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ON POSITIVE AND POSITIVE PARTIAL TRANSPOSE MATRICES*

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Abstract. A block matrix $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]$ is positive partial transpose (PPT) if both $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} A & X^* \\ X & B \end{smallmatrix}\right]$ are positive semi-definite. This class is significant in studying the separability criterion for density matrices. The current paper presents new relations for such matrices. This includes some equivalent forms and new related inequalities that extend some results from the literature. In the end of the paper, we present some related results for positive semi-definite block matrices, which have similar forms as those presented for PPT matrices, with applications that include significant improvement of numerical radius inequalities.

Key words. Positive partial transpose, block matrix, inequality, geometric mean.

AMS subject classifications. Primary 15A45, 47A63, Secondary 47A30, 47A64, 47B15.

1. Introduction and preliminaries. While studying the separability criterion for density matrices, Peres [18] introduced the notion of positive partial transpose (PPT) matrices, as follows. Let $\mathbb{M}_n$ be the algebra of all $n \times n$ complex matrices, with zero matrix O. If $T \in \mathbb{M}_n$, we say that T is positive semi-definite, and we write $T \geq O$, if $\langle Tx, x \rangle \geq 0$, for all $x \in \mathbb{C}^n$.

For a general matrix $T \in \mathbb{M}_n$, if $T \geq O$, then it does not follow that $T^t \geq O$ necessarily, where T^t denotes the transpose of T. Such discussion has its significance in mathematical physics; see [9, 18].

If $A, B, X \in \mathbb{M}_n$, then the matrix $T := \left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]$ is said to be PPT if both T and T^t are positive semi-definite. That is,

$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \text{ is PPT } \Leftrightarrow \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \geq O \text{ and } \begin{bmatrix} A & X^* \\ X & B \end{bmatrix} \geq O.$$

We notice that the block matrix $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]$ is in the class $\mathbb{M}_{2n}$ or $\mathbb{M}_2(\mathbb{M}_n)$. The latter notation indicates that each block is indeed in $\mathbb{M}_n$.

Block matrices have played a significant role in understanding the geometry of the algebra $\mathbb{M}_n$. We refer the reader to [6, 8] as a list of references emphasizing this assertion.

The block matrix $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]$ has received a special attention in the literature due to its applications in matrix theory and mathematical physics. For example, the following lemma which presents a mixed Cauchy–Schwarz inequality uses this matrix as a criterion. We remark that in Theorem 3.3 below, we present a better result than this lemma.

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LEMMA 1.1. [10, *Lemma* 1] *Let* $A, B, C \in \mathbb{M}_n$ *be such that* $A, B \geq O$. *Then*

$$\begin{bmatrix} A & C \\ C^* & B \end{bmatrix} \geq O \Leftrightarrow |\langle C^* x, y \rangle|^2 \leq \langle Ax, x \rangle \langle By, y \rangle, \forall x, y \in \mathbb{C}^n.$$

Related to the inner product, we also have the following.

LEMMA 1.2. [19] *Let* $T \geq O$. *Then for any vectors* $x, y \in \mathbb{C}^n$,

$$|\langle Tx, y \rangle| \leq \frac{\|T\|}{2} \left(|\langle x, y \rangle| + \|y\| \, \|x\| \right),$$

where $\| \cdot \|$ *is the operator norm, defined by* $\|T\| = \sup\limits_{\|x\|=1} \|Tx\|$.

Related to the operator norm, and as an important application of this paper, is the so-called numerical radius norm. This is defined, for $T \in \mathbb{M}_n$, by $\omega(T) = \sup\limits_{\|x\|=1} |\langle Tx, x \rangle|$. The numerical radius and the operator norm are related via the relation:

$$\frac{1}{2} \|T\| \leq \omega(T) \leq \|T\|.$$

In the literature, numerous researchers have studied the problem of sharpening the above basic inequalities. We refer the reader to [1, 17, 20, 21, 22] as a sample of our recent work on this topic. In this paper, we present a significant improvement of one of the most valuable bounds in this regard in the literature; see Remark 3.5 below.

Another important and valuable application of this block matrix is the following extremal property of the geometric mean of positive definite matrices S, T (i.e., $S, T > O$).

