



ON POSITIVE PARTIAL TRANSPOSE MATRICES*

MEHMET GUMUS[†], JIANZHEN LIU[‡], SAMIR RAOUAFI[§], AND TIN-YAU TAM[†]

Dedicated to Professor Randall R. Holmes in honor of his retirement from Auburn University in 2019.

Abstract. This paper mainly focuses on the class of 2×2 block PPT matrices. The relationship between PPT matrices and the norm inequalities is further explored. Some properties of a non-PPT matrix in terms of its eigenvalues are investigated. Moreover, a number of useful sufficient conditions for a matrix to be PPT are provided.

Key words. Positive semi-definite matrix, Positive partial transpose, Block matrix, Unitarily invariant norm.

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1. Introduction. Let $\mathbb{C}^{n \times n}$ be the space of $n \times n$ complex matrices. Given Hermitian matrices $A, B \in \mathbb{C}^{n \times n}$, we shall write $A \succeq B$ (resp., $A \succ B$) if $A - B$ is positive semi-definite (resp., positive definite), i.e., $A - B \succeq 0$ (resp., $A - B \succ 0$). The identity matrix of appropriate size shall be denoted by I . A norm $\|\cdot\|$ over $\mathbb{C}^{n \times n}$ is called *unitarily invariant* if $\|UXV\| = \|X\|$ for any $X \in \mathbb{C}^{n \times n}$ and any unitary matrices $U, V \in \mathbb{C}^{n \times n}$. We shall denote the Ky-Fan norms [1, p. 35] of X by $\|X\|_{(k)}$ for $1 \leq k \leq n$.

Throughout this paper, we assume that M is a positive semi-definite matrix in block matrix form:

$$M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{C}^{2n \times 2n},$$

where $A, B, X \in \mathbb{C}^{n \times n}$. The matrix M is said to be *positive partial transpose*, or PPT for short in the sequel, if

$$M' = \begin{bmatrix} A & X^* \\ X & B \end{bmatrix} \succeq 0.$$

The study of PPT matrices is motivated by the theory of quantum information. In fact, the PPT property is also called the Peres-Horodecki criterion, which is a necessary condition for a bipartite quantum state on a composite Hilbert space $H_1 \otimes H_2$ to be separable. This condition is also sufficient in low dimensional composite spaces with $\dim H_1 = 2$ and $\dim H_2 = 2$ or 3 . For more details, we refer the reader to, for example, [4, 11] and the references therein.

As a stronger class of positive semi-definite block matrices, PPT matrices possess a number of useful properties. Therefore, this special class of block matrices has recently drawn much attention [2, 6, 7, 8, 9, 10, 12]. A characterization of PPT property involving spectral norm was provided in [2] for matrices M with $A+B = kI$, where $k \geq 0$. In [6, 8, 9, 10], trace, eigenvalues, singular values, and norm inequalities concerning

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[†]Department of Mathematics and Statistics, University of Nevada, Reno, Nevada 89557, USA (mgumus@unr.edu, ttam@unr.edu).

[‡]Department of Science, Mathematics and Technology, Medaille College, Buffalo, New York 14214, USA (jianzhen.liu@medaille.edu).

[§]Department of Mathematics and Statistics, Auburn University, Auburn, Alabama 36849, USA (sizr0067@auburn.edu).

PPT matrices were investigated. Recently, Zhang [12] showed that the image of positive semi-definite block matrices under the completely PPT map $\Phi(X) = \min\{m, n\} \text{tr}(X)I - X$, see [7], is a set of PPT matrices.

Exploiting the PPT property, a number of important results were derived in aforementioned papers. Most of these results yield necessary conditions for M to be PPT. To the best of our knowledge, sufficient conditions have not been studied well in the literature. In this work, we consider this problem by examining the positive semi-definite block matrices which are not PPT. These matrices are named here as non-PPT matrices. They were also considered by Lin [9] who presented some inequalities between the singular values of the off diagonal blocks and the eigenvalues of the geometric mean of the diagonal blocks. In Section 2, we discuss some intriguing properties of a non-PPT block matrix in terms of its eigenvalues. Our observation turns out to be quite useful criterion for determining PPT property of a positive semi-definite block matrix under some special cases. In Section 3, a characterization of non-PPT matrices is presented in terms of Ky-Fan norms. In addition, we give several sufficient conditions for the PPT property.

