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POSITIVE SEMIDEFINITE $3 \times 3$ BLOCK MATRICES

MINGHUA LIN† AND P. VAN DEN DRIESSCHE‡

Abstract. Several results related to positive semidefinite $3 \times 3$ block matrices are presented. In particular, a question of Audenaert [K.M.R. Audenaert. A norm compression inequality for block partitioned positive semidefinite matrices. Linear Algebra Appl., 413:155–176, 2006.] is answered affirmatively and some determinantal inequalities are proved.

Key words. Positivity, Block matrix, Principal angle.

AMS subject classifications. 15A45, 15A60.

1. Introduction. Positive semidefinite $2 \times 2$ block matrices are well studied. Such a partition not only leads to beautiful theoretical results, but also provides powerful techniques for various practical problems; see [6, 21] for excellent surveys. However, an analogous partition into $3 \times 3$ blocks seems not to be extensively investigated. In this article, we present several results on positive semidefinite $3 \times 3$ block matrices. We do not consider partitioning into $4 \times 4$ or higher numbers of blocks as results do not apply or are known to be false.

For a matrix $A$ with real or complex entries, the absolute value of $A$ is defined to be the matrix $|A| = (A^*A)^{1/2}$, where $A^*$ denotes the conjugate transpose of $A$; that is, $|A|$ is the principal square root of $A^*A$. The Schatten $p$-norm ($p \geq 1$) of $A$ is given by $\|A\|_p = (\text{tr}[|A|^p])^{1/p}$, where tr denotes the trace. When $p = 1, 2, \infty$, these are the trace norm, Frobenius norm, spectral norm, respectively. The identity matrix is denoted by $I$, with order determined from the context.

Our main consideration is the following positive semidefinite $3 \times 3$ block matrix

\begin{equation}
\mathbf{H} = \begin{bmatrix}
H_{11} & H_{12} & H_{13} \\
H_{12}^* & H_{22} & H_{23} \\
H_{13}^* & H_{23}^* & H_{33}
\end{bmatrix},
\end{equation}

where the diagonal blocks are square and of arbitrary order. As is well known, $\mathbf{H}$ can

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be identified with

\[
H = \begin{bmatrix}
X^*X & X^*Y & X^*Z \\
Y^*X & Y^*Y & Y^*Z \\
Z^*X & Z^*Y & Z^*Z
\end{bmatrix},
\]

for certain matrices \(X, Y, Z\).

If each block of \(H\) is square, then since \(\langle X, Y \rangle = \text{tr} Y^*X\) defines an inner product on the matrix space, (1.2) immediately shows that

\[
H_1 = \begin{bmatrix}
\text{tr} H_{11} & \text{tr} H_{12} & \text{tr} H_{13} \\
\text{tr} H_{12}^* & \text{tr} H_{22} & \text{tr} H_{23} \\
\text{tr} H_{13} & \text{tr} H_{23}^* & \text{tr} H_{33}
\end{bmatrix},
\]

is a Gram matrix and so is positive semidefinite.

An interesting observation due to Marcus and Watkins [19] is that the matrix

\[
H_2 = \begin{bmatrix}
|\text{tr} H_{11}| & |\text{tr} H_{12}| & |\text{tr} H_{13}| \\
|\text{tr} H_{12}^*| & |\text{tr} H_{22}| & |\text{tr} H_{23}| \\
|\text{tr} H_{13}^*| & |\text{tr} H_{23}^*| & |\text{tr} H_{33}|
\end{bmatrix}
\]

is again positive semidefinite, but this is not the case for higher numbers of blocks. Using this observation, we prove in Section 2 that the angle determined by the product of the cosines of principal angles defines a metric. Ando and Petz [1] Theorems 5 proved a determinantal inequality involving a positive semidefinite \(3 \times 3\) block matrix. In Section 3, we give a stronger inequality when all blocks are square with a simpler proof. Moreover, our method of proof also provides a proof of Dodgson’s condensation formula (see, e.g. [3]). In Section 4, we answer in the affirmative a question raised by Audenaert [2]. In our notation, this is