LEMMA 1.3. [3, *Theorem* 4.1.3] *Let* $S, T \in \mathbb{M}_n$ *be positive definite. Then,*

$$S \sharp T = \max \left\{ Y \colon Y = Y^*, \begin{bmatrix} S & Y \\ Y & T \end{bmatrix} \geq O \right\},$$

where $S \sharp T = S^{\frac{1}{2}} \left(S^{-\frac{1}{2}} T S^{-\frac{1}{2}} \right)^{\frac{1}{2}} S^{\frac{1}{2}}$ *is the geometric mean of* S, T.
In particular, $\left[\begin{smallmatrix} S & S\sharp T \\ S\sharp T & T \end{smallmatrix} \right] \geq O$.

In this context, we remind the reader of operator means. An operator mean σ in the sense of Kubo–Ando [13] is defined by a positive operator monotone function f on the half interval $(0, \infty)$ with $f(1) = 1$ as:

$$A \sigma B = A^{\frac{1}{2}} f \left(A^{-\frac{1}{2}} B A^{-\frac{1}{2}} \right) A^{\frac{1}{2}}, \tag{1.1}$$

where $A, B > O$. The function being operator monotone means that $f(B) \geq f(A)$ when $A, B \in \mathbb{M}_n$ are such that $B \geq A > O$. Here, the ordering $B \geq A$ means $B - A \geq O$, the Löwner partial order.

The function f is called the representing function of σ. Let σ be an operator mean with representing function f. For a nonzero connection σ, the adjoint σ^* and the dual $\sigma^\perp$ are respectively defined by:

$$A \sigma^* B = \left(A^{-1} \sigma B^{-1} \right)^{-1} \quad \text{and} \quad A \sigma^\perp B = \left(B^{-1} \sigma A^{-1} \right)^{-1}. \tag{1.2}$$

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One can easily verify that when σ is an operator mean, we have the congruence invariance:

$$X^*\left(A\sigma B\right)X=\left(X^*AX\right)\sigma\left(X^*BX\right);\ \text{ for invertible } X. \tag{1.3}$$

Besides, the following form of (1.3) holds [5]

$$X^*\left(A\sigma B\right)X\le\left(X^*AX\right)\sigma\left(X^*BX\right);\ \text{ for any } X. \tag{1.4}$$

We also have the following characterization of the positivity of block matrices.

Lemma 1.4. [3, *Theorem* 1.3.3] *Let $A,B\in\mathbb{M}_n$ be positive definite. Then the block matrix* $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}\ge O$ *if and only if $A\ge XB^{-1}X^*$.*

Lemma 1.5. [3, *Proposition* 1.3.2] *Let $A,B\ge O$. Then $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]\ge O$ if and only if $X=A^{\frac12}KB^{\frac12}$ for some contraction K.*

We recall that a norm $\|\cdot\|_u$ on $\mathbb{M}_n$ is said to be a unitarily invariant norm if $\|UXV\|_u=\|X\|_u$ for any $X\in\mathbb{M}_n$ and all unitary matrices U,V. We refer the reader to [3] for further details of these norms and their applications.

There are many other implications of the positivity of the block matrix $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$. For example, Tao [23, Theorem 1] proved the following result: Let $A,B,X\in\mathbb{M}_n$ be such that $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]\ge O$. Then

$$2\|X\|_u\le\left\|\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}\right\|_u,$$

for any unitarily invariant norm $\|\cdot\|_u$.

In what follows, if no norm is explicitly stated, we implicitly understand that the notation $\|\cdot\|_u$ refers to an arbitrary chosen invariant norm.

Discussing similar relations for PPT matrices, it follows from [7] (see also [16, Lemma 3.1]) that if $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]$ is PPT, then

$$\left\|\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}\right\|_u\le\|A+B\|_u.$$

Further, it has been shown in [16, Remark 3.5] that if $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]\ge O$, then

$$\|\Re X\|_u\le\frac12\|A+B\|_u,$$

where $\Re X=\frac{X+X^*}{2}$ is the real part of the matrix X.