2. Eigenvalues of non-PPT matrices. In this section, we consider two types of non-PPT matrices. We show that M' has exactly one negative eigenvalue under the condition that either the dimension of M is 4×4 or a certain rank condition among the blocks of M holds. This observation leads to a characterization of PPT property in terms of a single determinantal condition for these cases.

We need the following characterization of the positive semi-definite 2×2 block matrices.

LEMMA 2.1. [13, Theorem 7.14] *Let $A \in \mathbb{C}^{n \times n}$ be positive definite and $X \in \mathbb{C}^{n \times m}$. Then for any positive semi-definite $B \in \mathbb{C}^{m \times m}$,*

$$M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \succeq 0 \quad \text{if and only if} \quad B \succeq X^* A^{-1} X.$$

Let us first consider the positive semi-definite block matrices with dimension 4×4 .

THEOREM 2.2. *Let $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{C}^{4 \times 4}$ be positive semi-definite with $A, B, X \in \mathbb{C}^{2 \times 2}$. If M is non-PPT, then M' has only one negative eigenvalue.*

Proof. By a continuity argument we may assume that $A \succ 0$. Since A is a positive definite and is a principal submatrix of M' , the Interlacing Eigenvalues Theorem, [3, Theorem 4.3.15], implies that M' has at most two negative eigenvalues. Suppose for a contradiction that M' has two negative eigenvalues. Since $M \succeq 0$, from Lemma 2.1 we get $B - X^* A^{-1} X \succeq 0$. Thus,

$$A^{-\frac{1}{2}}(B - X^* A^{-1} X)A^{-\frac{1}{2}} = A^{-\frac{1}{2}}BA^{-\frac{1}{2}} - A^{-\frac{1}{2}}X^*A^{-\frac{1}{2}}A^{-\frac{1}{2}}XA^{-\frac{1}{2}} \succeq 0,$$

and hence,

$$\text{tr}(A^{-\frac{1}{2}}(B - X^* A^{-1} X)A^{-\frac{1}{2}}) = \text{tr}(A^{-\frac{1}{2}}BA^{-\frac{1}{2}} - A^{-\frac{1}{2}}X^*A^{-\frac{1}{2}}A^{-\frac{1}{2}}XA^{-\frac{1}{2}}) \geq 0.$$

Therefore,

$$(2.1) \quad \text{tr}(A^{-\frac{1}{2}}(B - XA^{-1}X^*)A^{-\frac{1}{2}}) \geq 0.$$

On the other hand, we have $\det(M') \geq 0$ since M' has two negative eigenvalues. Schur Complement Formula, [13, p. 217], implies that $\det(B - XA^{-1}X^*) \geq 0$. This leads to

$$(2.2) \quad \det(A^{-\frac{1}{2}}(B - XA^{-1}X^*)A^{-\frac{1}{2}}) \geq 0.$$

Finally, (2.1) and (2.2) imply that $A^{-\frac{1}{2}}(B - XA^{-1}X^*)A^{-\frac{1}{2}} \succeq 0$, and so $B - XA^{-1}X^* \succeq 0$, which is a contradiction to the assumption of M' not being positive semi-definite. \square

The following corollary is an immediate consequence of Theorem 2.2.

