INEQUALITIES RELATED TO 2×2 BLOCK PPT MATRICES

Minghua Lin

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Abstract. A 2×2 block matrix $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is positive partial transpose (PPT) if both $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ and $\begin{bmatrix} A & X^* \\ X & B \end{bmatrix}$ are positive semidefinite. This article presents some inequalities related to this class of matrices. Among others, we show that the Hua matrix, which is PPT, reveals a remarkable singular value inequality for contractive matrices.

1. Introduction

Positive (semidefinite) matrices partitioned into 2×2 blocks play an important role in matrix analysis. A recent monograph [6] contains an excellent exposition of this point. We start by fixing some notation: Let $\mathbb{M}_{m \times n}$ be the set of all $m \times n$ complex matrices and let $\mathbb{M}_n = \mathbb{M}_{n \times n}$; the identity matrix of \mathbb{M}_n is I_n . Capital letters are used to denote the elements in $\mathbb{M}_{m \times n}$. The (conjugate) transpose of A is denoted by A^* . If A is positive, we put $A \ge 0$, then it has unique square root $A^{1/2}$ which is positive. For two Hermitian matrices A and B, $A \ge B$ is understood as $A - B \ge 0$. It is well known that the transpose map is not 2-positive, that is, assuming each block is square,

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

Motivated by the theory of quantum information (for example, to decide the separability of mixed states [11, 16]), there is a need to introduce a stronger class of positive matrices, that is, matrices whose partial transpose are also positive. In 2×2 block case, we say $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is positive partial transpose (PPT for short) if

$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \ge 0 \quad \text{and} \quad \begin{bmatrix} A & X^* \\ X & B \end{bmatrix} \ge 0.$$

Thus whenever we say $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is PPT, the off diagonal blocks are necessarily square.

In this paper, we present some inequalities related to 2×2 block PPT matrices. Our study follows a natural thought that conclusions drawn under the PPT assumption should be stronger than those drawn under only the usual positivity assumption. Moreover, we believe the new result presented in this work is of interest in its own right and may serve for a better understanding of the intrinsic properties of PPT matrices.

Keywords and phrases: Positive partial transpose, inequality, trace, singular value.



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2. Trace inequality

Let $A \in \mathbb{M}_n$, the trace of A is denoted by trA. In [4], Besenyei formulated the following remarkable trace inequality: if $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \ge 0$ with X square, then

$$trAB - trX^*X \leqslant trAtrB - |trX|^2.$$
(2.1)

Inequality (2.1) arises from the subadditivity of q-entropies; see [3, Theorem 2] and references therein for more details.

If $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \ge 0$ with X square, then it is clear that $\operatorname{tr} A \operatorname{tr} B - |\operatorname{tr} X|^2 \ge 0$, since trace functional is Liebian; see [17, p. 70]. However, $\operatorname{tr} AB - \operatorname{tr} X^*X$ may take a negative value. For example, taking

$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \ge 0,$$

then $\operatorname{tr} AB - \operatorname{tr} X^* X = -1$.

The following result proposes a condition for the positivity of $trAB - trX^*X$.

THEOREM 2.1. Let
$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{M}_{2n}$$
 be PPT. Then
 $\operatorname{tr} X^* X \leqslant \operatorname{tr} AB.$ (2.2)

Proof. Without loss of generality, we may assume A to be positive definite. As $\begin{bmatrix} A & X \\ X^* & B \end{bmatrix}$ is PPT, we have $B \ge XA^{-1}X^*$ and $B \ge X^*A^{-1}X$, thus

$$A^{1/2}BA^{1/2} \ge (A^{1/2}XA^{-1/2})(A^{1/2}XA^{-1/2})^*$$

and

$$A^{1/2}BA^{1/2} \ge (A^{-1/2}XA^{1/2})^*(A^{-1/2}XA^{1/2}).$$

Taking trace and adding up gives

$$2 \text{tr} AB \geqslant \|A^{1/2} X A^{-1/2}\|_F^2 + \|A^{-1/2} X A^{1/2}\|_F^2$$

where $\|\cdot\|_F$ means the Frobenius norm. Thus it suffices to show

$$\|A^{1/2}XA^{-1/2}\|_F^2 + \|A^{-1/2}XA^{1/2}\|_F^2 \ge 2\|X\|_F^2 = 2\operatorname{tr} X^*X.$$