In the sequel, we will present some results in terms of the so-called Heinz means, which are defined for positive definite A,B by [2]:

$$H_t\left(A,B\right)=\frac{A\sharp_t B+A\sharp_{1-t}B}{2};\ 0\le t\le 1,$$

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where $\sharp_t$ refers to the weighted geometric mean, whose representing function is $f(x) = x^t, 0 \le t \le 1$, as in (1.1). We notice that when $t = 0, 1$, $H_t(A, B) = \frac{A+B}{2}$. This latter quantity is known as the arithmetic mean of A, B and is usually denoted as $A\nabla B$. In general, if $0 \le t \le 1$, the weighted arithmetic mean of A, B is defined by $A\nabla_t B = (1-t)A + tB$.

Our target in this paper is to discuss possible related relations for PPT matrices. In [15, Lemma 4.2], it was shown that if $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is PPT, then $\begin{bmatrix} A\sharp B & X \\ X^* & A\sharp B \end{bmatrix}$ is PPT. In our first main result, we will show more general necessary and sufficient conditions; see Theorem 2.1 below.

Further, it has been proved, in [14, Theorem 2.1], that $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is PPT, then for some unitary $U \in \mathbb{M}_n$,

$$|X| \le \frac{1}{2}\left(A\sharp B + U^*(A\sharp B)U\right). \tag{1.5}$$

This result will be generalized too. Other developments will also be presented with operator means and operator monotone functions. In the end, we give some related results for positive block matrices.

2. PPT matrices. In this section, we present our main results for PPT matrices. We begin with the following extension of [15, Lemma 4.2].

THEOREM 2.1. *Let $A, B, X \in \mathbb{M}_n$ be such that $A, B > O$. Then $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is PPT if and only if $\begin{bmatrix} A\sharp_t B & X \\ X^* & A\sharp_{1-t} B \end{bmatrix}$ is PPT, for any $0 \le t \le 1$.*

Proof. Assume first that $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is PPT. We know that positivity of the matrix $\begin{bmatrix} A & X^* \\ X & B \end{bmatrix}$ is equivalent to positivity of $\begin{bmatrix} B & X \\ X^* & A \end{bmatrix}$. This, together with the fact that $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is PPT, implies

$$\begin{bmatrix} A & X^* \\ X & B \end{bmatrix} \ge O \ \text{ and } \ \begin{bmatrix} B & X^* \\ X & A \end{bmatrix} \ge O. \tag{2.6}$$

Noting Lemma 1.4, (2.6) implies

$$X^*A^{-1}X \le B \ \text{ and } \ X^*B^{-1}X \le A. \tag{2.7}$$

On the other hand, (1.4) implies

$$H^*\left(S\sharp_t T\right)H \le (H^*SH)\sharp_t(H^*TH), \tag{2.8}$$

for all $H \in \mathbb{M}_n$ and $S, T > O$. Consequently,

$$\begin{aligned} X^*(A\sharp_t B)^{-1}X &= X^*\left(A^{-1}\sharp_t B^{-1}\right)X \\ &\le (X^*A^{-1}X)\sharp_t(X^*B^{-1}X) \quad \text{(by the property (2.8))} \\ &\le B\sharp_t A \quad \text{(by (2.7))} \\ &= A\sharp_{1-t}B. \end{aligned}$$

Thus, we have shown that

$$X^*(A\sharp_t B)^{-1}X \le A\sharp_{1-t}B.$$

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Again, using Lemma 1.4 we have $\begin{bmatrix} A\sharp_{1-t}B & X^* \\ X & A\sharp_t B \end{bmatrix} \geq O$, which implies

$$\begin{bmatrix} A\sharp_t B & X \\ X^* & A\sharp_{1-t}B \end{bmatrix} \geq O. \tag{2.9}$$

On the other hand, by the assumption, we know that

$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \geq O \Leftrightarrow \begin{bmatrix} B & X^* \\ X & A \end{bmatrix} \geq O \Leftrightarrow B \geq X^* A^{-1} X.$$

If we apply the same procedure as in the above, we get

$$\begin{bmatrix} A\sharp_t B & X^* \\ X & A\sharp_{1-t}B \end{bmatrix} \geq O.$$