\[
\|H_1\|_p \geq \|H_2\|_p
\]

for \(1 \leq p \leq 2\), with the inequality reversed for \(p \geq 2\). Placing the absolute value inside the trace in (1.3) gives the matrix

\[
H_3 = \begin{bmatrix}
|\text{tr} H_{11}| & |\text{tr} H_{12}| & |\text{tr} H_{13}| \\
|\text{tr} H_{12}^*| & |\text{tr} H_{22}| & |\text{tr} H_{23}| \\
|\text{tr} H_{13}^*| & |\text{tr} H_{23}^*| & |\text{tr} H_{33}|
\end{bmatrix}.
\]

This matrix was recently shown by Drury [8] to be positive semidefinite. Motivated by Drury’s result, we conclude with a conjecture in Section 5.

2. Product cosines of angles. Let \(\mathcal{X}, \mathcal{Y}\) be subspaces of \(\mathbb{C}^n\) with the same dimension \(\ell\). The principal angles between \(\mathcal{X}\) and \(\mathcal{Y}\), say \(\alpha_k, k = 1, \ldots, \ell\), completely
describe the relative position of these subspaces. See Golub and Van Loan [13, p. 603] for the definition of principal angles between subspaces. Let \( X, Y \) be matrices whose columns are orthonormal bases for \( \mathcal{X}, \mathcal{Y} \), respectively. It is known [13, p. 604] that the cosines of principal angles between \( \mathcal{X} \) and \( \mathcal{Y} \) are equal to the singular values of \( X^*Y \).

The notion of the product of the cosines of the principal angles between subspaces was introduced by Miao and Ben-Israel in [20]. Let

\[
\cos \Phi_{X,Y} := \prod_{k=1}^{\ell} \cos \alpha_k, \quad \Phi_{X,Y} \in [0, \pi/2],
\]

denote the product of the cosines of principal angles \( \alpha_k \) \((k = 1, \ldots, \ell)\) between the subspaces \( \mathcal{X} \) and \( \mathcal{Y} \).

Thus,

\[
\cos \Phi_{X,Y} = \prod_{k=1}^{\ell} \sigma_k(X^*Y) = |\det X^*Y|,
\]

where \( \sigma_k \) denotes a singular value. Recall that the usual angle \( \theta_{xy} \) between two nonzero vectors \( x, y \in \mathbb{C}^n \) is determined by \( \cos \theta_{xy} = \frac{|x^*y|}{\|x\|\|y\|} \). It is well known that \( \theta_{xy} \) defines a metric. Thus, a natural question is whether the angle \( \Phi_{X,Y} \) also defines a metric. This is the content of the following theorem, as clearly \( \Phi_{X,Y} = \Phi_{Y,X} \) and \( \Phi_{X,X} = 0 \).

**Theorem 2.1.** Let \( \mathcal{X}, \mathcal{Y}, \mathcal{Z} \) be subspaces of \( \mathbb{C}^n \) with the same dimension. Then

\[
\Phi_{X,Z} \leq \Phi_{X,Y} + \Phi_{YZ}.
\]

**Proof.** The idea of the proof is similar to the proof of Krein’s inequality; see e.g. [13, p. 56] and [18]. Since \( \cos \alpha \) is a decreasing function of \( \alpha \in [0, \pi] \), it suffices to prove

\[
\cos \Phi_{X,Z} \geq \cos(\Phi_{X,Y} + \Phi_{YZ})
\]

or equivalently,

\[
|\det X^*Z| \geq |\det X^*Y| \cdot |\det Y^*Z| - \sqrt{1 - |\det X^*Y|^2} \cdot \sqrt{1 - |\det Y^*Z|^2}.
\]

