Matrices

Many properties of the pair (X, Y) correspond naturally with properties of $Z_{X,Y}$:

- $Z_{X,Y}$ is separable if and only if (X, Y) is pairwise completely positive.
- $Z_{X,Y}$ is positive semidefinite if and only if X is positive semidefinite and Y is real and entrywise non-negative. (Properties (a) and (b) in Theorem (†).)
- $Z_{X,Y}^\Gamma$ is positive semidefinite if and only if $|x_{i,j}|^2 \leq y_{i,j}y_{j,i}$ for all $1 \leq i, j \leq n$. (Property (d) in Theorem (†).)

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However, the sufficient condition for PCP-ness that we presented gives us a completely new way of showing that matrices of this special form are separable:

Theorem

If each of $Z_{X,Y}$, $Z_{X,Y}^\Gamma$, and $M(Z_{X,Y})$ are positive semidefinite, then $Z_{X,Y}$ is separable.

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Absolute Separability

OK, but why do we care about matrices of the form $Z_{X,Y}$ in the first place? This separability test only applies to very specially cooked up states. Well...

Definition

A matrix $Z \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ is called *absolutely separable* if UZU^* is separable for all unitary $U \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$.

- For example, identity matrix is absolutely separable, but (somewhat surprisingly?), so are many other matrices.

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Absolute PPT

Very little is known about absolute separability, but (as usual) there is a simple necessary condition for absolute separability:

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A matrix $Z \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ is called *absolutely PPT* if UZU^* is PPT for all unitary $U \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$.

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It is known that, for absolute PPT, we do not need to check that each UZU^* is PPT—there is a (finite!) list of unitaries $\{U_i\}$ such that Z is absolutely PPT if and only if $U_i Z U_i^*$ is PPT for all i .

- Question: Can we find an entangled but PPT $U_i Z U_i^*$?
- Answer: No. Every single $U_i Z U_i^*$ has the form of the $Z_{X,Y}$ matrices, and our sufficient condition shows that if they are PPT, they are separable.
- The Upshot: If there is a gap between absolute separability and absolute PPT, we have to look at some other weird unitaries to find it.

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Thank you!

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N. Johnston and O. MacLean. Pairwise completely positive matrices and conjugate local diagonal unitary quantum states. *Electronic Journal of Linear Algebra*, 35:156–180, 2019. [arXiv:1807.06897](https://arxiv.org/abs/1807.06897) [quant-ph]