This, together with (2.9), completes the sufficiency proof. Now for necessity, assume that $\begin{bmatrix} A\sharp_t B & X \\ X^* & A\sharp_{1-t}B \end{bmatrix}$ is PPT for any $0 \leq t \leq 1$. Letting $t = 0$ we reach the desired assertion, thanks to the simple identities $A\sharp_0 B = A$ and $B\sharp_0 A = B$. ∎

Corollary 2.2. *Let $A, B \in \mathbb{M}_n$ be positive definite. Then $\begin{bmatrix} A\sharp_t B & A\sharp B \\ A\sharp B & A\sharp_{1-t}B \end{bmatrix} \geq O$ for any $0 \leq t \leq 1$.*

Proof. By Lemma 1.3, the matrix $\begin{bmatrix} A & A\sharp B \\ A\sharp B & B \end{bmatrix} \geq O$. This implies that this latter matrix is PPT. Using Theorem 2.1, with $X = A\sharp B$ implies the desired result. ∎

If we apply the same method as in the proof of Theorem 2.1, we infer the following generalization of Theorem 2.1, thanks to (1.2) and (1.4).

Theorem 2.3. *Let $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ be PPT with $A, B, X \in \mathbb{M}_n$ and let σ be an operator mean. Then $\begin{bmatrix} A\sigma^* B & X \\ X^* & B\sigma A \end{bmatrix}$ is PPT.*

The following result generalizes (1.5), which was shown in [14, Theorem 2.1].

Theorem 2.4. *Let $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ be PPT with $A, B, X \in \mathbb{M}_n$ and let $X = U|X|$ be the polar decomposition of X. Then for any $0 \leq t \leq 1$,*

$$|X| \leq \frac{1}{2}\left(A\sharp_{1-t}B + U^* A\sharp_t B U\right) \quad \textit{and} \quad |X| \leq \frac{1}{2}\left(A\sharp_t B + U^* A\sharp_{1-t} B U\right).$$

Proof. Since $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is PPT, it follows from Theorem 2.1 that

$$\begin{bmatrix} A\sharp_t B & X \\ X^* & A\sharp_{1-t}B \end{bmatrix} \geq O \text{ and } \begin{bmatrix} A\sharp_t B & X^* \\ X & A\sharp_{1-t}B \end{bmatrix} \geq O, \tag{2.10}$$

for $0 \leq t \leq 1$. Thus,

$$\begin{bmatrix} -U^* & I \end{bmatrix} \begin{bmatrix} A\sharp_t B & X \\ X^* & A\sharp_{1-t}B \end{bmatrix} \begin{bmatrix} -U \\ I \end{bmatrix} \geq O \text{ and } \begin{bmatrix} I & -U^* \end{bmatrix} \begin{bmatrix} A\sharp_t B & X^* \\ X & A\sharp_{1-t}B \end{bmatrix} \begin{bmatrix} I \\ -U \end{bmatrix} \geq O.$$

Since U is the unitary factor in the polar decomposition $X = U|X|$, we get the result. ∎

We notice that the two inequalities in Theorem 2.4 are equivalent.

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Corollary 2.5. *Let* $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ *be PPT with* $A, B, X \in \mathbb{M}_n$. *Then for any* $0 \le t \le 1$,

i) $\begin{bmatrix} A\sharp_t B & \Re X \\ \Re X & A\sharp_{1-t} B \end{bmatrix} \ge O.$

ii) $\begin{bmatrix} H_t(A,B)+\Re X & \frac{A\sharp_{1-t}B - A\sharp_t B}{2} \\ \frac{A\sharp_{1-t}B - A\sharp_t B}{2} & H_t(A,B)-\Re X \end{bmatrix} \ge O.$

iii) $\begin{bmatrix} \frac{A+B}{2}+\Re X & \frac{A-B}{2} \\ \frac{A-B}{2} & \frac{A+B}{2}-\Re X \end{bmatrix} \ge O$ *and* $\begin{bmatrix} \frac{A+B}{2}+\Re X & O \\ O & \frac{A+B}{2}-\Re X \end{bmatrix} \ge O.$