COROLLARY 2.3. *Let $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{C}^{4 \times 4}$ be positive definite with $A, B, X \in \mathbb{C}^{2 \times 2}$. Then M is PPT if and only if $\det(M') \geq 0$.*

Proof. Necessity is obvious. For the sufficiency, assume that M is non-PPT. By Theorem 2.2, M' has at most one negative eigenvalue. Therefore, $\det M' \leq 0$. However, $\det M' \neq 0$. If on the contrary $\det M' = 0$, M' has a zero eigenvalue. Then we can choose a sufficiently small $\epsilon > 0$ such that $M - \epsilon I \succ 0$ and $M' - \epsilon I \not\prec 0$ with having two negative eigenvalues. This gives us a contradiction from Theorem 2.2. Hence, $\det M' < 0$, and the result follows. \square

Now we turn to a particular class of block matrices with arbitrary dimension. Let us write the eigenvalues of M and M' in increasing order:

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{2n-1} \leq \lambda_{2n}$$

and

$$\mu_1 \leq \mu_2 \leq \dots \leq \mu_{2n-1} \leq \mu_{2n},$$

respectively.

THEOREM 2.4. *Let $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{C}^{2n \times 2n}$ be positive semi-definite with $A, B, X \in \mathbb{C}^{n \times n}$. If*

$$\min \left\{ \text{rank}(A - B), \min_{\theta \in \mathbb{R}} \text{rank}(X + e^{i\theta}X^*) \right\} = 1,$$

then $\mu_2 \geq \lambda_1$.

Proof. First assume that $\text{rank}(A - B) = 1$. Let $P = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \in \mathbb{C}^{2n \times 2n}$. Then M' and $P^T M' P = \begin{bmatrix} B & X \\ X^* & A \end{bmatrix}$ have the same eigenvalues. We can write

$$\begin{bmatrix} B & X \\ X^* & A \end{bmatrix} = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} + \begin{bmatrix} B - A & 0 \\ 0 & A - B \end{bmatrix}.$$

Since $\text{rank}(B - A) = 1$, $\sigma(B - A) = \{t, 0, \dots, 0\}$ for some nonzero t . Therefore, the latter matrix in the above equation has the eigenvalues:

$$-t \leq 0 \leq \dots \leq 0 \leq t.$$

By Weyl's Theorem, [3, Theorem 4.3.1],

$$\lambda_1 + 0 \leq \mu_2,$$

and the result follows.

Now assume that $\text{rank}(X + e^{i\theta}X^*) = 1$ for some $\theta \in \mathbb{R}$. Let $U = \begin{bmatrix} I & 0 \\ 0 & e^{-i\theta}I \end{bmatrix} \in \mathbb{C}^{2n \times 2n}$ and $V = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} \in \mathbb{C}^{2n \times 2n}$. Then

$$UM'U^* = \begin{bmatrix} A & e^{i\theta}X^* \\ e^{-i\theta}X & B \end{bmatrix} \quad \text{and} \quad VMV^* = \begin{bmatrix} A & -X \\ -X^* & B \end{bmatrix}$$

share the same eigenvalues with M' and M , respectively. We can write

$$\begin{bmatrix} A & e^{i\theta} X^* \\ e^{-i\theta} X & B \end{bmatrix} = \begin{bmatrix} A & -X \\ -X^* & B \end{bmatrix} + \begin{bmatrix} 0 & X + e^{i\theta} X^* \\ e^{-i\theta} X + X^* & 0 \end{bmatrix}.$$

Since $\text{Rank}(X + e^{i\theta} X^*) = 1$, it has only one nonzero singular value, $\sigma_1 > 0$. Therefore, the latter matrix in above equation has the eigenvalues:

$$-\sigma_1 \leq 0 \leq \dots \leq 0 \leq \sigma_1.$$

Again by Weyl's Theorem,

$$\lambda_1 + 0 \leq \mu_2,$$

and the result follows. □

The above eigenvalue relationship yields the following results.

COROLLARY 2.5. *Let $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{C}^{2n \times 2n}$ be positive semi-definite with $A, B, X \in \mathbb{C}^{n \times n}$, and*

$$\min \left\{ \text{rank}(A - B), \min_{\theta \in \mathbb{R}} \text{rank}(X + e^{i\theta} X^*) \right\} = 1.$$

If M is non-PPT, then M' has only one negative eigenvalue.