This is equivalent to

\[
(2.1) \quad \sqrt{1 - |\det X^*Y|^2} \cdot \sqrt{1 - |\det Y^*Z|^2} \geq |\det X^*Y| \cdot |\det Y^*Z| - |\det X^*Z|.
\]
If the right-hand side of (2.1) is negative, then (2.1) holds. Otherwise, we need to prove
\[
(1 - |\det X^*Y|^2) \cdot (1 - |\det Y^*Z|^2) \geq \left( |\det X^*Y| \cdot |\det Y^*Z| - |\det X^*Z| \right)^2
\]
or equivalently,
\[
1 - |\det X^*Y|^2 - |\det Y^*Z|^2 - |\det X^*Z|^2 + 2|\det X^*Y| \cdot |\det Y^*Z| \cdot |\det X^*Z| \geq 0.
\]

It suffices to show
\[
\begin{bmatrix}
1 & |\det X^*Y| & |\det X^*Z| \\
|\det Y^*X| & 1 & |\det Y^*Z| \\
|\det Z^*X| & |\det Z^*Y| & 1
\end{bmatrix}
\]
is positive semidefinite. By the observation of Marcus and Watkins [19], this follows if
\[
\begin{bmatrix}
1 & \det X^*Y & \det X^*Z \\
\det Y^*X & 1 & \det Y^*Z \\
\det Z^*X & \det Z^*Y & 1
\end{bmatrix}
\]
is positive semidefinite. But this matrix is just a principal submatrix of a compound matrix (see, e.g. [15, p. 19]) of
\[
\begin{bmatrix}
I & X^*Y & X^*Z \\
Y^*X & I & Y^*Z \\
Z^*X & Z^*Y & I
\end{bmatrix},
\]
which is obviously positive semidefinite. \qed


**Theorem 3.1.** [1, Theorem 5] Let $H$ as defined in (1.1) be positive definite. Then
\[
(3.1) \quad \det H \cdot \det H_{22} \leq \det \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{bmatrix}, \det \begin{bmatrix} H_{22} & H_{23} \\ H_{23}^* & H_{33} \end{bmatrix}.
\]

Equality holds if and only if $H_{13} = H_{13} H_{22}^{-1} H_{23}$. Indeed, the above inequality had already appeared in Exercise 14 on p. 485 of [15]. Here we provide a refinement of (3.1) when all blocks of $H$ are square. We use the following observation by Everitt.
Lemma 3.2. \[ \text{Eq.(5.1)} \] Let \[
\begin{bmatrix}
A & X \\
X^* & B
\end{bmatrix}
\]
be positive semidefinite with all blocks square. Then
\[
\det \begin{bmatrix}
A & X \\
X^* & B
\end{bmatrix} \leq \det A \cdot \det B - |\det X|^2.
\]
Equality holds if and only if \(X\) is a zero matrix.

Theorem 3.3. Let \(H\) as defined in \((1.1)\) be positive definite. If each block of \(H\) is square, then
\[
\det H \cdot \det H_{22} \leq \det \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{bmatrix} \cdot \det \begin{bmatrix} H_{22} & H_{23} \\ H_{23}^* & H_{33} \end{bmatrix} - \left| \det \begin{bmatrix} H_{12} & H_{13} \\ H_{22} & H_{23} \end{bmatrix} \right|^2.
\]
Equality holds if and only if \(H_{13} = H_{12} H_{22}^{-1} H_{23}\).