Proof. The first assertion follows by adding the two inequalities in (2.10). To prove the second desired statement, let $J = \begin{bmatrix} \frac{I}{\sqrt{2}} & -\frac{I}{\sqrt{2}} \\ \frac{I}{\sqrt{2}} & \frac{I}{\sqrt{2}} \end{bmatrix}$. Then,

$$J^* \begin{bmatrix} A\sharp_t B & \Re X \\ \Re X & A\sharp_{1-t} B \end{bmatrix} J = \begin{bmatrix} H_t(A,B)+\Re X & \frac{A\sharp_{1-t}B - A\sharp_t B}{2} \\ \frac{A\sharp_{1-t}B - A\sharp_t B}{2} & H_t(A,B)-\Re X \end{bmatrix} \ge O.$$

This proves the second assertion. The third desired statement follows by letting $t = 1$ and $t = \frac{1}{2}$ in the second statement. Indeed, when $t = \frac{1}{2}$, part *ii*) implies

$$\begin{bmatrix} A\sharp B + \Re X & O \\ O & A\sharp B - \Re X \end{bmatrix} \ge O.$$

The fact that $\frac{A+B}{2} \ge A\sharp B$ implies the second inequality in *iii*). This completes the proof. ∎

Now Lemma 1.3, together with i) of Corollary 2.5, ensures the following.

Corollary 2.6. *Let* $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ *be PPT with* $A, B, X \in \mathbb{M}_n$. *Then for any* $0 \le t \le 1$,

$$\Re X \le (A\sharp_t B)\,\sharp\,(A\sharp_{1-t} B)\,.$$

In particular, if X *is Hermitian, then*

$$X \le (A\sharp_t B)\,\sharp\,(A\sharp_{1-t} B)\,.$$

We have seen how the positivity of block matrices is related to inner product inequalities, as we have in Lemma 1.1. In the following, we present the following similar conclusion for PPT matrices.

Theorem 2.7. *Let* $A, B, X \in \mathbb{M}_n$. *Then* $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ *is PPT if and only if*

$$|\langle Xx, y\rangle|\,, |\langle X^*x, y\rangle| \le \sqrt{\langle A\sharp_t Bx, x\rangle \,\langle A\sharp_{1-t} By, y\rangle}; \quad 0 \le t \le 1$$

for any vectors $x, y \in \mathbb{C}^n$.

Proof. By Theorem 2.1, one can directly see that

$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \text{ is PPT } \Leftrightarrow \begin{bmatrix} A\sharp_t B & X \\ X^* & A\sharp_{1-t} B \end{bmatrix} \text{ is PPT }.$$

By [10, Lemma 1], we have

$$\begin{bmatrix} A\sharp_t B & X \\ X^* & A\sharp_{1-t} B \end{bmatrix} \ge O \;\Leftrightarrow\; |\langle X^*x, y\rangle|^2 \le \langle A\sharp_t Bx, x\rangle \,\langle A\sharp_{1-t} By, y\rangle\,,$$

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and

$$\begin{bmatrix} A\sharp_t B & X^* \\ X & A\sharp_{1-t} B \end{bmatrix} \geq O \Leftrightarrow |\langle Xx, y\rangle|^2 \leq \langle A\sharp_t Bx, x\rangle \langle A\sharp_{1-t} By, y\rangle,$$

for any vector $x, y \in \mathbb{C}^n$. The required result follows. □

Real-valued functions applied to matrices through functional calculus have received considerable attention in the literature. For example, we have seen how operator means are defined using such an argument. We present a PPT matrix related to operator concave functions in the following. We recall that a function $f : J \to \mathbb{R}$ is called operator concave on the interval J if $f(A\nabla B) \geq f(A)\nabla f(B)$, for any Hermitian matrices A, B with spectra in J.

THEOREM 2.8. *Let $f : [0, \infty) \to (0, \infty)$ be an operator concave function, and let $\left[\begin{smallmatrix} f(A) & X \\ X^* & f(B) \end{smallmatrix}\right]$ be PPT with $A, B, X \in \mathbb{M}_n$ and such that $A, B \geq O$. Then $\left[\begin{smallmatrix} f(A)\nabla_t f(B) & X \\ X^* & f(A\nabla_t B) \end{smallmatrix}\right]$ is PPT, for $0 \leq t \leq 1$.*

Proof. We notice first the matrix $\left[\begin{smallmatrix} f(A) & X \\ X^* & f(B) \end{smallmatrix}\right]$ being PPT implies

$$\begin{bmatrix} f(A) & X \\ X^* & f(B) \end{bmatrix} \geq O, \begin{bmatrix} f(A) & X^* \\ X & f(B) \end{bmatrix} \geq O, \begin{bmatrix} f(B) & X \\ X^* & f(A) \end{bmatrix} \geq O, \begin{bmatrix} f(B) & X^* \\ X & f(A) \end{bmatrix} \geq O,$$

by Lemma 1.4.