One may ask whether there exists matrices satisfying the condition of the above corollary. Take, for instance,

$$(2.3) \quad M = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 1 & 1 & 0 & i \\ 1 & 0 & 2 & -i \\ 0 & -i & i & 3 \end{bmatrix} \succeq 0,$$

which is non-PPT. Note that

$$\text{rank}(A - B) = \text{rank} \begin{bmatrix} 0 & 1 + i \\ 1 - i & -2 \end{bmatrix} = 2$$

and

$$\text{rank}(X + e^{i\theta} X^*) = \text{rank} \begin{bmatrix} 1 + e^{i\theta} & 0 \\ 0 & i - e^{i\theta} i \end{bmatrix} \geq 1$$

for any $\theta \in \mathbb{R}$. When $\theta = 0$ or $\theta = \pi$, $\text{rank}(X + e^{i\theta} X^*) = 1$, which means that M satisfies the condition of Corollary 2.5.

For the other case, consider

$$M = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \succeq 0,$$

where $\text{rank}(A - B) = \text{rank} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = 1$ and $\text{rank}(X + e^{i\theta} X^*) = \text{rank} \begin{bmatrix} 0 & 1 \\ e^{i\theta} & 0 \end{bmatrix} = 2$ for any $\theta \in \mathbb{R}$. However, M is non-PPT.

COROLLARY 2.6. Let $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{C}^{2n \times 2n}$ be positive definite with $A, B, X \in \mathbb{C}^{n \times n}$, and

$$\min \left\{ \text{rank}(A - B), \min_{\theta \in \mathbb{R}} \text{rank}(X + e^{i\theta} X^*) \right\} = 1.$$

Then M is PPT if and only if $\det M' \geq 0$.

Proof. Proof is similar to the proof of Corollary 2.3. □

REMARK 2.7. Let

$$k = \min \left\{ \text{rank}(A - B), \min_{\theta \in \mathbb{R}} \text{rank}(X + e^{i\theta} X^*) \right\}.$$

Replacing μ_2 by μ_{k+1} in the proof of Theorem 2.4, we obtain $\mu_{k+1} \geq \lambda_1$. Therefore, M' has at most k negative eigenvalues. In particular, if $k = 0$, then M is PPT.

REMARK 2.8. In general, M' may have $n - 1$ negative eigenvalues when M is non-PPT; see [5] for more details.

3. Sufficient conditions for PPT matrices. In this section, we establish a characterization of non-PPT matrices in terms of Ky-Fan norms. We also provide a number of sufficient conditions for the PPT property as applications of this result.

We need the following lemma for the proofs of the main results in this section.

LEMMA 3.1. Let $A, B \in \mathbb{C}^{n \times n}$ be positive semi-definite. Then, $A \succeq B$ if and only if for any $C \succ 0$,

$$\|CAC\| \geq \|CBC\|$$

for any unitarily invariant norm.

Proof. Necessity: Assume that $A \succeq B$. Then for any $C \succ 0$, $CAC \succeq CBC$. We conclude that $\lambda_k(CAC) \geq \lambda_k(CBC)$, $k = 1, \dots, n$, where $\lambda_k(CAC)$ and $\lambda_k(CBC)$ denote the k^{th} eigenvalues in decreasing order of CAC and CBC respectively. Since $CAC, CBC \succeq 0$, we get $\|CAC\|_{(k)} \geq \|CBC\|_{(k)}$ for all $k = 1, \dots, n$. Hence, the result follows by Ky-Fan Dominance Theorem, see [1, Theorem IV.2.2].

Sufficiency: Suppose for a contradiction that $A \not\succeq B$. Then there exists $y \in \mathbb{C}^n$ such that

$$y^*(A - B)y = \text{tr}((A - B)yy^*) < 0.$$

We can choose a sufficiently small $\epsilon > 0$ such that

$$\text{tr}((A - B)(yy^* + \epsilon I)) = \text{tr}((yy^* + \epsilon I)^{1/2}(A - B)(yy^* + \epsilon I)^{1/2}) < 0.$$

Let $C = (yy^* + \epsilon I)^{1/2} \succ 0$. Then

$$(3.1) \quad \text{tr}(CAC) < \text{tr}(CBC).$$

Let $\lambda_1, \dots, \lambda_n$ and μ_1, \dots, μ_n be the eigenvalues of CAC and CBC , respectively. Inequality (3.1) implies that

$$\sum_{i=1}^n \lambda_i < \sum_{i=1}^n \mu_i.$$

Since $CAC, CBC \succeq 0$, there exists $1 \leq k \leq n$ such that

$$\|CAC\|_{(k)} < \|CBC\|_{(k)},$$

which contradicts the assumption. □

In the following theorem, we do not assume that $M \succeq 0$.