Let $A = UDU^*$ be the spectral decomposition of A with U unitary and $D = \text{diag}(d_1, \dots, d_n)$ a diagonal matrix. Let also $Y = [y_{ij}]_{i,j=1}^n = U^*XU$. Then

$$\begin{split} \|A^{1/2}XA^{-1/2}\|_{F}^{2} + \|A^{-1/2}XA^{1/2}\|_{F}^{2} &= \|D^{1/2}YD^{-1/2}\|_{F}^{2} + \|D^{-1/2}YD^{1/2}\|_{F}^{2} \\ &= \sum_{i,j=1}^{n} \frac{d_{i}}{d_{j}}|y_{ij}|^{2} + \sum_{i,j=1}^{n} \frac{d_{j}}{d_{i}}|y_{ij}|^{2} \\ &= \sum_{i,j=1}^{n} \left(\frac{d_{i}}{d_{j}} + \frac{d_{j}}{d_{i}}\right)|y_{ij}|^{2} \\ &\geqslant 2\sum_{i,j=1}^{n} |y_{ij}|^{2} \\ &= 2\|Y\|_{F}^{2} = 2\|X\|_{F}^{2} = 2\mathrm{tr}X^{*}X, \end{split}$$

from which (2.2) follows. \Box

We remark that inequality (2.2) is an extension of [12, Lemma 2.10].

Recall that $A \in \mathbb{M}_{m \times n}$ is contractive if $I_n \ge A^*A$ and strict contractive if $I_n - A^*A$ is further invertible. In studying the theory of functions of several complex variables, L.-K. Hua [10] discovered an intriguing positive matrix which now carries his name (e.g., [1, 18]). The Hua matrix is given by

$$\mathbf{H} = \begin{bmatrix} (I_n - A^*A)^{-1} & (I_n - B^*A)^{-1} \\ (I_n - A^*B)^{-1} & (I_n - B^*B)^{-1} \end{bmatrix},$$

where $A, B \in \mathbb{M}_{m \times n}$ are strictly contractive. It was only recently observed that **H** is PPT; see [1]. Thus, thanks to Theorem 2.1, we have the following corollary.

COROLLARY 2.2. Let $A, B \in \mathbb{M}_{m \times n}$ be strictly contractive. Then

$$\operatorname{tr}(I_n - A^*B)^{-1}(I_n - B^*A)^{-1} \leq \operatorname{tr}(I_n - A^*A)^{-1}(I_n - B^*B)^{-1}.$$

A generalization of Theorem 2.1 is given in Section 4.

3. Eigenvalue/singular value inequality

A norm $\|\cdot\|$ on \mathbb{M}_n is called unitarily invariant if $\|UAV\| = \|A\|$ for any $A \in \mathbb{M}_n$ and any unitary matrices $U, V \in \mathbb{M}_n$. The following result is implicit in [14]:

PROPOSITION 3.1. Let
$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{M}_{2n}$$
 be PPT. Then
$$2\|X\| \leq \|A+B\|$$
(3.1)

for any unitarily invariant norm.

Again, the example in Section 2 shows that (3.1) may fail without the PPT assumption.

As the Hua matrix is PPT, Proposition 3.1 entails

COROLLARY 3.2. [14, Theorem 3.3] Let $A, B \in \mathbb{M}_{m \times n}$ be strictly contractive. Then

$$2\|(I_n - A^*B)^{-1}\| \leq \|(I_n - A^*A)^{-1} + (I_n - B^*B)^{-1}\|$$
(3.2)

for any unitarily invariant norm.

Under the same assumption as in Proposition 3.1, one may wonder whether a stronger level inequality (in the sense of Bhatia and Kittaneh [7])

$$2s_j(X) \leqslant s_j(A+B), \qquad j=1,\ldots,n$$

is true. Here $s_j(\cdot)$ denotes the *j*-th largest singular value. The answer is no. For example, $\begin{bmatrix} P^2 + Q^2 & PQ + QP \\ PQ + QP & P^2 + Q^2 \end{bmatrix} \in \mathbb{M}_{2n}$ is PPT whenever $P, Q \in \mathbb{M}_n$ are Hermitian. But it is known that $s_j(PQ + QP) \leq s_j(P^2 + Q^2)$ fails in general; see [7, p. 2182].

Nevertheless, for the Hua matrix the answer is affirmative. This looks surprising. We remark that a similar inequality was conjectured in [13]. The main result of this section is as follows.

THEOREM 3.3. Let $A, B \in \mathbb{M}_{m \times n}$ be strictly contractive. Then for j = 1, ..., n

$$2s_j\Big((I_n - A^*B)^{-1}\Big) \leqslant s_j\Big((I_n - A^*A)^{-1} + (I_n - B^*B)^{-1}\Big).$$
(3.3)

We need some lemmas. The first one is due to Fan and Hoffman and can be found in [5, p. 73].