The positivity of the second and fourth matrices above implies

$$X^* f(B)^{-1} X \leq f(A) \text{ and } X^* f(A)^{-1} X \leq f(B). \tag{2.11}$$

Further, since f is operator concave, we have $f(A\nabla_t B) \geq f(A)\nabla_t f(B)$, $0 \leq t \leq 1$. Since the function $g(x) = x^{-1}$ is operator monotone decreasing, the latter inequality implies $f(A\nabla_t B)^{-1} \leq (f(A)\nabla_t f(B))^{-1}$. Multiplying this latter inequality with X^* from left and X from right gives

$$\begin{aligned} X^* f(A\nabla_t B)^{-1} X &\leq X^* (f(A)\nabla_t f(B))^{-1} X \\ &\leq X^* \left(f(A)^{-1}\nabla_t f(B)^{-1}\right) X \quad (g(x) = x^{-1} \text{ is operator convex}) \\ &= \left(X^* f(A)^{-1} X\right) \nabla_t \left(X^* f(B)^{-1} X\right) \quad \text{(direct calculations)} \\ &\leq f(B)\nabla_t f(A) \quad \text{(by (2.11))}. \end{aligned}$$

Applying Lemma 1.4 again implies that $\left[\begin{smallmatrix} f(B)\nabla_t f(A) & X^* \\ X & f(A\nabla_t B) \end{smallmatrix}\right] \geq O$. Repeating the same steps, except for the first step, where one should multiply with X from left then X^* from right implies positivity of $\left[\begin{smallmatrix} f(B)\nabla_t f(A) & X \\ X^* & f(A\nabla_t B) \end{smallmatrix}\right]$. This completes the proof. □

3. Positive semi-definite block matrices. Now we continue with positive semi-definite block matrices. In particular, we discuss similar results as those presented for PPT matrices in the previous section.

THEOREM 3.1. *Let $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right] \geq O$ with $A, B, X \in \mathbb{M}_n$ and let $X = U|X|$ be the polar decomposition X. Then $\left[\begin{smallmatrix} U^*AU\sharp_t B & |X| \\ |X| & U^*AU\sharp_{1-t} B \end{smallmatrix}\right] \geq O$ for any $0 \leq t \leq 1$.*

Proof. Let X have the polar decomposition $X = U|X|$, for some unitary U. Since

$$\begin{bmatrix} U^*AU & |X| \\ |X| & B \end{bmatrix} = \begin{bmatrix} U^* & O \\ O & I \end{bmatrix} \begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \begin{bmatrix} U & O \\ O & I \end{bmatrix},$$

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positivity of $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right]$ implies that $\left[\begin{smallmatrix} U^*AU & |X| \\ |X| & B \end{smallmatrix}\right] \geq O$. Following the proof of Theorem 2.1, we have

$$\begin{bmatrix} U^*AU & |X| \\ |X| & B \end{bmatrix} \geq O \Rightarrow \begin{bmatrix} U^*AU\sharp_t B & |X| \\ |X| & U^*AU\sharp_{1-t}B \end{bmatrix} \geq O; \ \ (0 \leq t \leq 1)\,.$$

This completes the proof. ∎

In what follows, we use the fact that if U is unitary and $y \in \mathbb{C}^n$ is any vector, then $\|Uy\| = \|y\|$.