Proof. Let \(P = \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \end{bmatrix}\) be partitioned conformally with \(H\). It is easy to see that
\[
G = P^* HP = \begin{bmatrix} H_{11} & H_{13} & H_{12} \\ H_{13}^* & H_{33} & H_{23} \\ H_{12}^* & H_{23} & H_{22} \end{bmatrix}
\]
is again positive definite, as is its Schur complement (see, e.g., [21])
\[
G/H_{22} := \begin{bmatrix} H_{11} & H_{13} \\ H_{13} & H_{22} \\ H_{12} & H_{23} \end{bmatrix} - \begin{bmatrix} H_{12} \\ H_{23}^* \end{bmatrix} H_{22}^{-1} \begin{bmatrix} H_{12}^* & H_{23} \end{bmatrix}
\]
\[
= \begin{bmatrix} H_{11} - H_{12} H_{22}^{-1} H_{12}^* & H_{13} - H_{12} H_{22}^{-1} H_{23} \\ H_{13}^* - H_{23}^* H_{22}^{-1} H_{12}^* & H_{33} - H_{23}^* H_{22}^{-1} H_{23} \end{bmatrix}.
\]
By Lemma 5.2,
\[
\det(G/H_{22}) \leq \det(H_{11} - H_{12} H_{22}^{-1} H_{12}^*) \cdot \det(H_{33} - H_{23}^* H_{22}^{-1} H_{23})
\]
\[
- \left| \det(H_{13} - H_{12} H_{22}^{-1} H_{23}) \right|^2
\]
with equality if and only if the off-diagonal blocks \(G/H_{22}\) vanish, that is, \(H_{13} = H_{12} H_{22}^{-1} H_{23}\).

The assertion follows by observing that
\[
\det H = \det G = \det H_{22} \cdot \det(G/H_{22})
\]
and
\[
\det \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{bmatrix} = \det H_{22} \cdot \det(H_{11} - H_{12} H_{22}^{-1} H_{12}^*),
\]
\[
\det \begin{bmatrix} H_{22} & H_{23} \\ H_{23}^* & H_{33} \end{bmatrix} = \det H_{22} \cdot \det(H_{33} - H_{23}^* H_{22}^{-1} H_{23}). \]
Remark 3.4. By a continuity argument, (3.1) and (3.2) remain valid if $H$ is assumed to be only positive semidefinite.

The equalities in the previous proof may also be applied to give a proof of Dodgson’s condensation formula (see, e.g. [3]); if

$$A = \begin{bmatrix} a_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & a_{33} \end{bmatrix},$$

with $a_{11}, a_{33}$ scalars and $A_{22}$ a square matrix, then

$$\det A \cdot \det A_{22} = \det \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \cdot \det \begin{bmatrix} A_{22} & A_{23} \\ A_{32} & a_{33} \end{bmatrix} - \det \begin{bmatrix} 0 & A_{13} \\ A_{22} & A_{23} \end{bmatrix} \cdot \det \begin{bmatrix} A_{12} & A_{13} \\ A_{21} & A_{22} \end{bmatrix}.$$

In the remaining part of this section, we give an application of (3.1) to find a bound for the determinant of the $k$-subdirect sum of two positive semidefinite matrices of the same order.

Consider

$$(3.3) \quad A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} B_{22} & B_{23} \\ B_{32} & B_{33} \end{bmatrix}$$

partitioned such that $A_{22}, B_{22}$ are $k \times k$. The $k$-subdirect sum of $A$ and $B$ is defined as

$$A \oplus_k B := \begin{bmatrix} A_{11} & A_{12} & 0 \\ A_{21} & A_{22} + B_{22} & B_{23} \\ 0 & B_{32} & B_{33} \end{bmatrix};$$

see for example [10]. Thus, $A \oplus_k B$ is a $3 \times 3$ block matrix.

Theorem 3.5. Let $A, B$ as defined in (3.3) be positive semidefinite of the same order. Then

$$\det(A \oplus_k B) \cdot \det(A_{22} + B_{22}) \leq \det(A + B)^2.$$

Proof. It is known that $A \oplus_k B$ is again positive semidefinite [10, Theorem 2.2]. Applying (3.1) to $A \oplus_k B$ gives

$$(3.4) \quad \det(A \oplus_k B) \cdot \det(A_{22} + B_{22}) \leq \det \begin{bmatrix} A_{11} & A_{12} \\ A_{12} & A_{22} + B_{22} \end{bmatrix} \cdot \det \begin{bmatrix} A_{22} + B_{22} & B_{23} \\ B_{23} & B_{33} \end{bmatrix}.$$
Without loss of generality, assume $A$ is positive definite. As $A^{-1/2}B$ is a principal submatrix of $A^{-1/2}BA^{-1/2}$, the eigenvalues of $A^{-1/2}B$ are dominated by those of $A^{-1/2}BA^{-1/2}$ (\cite{15} p. 189), so

$$\det \left( I + A^{-1/2}B \right) \leq \det \left( I + A^{-1/2}BA^{-1/2} \right).$$