LEMMA 3.4. For every $A \in \mathbb{M}_n$ with $\Re A \ge 0$,

$$s_j(\Re A) \leqslant s_j(A), \qquad j = 1, \dots, n.$$
 (3.4)

Here $\Re A = \frac{1}{2}(A + A^*).$

With Lemma 3.4, we can present the following result, which can be regarded as a complement of (3.3).

LEMMA 3.5. Let $A, B \in \mathbb{M}_{m \times n}$ be contractive. Then for j = 1, ..., n

$$2s_j \left(I_n - A^* B \right) \ge s_j \left((I_n - A^* A) + (I_n - B^* B) \right).$$

$$(3.5)$$

Proof. It is clear that

$$A^*A + B^*B \ge A^*B + B^*A = 2\Re A^*B,$$

thus

$$\Re(I_n - A^*B) = I_n - \Re A^*B \ge I_n - \frac{1}{2}(A^*A + B^*B) \ge 0.$$

Hence by Lemma 3.4, we have

$$s_{j}\left(\frac{(I_{n}-A^{*}A)+(I_{n}-B^{*}B)}{2}\right) \leqslant s_{j}\left(\Re(I_{n}-A^{*}B)\right)$$
$$\leqslant s_{j}\left(I_{n}-A^{*}B\right), \qquad j=1,\ldots,n,$$

so the required result follows. \Box

We need to invoke the following powerful tool, which was recently established by Drury [9] as a solution to the question raised in [7].

LEMMA 3.6. Let $A, B \in \mathbb{M}_n$ be positive. Then for j = 1, ..., n

$$2\sqrt{s_j(AB)} \leqslant s_j(A+B).$$

Now we are in a position to present

Proof of Theorem 3.3. For any j = 1, ..., n, by Lemma 3.6, it suffices to show

$$\sqrt{s_j \Big((I_n - A^* A)^{-1} (I_n - B^* B)^{-1} \Big)} \ge s_j \Big((I_n - A^* B)^{-1} \Big),$$

which is equivalent to

$$\sqrt{s_j \left((I_n - B^* B) (I_n - A^* A) \right)} \leqslant s_j \left(I_n - A^* B \right), \tag{3.6}$$

since $s_j(X^{-1}) = \frac{1}{s_{n-j+1}(X)}$ for every invertible $X \in \mathbb{M}_n$. Again by Lemma 3.6, (3.6) would follow if

$$s_j\left(\frac{(I_n-B^*B)+(I_n-A^*A)}{2}\right)\leqslant s_j\left(I_n-A^*B\right),$$

but this is the content of Lemma 3.5. Therefore, Theorem 3.3 is proved. \Box

As a byproduct of our proof, we have the following proposition.

PROPOSITION 3.7. Let $A, B \in \mathbb{M}_{m \times n}$ be strictly contractive. Then for j = 1, ..., n

$$s_j\Big((I_n - A^*B)^{-1}(I_n - B^*A)^{-1}\Big) \leq s_j\Big((I_n - A^*A)^{-1}(I_n - B^*B)^{-1}\Big),$$

or equivalently,

$$s_j\Big((I_n-A^*B)(I_n-B^*A)\Big) \ge s_j\Big((I_n-A^*A)(I_n-B^*B)\Big).$$

To finish this section, we show that Proposition 3.7 implies the following result of Marcus [15]. If $A \in \mathbb{M}_n$, we let the eigenvalues of A be so arranged such that $|\lambda_1(A)| \ge |\lambda_2(A)| \ge \cdots \ge |\lambda_n(A)|$.

PROPOSITION 3.8. Let $A, B \in \mathbb{M}_{m \times n}$ be contractive. Then for each k satisfying $1 \leq k \leq n$,

$$\prod_{j=1}^{k} |\lambda_{n-j+1}(I_n - A^*B)|^2 \ge \prod_{j=1}^{k} (1 - \lambda_j(A^*A))(1 - \lambda_j(B^*B)).$$

Proof. It is well known [5, p. 43, p. 72] that for any $X, Y \in \mathbb{M}_n$, $\prod_{j=1}^k s_j(X) \ge \prod_{j=1}^k |\lambda_j(X)|$ and $\prod_{j=1}^k s_j(X)s_j(Y) \ge \prod_{j=1}^k s_j(XY)$ for each k satisfying $1 \le k \le n-1$ with equality at k = n. This implies

$$\prod_{j=1}^k s_{n-j+1}(X) \leqslant \prod_{j=1}^k |\lambda_{n-j+1}(X)|$$

and

$$\prod_{j=1}^{k} s_{n-j+1}(X) s_{n-j+1}(Y) \leqslant \prod_{j=1}^{k} s_{n-j+1}(XY)$$