PROPOSITION 3.2. *Let $A \in \mathbb{M}_n$ with the polar decomposition $A = U\,|A|$. Then for any vectors $x, y \in \mathbb{C}^n$,*

$$|\langle Ax, y\rangle| \leq \frac{\|A\|}{2}\left(|\langle x, U^*y\rangle| + \|y\|\,\|x\|\right).$$

Proof. Lemma 1.2 gives

$$|\langle |A|\,x, y\rangle| \leq \frac{\|\,|A|\,\|}{2}\left(|\langle x, y\rangle| + \|y\|\,\|x\|\right) = \frac{\|A\|}{2}\left(|\langle x, y\rangle| + \|y\|\,\|x\|\right) \tag{3.12}$$

for any $A \in \mathbb{M}_n$. Assume that $A = U\,|A|$ be the polar decomposition of A. If we replace y by U^*y, in the inequality (3.12), we get

$$\begin{aligned} |\langle Ax, y\rangle| &= |\langle U\,|A|\,x, y\rangle| \\ &= |\langle |A|\,x, U^*y\rangle| \\ &\leq \frac{\|A\|}{2}\left(|\langle x, U^*y\rangle| + \|y\|\,\|x\|\right), \end{aligned}$$

from which the required result follows. ∎

In the following, we present a refinement of Lemma 1.1.

THEOREM 3.3. *Let $A, X, B \in \mathbb{M}_n$. Then $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right] \geq O$, if and only if for any vectors $x, y \in \mathbb{C}^n$,*

$$|\langle Xx, y\rangle| \leq \frac{1}{2}\left(\left|\left\langle A^{\frac{1}{2}}UB^{\frac{1}{2}}x, y\right\rangle\right| + \sqrt{\langle Ay, y\rangle\,\langle Bx, x\rangle}\right)$$

for some unitary U.

Proof. Suppose that $\left[\begin{smallmatrix} A & X \\ X^* & B \end{smallmatrix}\right] \geq O$. So, a contraction K exists such that

$$\begin{aligned} |\langle Xx, y\rangle| &= \left|\left\langle A^{\frac{1}{2}}KB^{\frac{1}{2}}x, y\right\rangle\right| \quad \text{(by Lemma 1.5)} \\ &\leq \frac{\|K\|}{2}\left(\left|\left\langle A^{\frac{1}{2}}UB^{\frac{1}{2}}x, y\right\rangle\right| + \left\|A^{\frac{1}{2}}y\right\|\left\|B^{\frac{1}{2}}x\right\|\right) \quad \text{(by Proposition 3.2)} \\ &\leq \frac{1}{2}\left(\left|\left\langle A^{\frac{1}{2}}UB^{\frac{1}{2}}x, y\right\rangle\right| + \left\|A^{\frac{1}{2}}y\right\|\left\|B^{\frac{1}{2}}x\right\|\right) \quad \text{(since } \|K\| \leq 1) \\ &= \frac{1}{2}\left(\left|\left\langle A^{\frac{1}{2}}UB^{\frac{1}{2}}x, y\right\rangle\right| + \sqrt{\langle Ay, y\rangle\,\langle Bx, x\rangle}\right) \end{aligned}$$

for any vectors $x, y \in \mathbb{C}^n$.

For the other side, if for any $x, y \in \mathbb{C}^n$,

$$|\langle Xx, y\rangle| \leq \frac{1}{2}\left(\left|\left\langle A^{\frac{1}{2}}UB^{\frac{1}{2}}x, y\right\rangle\right| + \sqrt{\langle Ay, y\rangle\,\langle Bx, x\rangle}\right)$$

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holds, for some unitary U, then by the Cauchy–Schwarz inequality, we have

$$\begin{aligned}\left|\left\langle A^{\frac{1}{2}}UB^{\frac{1}{2}}x,y\right\rangle\right| &= \left|\left\langle UB^{\frac{1}{2}}x,A^{\frac{1}{2}}y\right\rangle\right| \\ &\le \left\|B^{\frac{1}{2}}x\right\|\left\|A^{\frac{1}{2}}y\right\| \\ &= \sqrt{\left\langle B^{\frac{1}{2}}x,B^{\frac{1}{2}}x\right\rangle\left\langle A^{\frac{1}{2}}y,A^{\frac{1}{2}}y\right\rangle} \\ &= \sqrt{\langle Bx,x\rangle\langle Ay,y\rangle}.\end{aligned} \tag{3.13}$$