Multiplying both sides by $\det A$ gives

$$\begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} \leq \det(A + B).$$

Similarly, $\begin{vmatrix} A_{22} & A_{23} \\ B_{23} & B_{33} \end{vmatrix} \leq \det(A + B)$. Using these in (3.4) gives the required inequality.

4. A norm inequality. In \cite{16}, King proved that for positive semidefinite $2 \times 2$ block matrices:

$$\begin{vmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{vmatrix} \geq \begin{vmatrix} \|H_{11}\|_p & \|H_{12}\|_p \\ \|H_{21}\|_p & \|H_{22}\|_p \end{vmatrix}, \quad 1 \leq p \leq 2,$$

while the reverse inequality holds for $p \geq 2$.

Even when the blocks $H_{ij}$ are scalars, the obvious generalisation of (4.1) to $4 \times 4$ and thus to higher numbers of blocks is still not true for non-integral $p$. Audenaert \cite{2} p. 158] gave a $4 \times 4$ positive semidefinite matrix counterexample, and remarked that it might be true for the $3 \times 3$ case. We provide in Theorem 4.3 a proof of this fact.

**Lemma 4.1.** Let $H_1$ and $H_2$ be defined as in Section 1. Then $\|H_1\|_{\infty} \leq \|H_2\|_{\infty}$.

**Proof.** As $H_2$ is a symmetric entrywise nonnegative matrix, by Perron-Frobenius theory \cite{15} p. 503], it follows that $\max_{\|x\|=1} |\text{tr} H_{ij}||x_i||x_j| = \max_{\|x\|=1} x^*H_2x$, where $x = [x_1, x_2, x_3]^T \in \mathbb{C}^3$. Compute

$$\|H_1\|_{\infty} = \max_{\|x\|=1} x^*H_1x = \max_{\|x\|=1} (\text{tr} H_{ij})x_i x_j$$

$$\leq \max_{\|x\|=1} |\text{tr} H_{ij}||x_i||x_j| = \max_{\|x\|=1} x^*H_2x = \|H_2\|_{\infty}. \quad \Box$$

The following elegant $p$-free $\ell^p$ inequality is due to Bennett.

**Lemma 4.2.** [4 Theorem 1] Suppose that $a, b, c$ and $x, y, z$ are positive numbers. Then the inequality

$$a^p + b^p + c^p \leq x^p + y^p + z^p$$
holds whenever \( p \geq 2 \) or \( 0 \leq p \leq 1 \), and reverses direction whenever \( p \leq 0 \) or \( 1 \leq p \leq 2 \), if and only if the following three conditions are satisfied:
\[
\begin{align*}
    a + b + c &= x + y + z \\
    a^2 + b^2 + c^2 &= x^2 + y^2 + z^2 \\
    \max\{a, b, c\} &\leq \max\{x, y, z\}.
\end{align*}
\]

**Theorem 4.3.** Let \( H_1 \) and \( H_2 \) be defined as in Section 1. Then
\[
\|H_1\|_p \leq \|H_2\|_p,
\]
for \( p \geq 2 \), while the reverse inequality holds for \( 1 \leq p \leq 2 \).

**Proof.** Let \( a, b, c \) be the singular values of \( H_1 \), and \( x, y, z \) be the singular values of \( H_2 \), respectively. Lemma 4.1 gives \( \max\{a, b, c\} \leq \max\{x, y, z\} \). It is obvious that \( \text{tr} H_1 = a + b + c = \text{tr} H_2 = x + y + z \) and \( \|H_1\|_2 = a^2 + b^2 + c^2 = \|H_2\|_2 = x^2 + y^2 + z^2 \). Without loss of generality, assume that both \( H_1 \) and \( H_2 \) are positive definite, thus Lemma 4.2 gives the desired result.

