2014

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Recommended Citation
DOI: https://doi.org/10.13001/1081-3810.2003

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POSITIVE SEMIDEFINITE 3 × 3 BLOCK MATRICES∗

MINGHUA LIN† AND P. VAN DEN DRIESSCHE‡

Abstract. Several results related to positive semidefinite 3 × 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 × 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 [16, 21] for excellent surveys. However, an analogous partition into 3 × 3 blocks seems not to be extensively investigated. In this article, we present several results on positive semidefinite 3 × 3 block matrices. We do not consider partitioning into 4 × 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 ≥ 1) of A is given by ∥A∥p = (tr |A|p)1/p, where tr denotes the trace. When p = 1, 2, ∞, 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 × 3 block matrix

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

where the diagonal blocks are square and of arbitrary order. As is well known, H can

∗Received by the editors on March 12, 2014. Accepted for publication on November 9, 2014. Handling Editor: Bryan L. Shader.
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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 \cite{MarcusWatkins} 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 \cite{AndoPetz} 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. \cite{Dodgson}). In Section 4 we answer in the affirmative a question raised by Audenaert \cite{Audenaert}. 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 \cite{Drury} 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

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

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

Thus,

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

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 \(\Phi_{XY}\) also defines a metric. This is the content of the following theorem, as clearly \(\Phi_{XY} = \Phi_{YX}\) and \(\Phi_{XX} = 0\).

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

\[
\Phi_{XZ} \leq \Phi_{XY} + \Phi_{YZ}.
\]

**Proof.** The idea of the proof is similar to the proof of Krein’s inequality; see e.g. [14, p. 56] and [18]. Since \(\cos \alpha\) is a decreasing function of \(\alpha \in [0, \pi]\), it suffices to prove

\[
\cos \Phi_{XZ} \geq \cos(\Phi_{XY} + \Phi_{YZ})
\]

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.


**Theorem 3.1.** [1 Theorem 5] Let \( H \) as defined in (1.1) be positive definite. Then
\[
(3.1) \quad \det H \cdot \det H_{22} \leq \det \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{bmatrix} \cdot \det \begin{bmatrix} H_{22} & H_{23} \\ H_{23}^* & H_{33} \end{bmatrix}.
\]
Equality holds if and only if \( H_{13} = H_{12}^{-1} H_{22} H_{23} \).

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.** [6, 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 $P = \begin{bmatrix} I & 0 & 0 \\ 0 & 0 & I \\ 0 & I & 0 \end{bmatrix}$ be partitioned conformally with $H$. It is easy to see that

$$G = P^* H P = \begin{bmatrix} H_{11} & H_{13} & H_{12} \\ H_{13}^* & H_{33} & H_{23} \\ H_{12}^* & H_{23} & H_{22} \end{bmatrix}$$

is again positive definite, as is its Schur complement (see, e.g. [21])

$$G/H_{22} = \begin{bmatrix} H_{11} & H_{13} \\ H_{13}^* & H_{33} \end{bmatrix} - \begin{bmatrix} H_{12} & H_{23}^{-1} \end{bmatrix} H_{22}^{-1} \begin{bmatrix} H_{12}^* & H_{23} \\ H_{23}^* & H_{33} \end{bmatrix}$$

$$= \begin{bmatrix} H_{11} - H_{12} H_{22}^{-1} H_{12}^* & H_{13} - H_{12} H_{22}^{-1} H_{23} \\ H_{13}^* - H_{23}^* H_{22}^{-1} H_{12}^* & H_{33} - H_{23}^* H_{22}^{-1} H_{23} \end{bmatrix}.$$  

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

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

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

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

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

$$\det(A \oplus_k B) \cdot \det(A_{22} + B_{22}) \leq \det \begin{bmatrix} A_{11} & A_{12} \\ A_{12} & A_{22} + B_{22} \end{bmatrix} \cdot \det \begin{bmatrix} A_{22} + B_{22} & B_{23} \\ B_{23} & B_{33} \end{bmatrix}.$$
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Without loss of generality, assume $A$ is positive definite. As $A^{-1/2}[0 \quad 0 \quad B_{22}]A^{-1/2}$
is a principal submatrix of $A^{-1/2}BA^{-1/2}$, the eigenvalues of $A^{-1/2}[0 \quad 0 \quad B_{22}]A^{-1/2}$
are dominated by those of $A^{-1/2}BA^{-1/2}$ ([15, p. 189]), so
\[
\det \left( I + A^{-1/2}[0 \quad 0 \quad B_{22}]A^{-1/2} \right) \leq \det \left( I + A^{-1/2}BA^{-1/2} \right).
\]
Multiplying both sides by $\det A$ gives $\det \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \leq \det \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$. Similarly, $\det \begin{bmatrix} A_{12} & B_{22} \\ A_{23} & B_{33} \end{bmatrix} \leq \det \begin{bmatrix} A_{12} & B_{22} \\ A_{23} & B_{33} \end{bmatrix}$. Using these in (3.4) gives the required inequality.

4. A norm inequality. In [16], King proved that for positive semidefinite $2 \times 2$
block matrices:
\[
\left\| \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \right\|_p \geq \left\| \begin{bmatrix} H_{11} \\ H_{21} \end{bmatrix} \right\|_p \left\| \begin{bmatrix} H_{12} \\ H_{22} \end{bmatrix} \right\|_p , \quad 1 \leq p \leq 2,
\]
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 [21 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 [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
\[
\|H_1\|_\infty = \max_{\|x\|=1} x^*H_1x = \max_{\|x\|=1} (\text{tr} H_{ij})x_i x_j \\
\leq \max_{\|x\|=1} |\text{tr} H_{ij}||x_i||x_j| \\
= \max_{\|x\|=1} x^*H_2x = \|H_2\|_\infty. \quad \square
\]

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 (4.2) when \( H_3 \) is involved.

It is clear that \( \|H_2\|_1 = \|H_3\|_1 \) and as in the proof of Lemma 4.2, it follows that \( \|H_2\|_\infty \leq \|H_3\|_\infty \). It is tempting to ask whether \( \|H_2\|_p \leq \|H_3\|_p \) for every \( p > 1 \). We remark that, however, it is in general not true that \( \|H_2\|_p \leq \|H_3\|_p \) for every unitarily invariant norm as the following example shows.

**Example 4.4.** Take

\[
X = \begin{bmatrix}
-0.8621 & -0.8174 \\
-2.0383 & 1.9741
\end{bmatrix},
\]

\[
Y = \begin{bmatrix}
0.5419 & -2.4834 \\
-0.0855 & -1.3874
\end{bmatrix}
\]

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 $A^p := [a_{ij}^p]$ 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

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

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

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

has negative determinant, and so is not positive semidefinite.

**Acknowledgment.** The authors are grateful to the referee for helpful comments.

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