for each *k* satisfying $1 \le k \le n$. Compute

$$\begin{split} \prod_{j=1}^{k} |\lambda_{n-j+1}(I_n - A^*B)|^2 &\ge \prod_{j=1}^{k} \left(s_{n-j+1}(I_n - A^*B) \right)^2 \\ &\geqslant \prod_{j=1}^{k} s_{n-j+1} \left((I_n - A^*A)(I_n - B^*B) \right) \\ &\geqslant \prod_{j=1}^{k} s_{n-j+1}(I_n - A^*A) s_{n-j+1}(I_n - B^*B) \\ &= \prod_{j=1}^{k} \lambda_{n-j+1}(I_n - A^*A) \lambda_{n-j+1}(I_n - B^*B) \\ &= \prod_{j=1}^{k} (1 - \lambda_j(A^*A))(1 - \lambda_j(B^*B)), \end{split}$$

in which Proposition 3.7 plays a role in the second inequality. \Box

4. More results

After finishing the first version this paper, J.-C. Bourin informed the author that a weak log majorization version of Theorem 2.1 is also valid. We thank J.-C. Bourin for allowing us to include his result.

THEOREM 4.1. (Bourin) Let
$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{M}_{2n}$$
 be PPT. Then
$$\prod_{j=1}^k s_j(X) \leqslant \prod_{j=1}^k s_j(A^{1/2}B^{1/2}), \quad k = 1, \dots, n.$$

Equivalently,

$$\prod_{j=1}^k \lambda_j(X^*X) \leqslant \prod_{j=1}^k \lambda_j(AB), \quad k = 1, \dots, n.$$

Proof. We have $X = A^{1/2}CB^{1/2}$ for some contraction $C \in \mathbb{M}_n$; see [6, p. 13]. Similarly, $X^* = A^{1/2}DB^{1/2}$ for some contraction $D \in \mathbb{M}_n$. Therefore,

$$\prod_{j=1}^{k} \lambda_j(X^*X) = \prod_{j=1}^{k} s_j(A^{1/2}DB^{1/2}A^{1/2}CB^{1/2}) \leqslant \prod_{j=1}^{k} s_j(DB^{1/2}A^{1/2}CB^{1/2}A^{1/2})$$
$$\leqslant \prod_{j=1}^{k} s_j(B^{1/2}A^{1/2})s_j(B^{1/2}A^{1/2}) = \prod_{j=1}^{k} \lambda_j(AB),$$

in which the first inequality is by the fact [5, p. 253] that $\prod_{j=1}^{k} s_k(PQ) \leq \prod_{j=1}^{k} s_j(QP)$, k = 1, 2, ..., whenever *PQ* is normal. \Box

In this connection, we shall show that Theorem 4.1 can be self-improved. The geometric mean of two positive definite matrices $A, B \in \mathbb{M}_n$, denoted by $A \sharp B$, is the positive definite solution of the Ricatti equation $XB^{-1}X = A$ and it has the explicit expression $A \sharp B = B^{1/2} (B^{-1/2}AB^{-1/2})^{1/2}B^{1/2}$. The notion of geometric mean can be uniquely extended to all $A, B \ge 0$ by a limit from above:

$$A \sharp B := \lim_{\varepsilon \to 0} (A + \varepsilon I_n) \sharp (B + \varepsilon I_n).$$

For more information about matrix geometric mean, we refer to [6, Chapter 4].

LEMMA 4.2. If
$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{M}_{2n}$$
 is PPT, then so is $\begin{bmatrix} A \ \# B & X \\ X^* & A \ \# B \end{bmatrix}$.

Proof. This follows immediately from [2, Lemma 3.1]. \Box

THEOREM 4.3. Let
$$\begin{bmatrix} A & X \\ X^* & B \end{bmatrix} \in \mathbb{M}_{2n}$$
 be PPT. Then
$$\prod_{j=1}^k s_j(X) \leqslant \prod_{j=1}^k s_j(A \sharp B) \leqslant \prod_{j=1}^k s_j(A^{1/2}B^{1/2}), \quad k = 1, \dots, n.$$

Proof. By Lemma 4.2, $\begin{bmatrix} A \# B \ X \\ X^* A \# B \end{bmatrix}$ is PPT. Now applying Theorem 4.1 to $\begin{bmatrix} A \# B \ X \\ X^* A \# B \end{bmatrix}$ gives the first inequality. The second inequality is well known and it has various generalizations; see for example [8, (18)]. It is also apparent that $\prod_{j=1}^{n} s_j(A \# B) \leq \prod_{i=1}^{n} s_j(A^{1/2}B^{1/2})$. \Box

We remark that Theorem 4.3 generalizes [2, Theorem 3.3].

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Minghua Lin Department of Mathematics, Shanghai University Shanghai, 200444, China e-mail: mlin87@ymail.com