THEOREM 3.2. *Let $A, B, X \in \mathbb{C}^{n \times n}$ such that $A \succ 0$ and $B \succeq 0$. The following statements are equivalent.*

- (i) $M' = \begin{bmatrix} A & X^* \\ X & B \end{bmatrix} \not\geq 0$.
- (ii) *There exists a matrix $C \succ 0$ such that $\|CBC\|_{(k)} < \|CXA^{-1}X^*C\|_{(k)}$ for some $1 \leq k \leq n$.*
- (iii) *There exists a matrix $C \succeq 0$ such that $\|CBC\|_{(k)} < \|CXA^{-1}X^*C\|_{(k)}$ for some $1 \leq k \leq n$.*

Proof. Obviously, (ii) implies (iii). We only need to show that (i) implies (ii), and (iii) implies (i).

(i) \Rightarrow (ii): Assume that $M' \not\geq 0$. Then Lemmas 2.1 and 3.1 imply that there exists $C \succ 0$ such that

$$\|CBC\| < \|CXA^{-1}X^*C\|$$

for some unitarily invariant norm $\|\cdot\|$. Hence, the result follows from Ky-Fan Dominance Theorem.

(iii) \Rightarrow (i): Assume that $M' \succeq 0$. By Lemma 2.1, $B \succeq XA^{-1}X^*$. Then for any $C \succeq 0$, $CBC \succeq CXA^{-1}X^*C$. Hence,

$$\|CBC\|_{(k)} \geq \|CXA^{-1}X^*C\|_{(k)}$$

for $k = 1, \dots, n$. □

We comment that if we consider M instead of M' in the above theorem, the norm inequality in (ii) and (iii) changes to $\|CBC\|_{(k)} < \|CX^*A^{-1}XC\|_{(k)}$.

Replacing B by $X^*A^{-1}X$ in (ii) of Theorem 3.2, we can derive a necessary condition for the non-PPT property or, equivalently, a sufficient condition for the PPT property involving only A and X .

THEOREM 3.3. *Let $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \succeq 0$ with $A, B, X \in \mathbb{C}^{n \times n}$ such that $A \succ 0$. If M is non-PPT, then there exists a matrix $C \succ 0$ such that*

$$\|CX^*A^{-1}XC\|_{(k)} < \|CXA^{-1}X^*C\|_{(k)}$$

for some $1 \leq k \leq n$.

Proof. Since M is non-PPT, we have $M' \not\geq 0$. Therefore, by Lemma 2.1,

$$B \succeq X^*A^{-1}X \quad \text{and} \quad B \not\geq XA^{-1}X^*.$$

We conclude that

$$X^*A^{-1}X \not\geq XA^{-1}X^*.$$

By Lemma 3.1, there exists $C \succ 0$ such that

$$\|CX^*A^{-1}XC\| < \|CXA^{-1}X^*C\|$$

for some unitarily invariant norm $\|\cdot\|$. The result then follows by Ky-Fan Dominance Theorem. □

It is well-known that

$$\|A + B\| \geq \|M\| \quad \text{and} \quad \|A + B\| \geq \|A + XA^{-1}X^*\|$$

for any unitarily invariant norm when M is PPT [10]. The converse is not true in general. We now give an extension to these norm inequalities which leads to a necessary and sufficient condition for M to be PPT.