Therefore,

$$|\langle Xx,y\rangle| \le \sqrt{\langle Ay,y\rangle\langle Bx,x\rangle}.$$

Now, the result follows by Lemma 1.1. □

COROLLARY 3.4. *Let $A,B\in\mathbb{M}_n$. Then there exists unitary U, such that*

$$\omega(A^*B) \le \frac{1}{2}\omega(|A|U|B|)+\frac{1}{4}\left\||A|^2+|B|^2\right\|.$$

Proof. Noting that

$$\begin{bmatrix}|A|^2 & A^*B\\ B^*A & |B|^2\end{bmatrix}\ge O.$$

Now, by Theorem 3.3, we infer for any vectors $x,y\in\mathbb{C}^n$,

$$|\langle A^*Bx,y\rangle| \le \frac{1}{2}\left(|\langle|A|U|B|x,y\rangle|+\sqrt{\left\langle|A|^2y,y\right\rangle\left\langle|B|^2x,x\right\rangle}\right) \tag{3.14}$$

for some unitary U. This inequality is of interest in itself. If we set $x=y$, in (3.14), we get

$$|\langle A^*Bx,x\rangle| \le \frac{1}{2}\left(|\langle|A|U|B|x,x\rangle|+\sqrt{\left\langle|A|^2x,x\right\rangle\left\langle|B|^2x,x\right\rangle}\right). \tag{3.15}$$

From the arithmetic–geometric mean inequality, we know that

$$\sqrt{\left\langle|A|^2x,x\right\rangle\left\langle|B|^2x,x\right\rangle} \le \frac{1}{2}\left\langle\left(|A|^2+|B|^2\right)x,x\right\rangle. \tag{3.16}$$

Combining the inequalities (3.15) and (3.16) gives

$$|\langle A^*Bx,x\rangle| \le \frac{1}{2}|\langle|A|U|B|x,x\rangle|+\frac{1}{4}\left\langle\left(|A|^2+|B|^2\right)x,x\right\rangle.$$

Now taking the supremum over $x\in\mathbb{C}^n$ with $\|x\|=1$ in the above inequality produces

$$\omega(A^*B) \le \frac{1}{2}\omega(|A|U|B|)+\frac{1}{4}\left\||A|^2+|B|^2\right\|,$$

as desired. □

REMARK 3.5. *Since*

$$\begin{aligned}|\langle|A|U|B|x,x\rangle| &\le \sqrt{\left\langle|A|^2x,x\right\rangle\left\langle|B|^2x,x\right\rangle} \quad \textit{(by (3.13))} \\ &\le \frac{1}{2}\left\langle\left(|A|^2+|B|^2\right)x,x\right\rangle \quad \textit{(by (3.16))}\end{aligned}$$

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we obtain

$$\omega\left(|A|\,U\,|B|\right) \le \frac{1}{2}\left\| |A|^2 + |B|^2 \right\|.$$

This inequality ensures that

$$\omega\left(A^*B\right) \le \frac{1}{2}\omega\left(|A|\,U\,|B|\right) + \frac{1}{4}\left\| |A|^2 + |B|^2 \right\| \le \frac{1}{2}\left\| |A|^2 + |B|^2 \right\|.$$

The above inequality provides an improvement of [11, (17)].

Applying the same method to the positive matrix $\begin{bmatrix} |T^*|^{2t} & T \\ T^* & |T|^{2(1-t)} \end{bmatrix}$, $(0 \le t \le 1)$ [10, Theorem 1] implies

$$\omega\left(T\right) \le \frac{1}{2}\omega\left(|T^*|^t U |T|^{1-t}\right) + \frac{1}{4}\left\| |T|^{2(1-t)} + |T^*|^{2t} \right\|$$

for some unitary U. This inequality nicely improves the celebrated inequality (see [12, (8)] and [4, Theorem 1])

$$\omega\left(T\right) \le \frac{1}{2}\left\| |T|^{2(1-t)} + |T^*|^{2t} \right\|.$$

We should remark here that the above inequality significantly improves the inequality $\omega(T) \le \frac{1}{2}\|\ |T| + |T^*|\ \|$. This latter inequality is a valuable result in the literature, being one of the sharpest bounds that have ever been found.

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