In general, \( \|H_2\|_2 < \|H_3\|_2 \), where \( H_2 \) and \( H_3 \) are defined in Section 1. In view of the second condition in Lemma 4.2, there is no analogy of (1.2) when \( H_3 \) is involved.

**Example 4.4.** Take \( X = \begin{bmatrix} -0.8621 & -0.8174 \\ -2.2038 & 1.1974 \end{bmatrix}, Y = \begin{bmatrix} 0.5419 & -2.4834 \\ -0.0855 & -1.3874 \end{bmatrix} \) and \( Z = \begin{bmatrix} 0.6275 & -3.1929 \\ -1.6270 & 1.2459 \end{bmatrix} \) to form the matrix \( H \) as in (1.2). A calculation gives the smallest singular value of \( H_2 \) is about 1.1033, while the smallest singular value of \( H_3 \) is about 2.1821. By the Fan Dominance Theorem (see, e.g. [5, p. 93]), the majorization between \( H_2 \) and \( H_3 \) is not possible.

**5. A conjecture.** Motivated by results of [8] and [19], we make the following conjecture.

**Conjecture 5.1.** Let \( H \) be defined as in (1.1) and \( 1 \leq p \leq 2 \). Then the \( 3 \times 3 \) matrix
\[
H = \begin{bmatrix}
    \|H_{11}\|_p & \|H_{12}\|_p & \|H_{13}\|_p \\
    \|H_{12}\|_p & \|H_{22}\|_p & \|H_{23}\|_p \\
    \|H_{13}\|_p & \|H_{23}\|_p & \|H_{33}\|_p
\end{bmatrix}
\]
is positive semidefinite.
When \( p = 1 \), Conjecture 5.1 is exactly the aforementioned result of Drury [8, Corollary 1.3]. For a short proof of this case, see [17]. Note that the authors in [11, Proposition 1] claimed a similar result, but there is a serious gap in the proof, which lies in [11, Lemma 2]. When \( p = 2 \), the result of Marcus and Watkins [19, Theorem 1] states that Conjecture 5.1 is also true for higher numbers of blocks. Fitzgerald and Horn [12] have shown that, if \( A = [a_{ij}] \) is an \( n \times n \) positive semidefinite matrix with \( a_{ij} \geq 0 \) for all \( i \) and \( j \), then \( A^{op} := [a_{ij}^p] \) is positive semidefinite for each \( p \geq n - 2 \). Thus, Conjecture 5.1 is true when each block of \( H \) defined in (1.1) is a scalar. We remark that the approaches in [8, 17] do not enable us to fully prove Conjecture 5.1, we expect a completely new approach is needed.

Numerical experiment suggests that in general \( H \) fails to be positive semidefinite for any finite \( p > 2 \). We borrow the following example from [7] to show that the result is also not true in general for \( p = \infty \).

**Example 5.2.** Consider

\[
H = \begin{bmatrix}
H_{11} & H_{12} & H_{13} \\
H_{12}^T & H_{22} & H_{23} \\
H_{13}^T & H_{23}^T & H_{33}
\end{bmatrix} = \begin{bmatrix}
1 & 0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1
\end{bmatrix},
\]

which is positive definite. However, with \( p = \infty \),

\[
H = \begin{bmatrix}
\|H_{11}\|_{\infty} & \|H_{12}\|_{\infty} & \|H_{13}\|_{\infty} \\
\|H_{12}\|_{\infty} & \|H_{22}\|_{\infty} & \|H_{23}\|_{\infty} \\
\|H_{13}\|_{\infty} & \|H_{23}\|_{\infty} & \|H_{33}\|_{\infty}
\end{bmatrix} = \begin{bmatrix}
1 & 0 & 1 \\
0 & 1 & 1 \\
1 & 1 & 1
\end{bmatrix}
\]

has negative determinant, and so is not positive semidefinite.

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M. Lin and P. van den Driessche