THEOREM 3.4. Let $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \succeq 0$ with $A, B, X \in \mathbb{C}^{n \times n}$ such that $A \succ 0$. Then, M is PPT if and only if for any $C \succ 0$,

$$\|C(A+B)C\| \geq \max\{\|KMK\|, \|C(A+XA^{-1}X^*)C\|\}$$

for any unitarily invariant norm, where $K = \begin{bmatrix} C & 0 \\ 0 & C \end{bmatrix} \in \mathbb{C}^{2n \times 2n}$.

Proof. Necessity: Assume that M is PPT. Let $C \succ 0$, and $K = \begin{bmatrix} C & 0 \\ 0 & C \end{bmatrix} \in \mathbb{C}^{2n \times 2n}$. Clearly,

$$KMK = \begin{bmatrix} CAC & CXC \\ CX^*C & CBC \end{bmatrix}$$

is also PPT. It follows that

$$\|C(A+B)C\| = \|CAC + CBC\| \geq \|KMK\|$$

for any unitarily invariant norm. On the other hand, we have $B \succeq XA^{-1}X^*$, and thus, $A+B \succeq A+XA^{-1}X^*$. By Lemma 3.1,

$$\|C(A+B)C\| \geq \|C(A+XA^{-1}X^*)C\|$$

for any unitarily invariant norm.

Sufficiency: Since $\|C(A+B)C\| \geq \|C(A+XA^{-1}X^*)C\|$ for any unitarily invariant norm, we observe from Lemma 3.1 that $A+B \succeq A+XA^{-1}X^*$. This leads to $B \succeq XA^{-1}X^*$. Hence, the result follows from Lemma 2.1. \square

Next, we give an application of Theorem 3.2, where $\mathbb{R}^{n \times n}$ stands for the space of $n \times n$ real matrices.

COROLLARY 3.5. Let $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \succeq 0$ such that $A, B \in \mathbb{R}^{n \times n}$ and $X \in \mathbb{C}^{n \times n}$ is diagonal. Then M is PPT.

Proof. Let $C \succ 0$. By Theorem 3.2, we need to show that

$$(3.2) \quad \|CBC\| \geq \|CXA^{-1}X^*C\|$$

for any unitarily invariant norm. Note that $C^T \succ 0$; see [3, p. 397]. By Theorem 3.2, since $M \succ 0$,

$$(3.3) \quad \|C^T BC^T\| \geq \|C^T X^* A^{-1} X C^T\|$$

for any unitarily invariant norm. Observe from the assumption that

$$(CBC)^T = C^T BC^T \quad \text{and} \quad (CXA^{-1}X^*C)^T = C^T X^* A^{-1} X C^T.$$

Since a matrix and its transpose share the same eigenvalues, (3.3) implies (3.2) by Ky-Fan Dominance Theorem. \square

Without the assumption of A and B being real in Corollary 3.5, the matrix M is not PPT in general. Consider the matrix M given in (2.3). Note that $A = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix} \succ 0$, $B = \begin{bmatrix} 2 & -i \\ i & 3 \end{bmatrix} \succ 0$ and $X = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$

is diagonal and unitary. However,

$$M' = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 1 & 1 & 0 & -i \\ 1 & 0 & 2 & -i \\ 0 & i & i & 3 \end{bmatrix} \not\geq 0.$$

We can also observe from the above example that the numerical range of X is a line segment, which is not sufficient for M to be PPT. However, when the numerical range of X is contained in a line passing through the origin, we now see in the next corollary that M is PPT. We denote the numerical range of X by $W(X)$.

COROLLARY 3.6. *Let $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{C}^{2n \times 2n}$ be a positive semi-definite matrix with $A, B, X \in \mathbb{C}^{n \times n}$. If $W(X)$ is contained in a line passing through the origin, then M is PPT.*

Proof. Suppose that $W(X)$ is contained in a line passing through the origin. Then, there exists $\theta \in \mathbb{R}$ such that $W(e^{\frac{1}{2}i\theta}X) = e^{\frac{1}{2}i\theta}W(X)$ is contained in the real line. Thus, $e^{\frac{1}{2}i\theta}X$ is Hermitian, and so $X^* = e^{i\theta}X$.

By a continuity argument, we may assume that $A \succ 0$. From Theorem 3.2, we have that $\|CBC\| \geq \|CX^*A^{-1}XC\|$ for any $C \succ 0$ and any unitarily invariant norm. Since $X^* = e^{i\theta}X$, we get

$$\|CX^*A^{-1}XC\| = \|CXA^{-1}e^{i\theta}XC\| = \|CXA^{-1}X^*C\|.$$

Then, again by Theorem 3.2,

$$\begin{bmatrix} A & X^* \\ X & B \end{bmatrix} \succeq 0$$

and M is PPT. □

We observe that the numerical range condition in Corollary 3.6 is also necessary for a special type of positive semi-definite block matrices to be PPT.

COROLLARY 3.7. *Let $M = \begin{bmatrix} A & X \\ X^* & X^*A^{-1}X \end{bmatrix}$ with $A, X \in \mathbb{C}^{n \times n}$ such that $A \succ 0$ and X is diagonal. Assume that all entries of A^{-1} are nonzero. Then, M is PPT if and only if $W(X)$ is contained in a line passing through the origin.*

Proof. Clearly, $M \succeq 0$. By Corollary 3.6, we only need to show the necessity part. Assume that $W(X)$ is not contained in a line passing through the origin. Then X has at least two eigenvalues d_i, d_j such that $\overline{d_i}d_j$ is not real. Let us denote the (i, j) entry of A^{-1} by $A_{i,j}^{-1}$. Then the (i, j) entry of the matrix $X^*A^{-1}X - XA^{-1}X^*$ is $A_{i,j}^{-1}(\overline{d_i}d_j - d_i\overline{d_j})$. Since $A_{i,j}^{-1} \neq 0$, we deduce that $A_{i,j}^{-1}(\overline{d_i}d_j - d_i\overline{d_j}) \neq 0$. Note from X being diagonal that all diagonal entries of $X^*A^{-1}X - XA^{-1}X^*$ are zero. Then $X^*A^{-1}X - XA^{-1}X^*$ has a principal submatrix with negative determinant. Therefore, $X^*A^{-1}X - XA^{-1}X^* \not\geq 0$. Thus, Lemma 3.1 implies that there exists $C \succ 0$ such that $\|CX^*A^{-1}XC\| < \|CXA^{-1}X^*C\|$ for some unitarily invariant norm $\|\cdot\|$. By Theorem 3.2, $M' \not\geq 0$, and so M is non-PPT. □

It is easy to see from Theorem 3.2 that if X is normal and X commutes with A , then M is PPT. In particular, $M = \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \succeq 0$ is PPT when $A = I$ and X is normal. However, without the normality assumption on X , M is not necessarily PPT despite the strong condition of A being I ; see Example 3.9.

As another application of Theorem 3.2, we now provide a norm condition that guarantees such an M to be non-PPT.

COROLLARY 3.8. Let $M = \begin{bmatrix} I & X \\ X^* & B \end{bmatrix} \succeq 0$ such that $B \succ 0$. If $\|B^{-\frac{1}{2}}X\|_{(1)} > 1$, then M is non-PPT.

Proof. Note that

$$\begin{aligned} \|B^{-\frac{1}{2}}XX^*B^{-\frac{1}{2}}\|_{(1)} &= \|(B^{-\frac{1}{2}}X)(B^{-\frac{1}{2}}X)^*\|_{(1)} \\ &= \|B^{-\frac{1}{2}}X\|_{(1)}^2 \\ &> 1 \\ &= \|B^{-\frac{1}{2}}BB^{-\frac{1}{2}}\|_{(1)}. \end{aligned}$$

By taking $C = B^{-\frac{1}{2}}$ in Theorem 3.2, we conclude that M is non-PPT. \square

We conclude this section with an example of a non-PPT matrix satisfying the requirements of the previous corollary.

EXAMPLE 3.9. Let

$$A = I, \quad B = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{bmatrix} \quad \text{and} \quad X = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

Then $\|B^{-\frac{1}{2}}X\|_{(1)} = \sqrt{2}$ and $M \succ 0$, but it is non-PPT.

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