Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.

# SINGULAR VALUES, EIGENVALUES AND DIAGONAL ELEMENTS OF THE COMMUTATOR OF $2 \times 2$ RANK ONE MATRICES*

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*Dedicated to Professor Yik-Hoi Au-Yeung*

**Abstract.** The region of singular values of the commutator $XY - YX$ for $2 \times 2$ rank one complex matrices $X$ and $Y$ is determined. This answers in affirmative a conjecture raised in [D. Wenzel. A strange phenomenon for the singular values of commutators with rank one matrices. *Electron. J. Linear Algebra*, 30:649–669, 2015.] when $2 \times 2$ matrices are concerned. The approach and proofs also lead to a complete relation between the singular values, eigenvalues and diagonal elements of the commutator under consideration.

**Key words.** Commutator, Singular value, Eigenvalue, Diagonal element.

**AMS subject classifications.** 15A18.

## 1. Introduction.

**1.1. Background and main results.** Let $\mathbb{F}$ denote the set of real numbers $\mathbb{R}$ or the set of complex numbers $\mathbb{C}$, and let $\mathbf{i} = \sqrt{-1}$. We use column vectors for vectors in $\mathbb{F}^n$, and use row $n$-tuples for points in $\mathbb{F}^n$. The Euclidean inner product and norm on $\mathbb{F}^n$ are denoted by $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$, respectively. Let $M_n(\mathbb{F})$ denote the set of $n \times n$ matrices with entries in $\mathbb{F}$. We use also $\| \cdot \|$ to denote the Frobenius norm on $M_n(\mathbb{F})$. For $X \in M_n(\mathbb{F})$, let $s_1(X) \geq \cdots \geq s_n(X)$ denote the singular values of $X$ arranged in non-increasing order, and let $s(X) = (s_1(X), \ldots, s_n(X))^T$. Let $\|X\|_1 = s_1(X) + \cdots + s_n(X)$ denote the trace norm (also known as Schatten 1-norm and Ky-Fan $n$-norm) of $X$. Be aware that two norms are used in this paper. By a norm one matrix $X$ it is always meant $\|X\| = 1$ unless otherwise stated. For $X, Y \in M_n(\mathbb{F})$, the commutator of $X$ and $Y$ is defined and denoted by

$$[X, Y] = XY - YX.$$

We assume $n > 1$ throughout the paper to avoid trivial situations.

Let

$$\Sigma_n(\mathbb{F}) = \{X : X \in M_n(\mathbb{F}), s(X) = (1, 0, \ldots, 0)^T\},$$

which is the set of rank one norm one matrices in $M_n(\mathbb{F})$. When $X, Y \in \Sigma_n(\mathbb{F})$, the rank of the commutator $[X, Y]$ is at most two. Let

$$\mathcal{S}_n^{\mathbb{F}} = \{(s_1([X, Y]), s_2([X, Y])) : X, Y \in \Sigma_n(\mathbb{F})\} \subset \mathbb{R}^2. \tag{1.1}$$

*Received by the editors on August 9, 2018. Accepted for publication on November 6, 2019. Handling Editor: Ilya Spitkovski. Corresponding Author: Che-Man Cheng. This research was supported by research grant MYRG2016-00121-FST from the University of Macau.

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Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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It is proved in [7] that the set $\mathcal{S}_n^{\mathbb{R}}$ is the region $\mathcal{R}$ (see Figure 2.1) bounded by the segment joining $(0,0)$ and $(1,1)$, the segment joining $(0,0)$ and $(1,0)$, the segment joining $(1,0)$ and $\left(\frac{\sqrt{2}+1}{2}, \frac{\sqrt{2}-1}{2}\right)$, and the curve

$$\frac{4\sqrt{\cos\phi\sin\phi}}{1+2\cos\phi\sin\phi}(\cos\phi,\sin\phi), \quad \phi\in\left[\tan^{-1}\left(\frac{\sqrt{2}-1}{\sqrt{2}+1}\right), \frac{\pi}{4}\right]. \tag{1.2}$$

For an alternative characterization of $\mathcal{S}_n^{\mathbb{R}}$, see Theorem 1.5 below. It is also conjectured in [7, Conjecture 3.6] that $\mathcal{S}_n^{\mathbb{C}} = \mathcal{R}$. Numerical experiments highly suggest that this is true. Sadly, the approach used in [7] relies heavily on real numbers (in the form of angles) and cannot directly be adopted to the complex case.

When $X, Y \in \Sigma_n(\mathbb{F})$, we may assume $X = \mathbf{a}\mathbf{b}^*$ and $Y = \mathbf{c}\mathbf{d}^*$ where $\mathbf{a},\mathbf{b},\mathbf{c},\mathbf{d}\in\mathbb{F}^n$ are unit vectors. It is shown in [7, Theorem 4.1] that $s_1([X,Y])$ and $s_2([X,Y])$ depend solely on

$$A=\langle\mathbf{a},\mathbf{c}\rangle,\quad B=\langle\mathbf{b},\mathbf{d}\rangle,\quad C=\langle\mathbf{c},\mathbf{b}\rangle,\quad D=\langle\mathbf{d},\mathbf{a}\rangle.$$

Based on these inner products, the result is proved. The main purpose of this paper is to prove in affirmative that the conjecture is true for $2\times 2$ matrices. During our investigation, we found that there is a point in the proof in [7] that is not clear when $2\times 2$ matrices are concerned. Let us first point out the difference between the cases $n=2$ and $n\geq 3$.

It is trivial that $\mathcal{S}_2^{\mathbb{F}}\subseteq\mathcal{S}_3^{\mathbb{F}}\subseteq\mathcal{S}_4^{\mathbb{F}}\subseteq\cdots$. When $n>4$ and $X,Y\in\Sigma_n(\mathbb{F})$, there exists a unitary (orthogonal if $\mathbb{F}=\mathbb{R}$) matrix $U\in M_n(\mathbb{F})$ such that $U^*XU,\ U^*YU\in M_4(\mathbb{F})\oplus 0_{n-4}$. Consequently we know that $\mathcal{S}_k^{\mathbb{F}}=\mathcal{S}_4^{\mathbb{F}}$ for all $k>4$. Using the following proposition, we can extend the result to $3\times 3$ matrices to have $\mathcal{S}_k^{\mathbb{F}}=\mathcal{S}_3^{\mathbb{F}}$ for all $k>3$.

Proposition 1.1. *Suppose* $\mathbf{a},\mathbf{b},\mathbf{c},\mathbf{d}\in\mathbb{F}^4$ *are unit vectors. Then there are unit vectors* $\mathbf{v}_1,\mathbf{v}_2,\mathbf{v}_3,\mathbf{v}_4\in\mathbb{F}^3$ *such that*

$$\langle\mathbf{v}_1,\mathbf{v}_3\rangle=\langle\mathbf{a},\mathbf{c}\rangle,\quad\langle\mathbf{v}_2,\mathbf{v}_4\rangle=\langle\mathbf{b},\mathbf{d}\rangle,\quad\langle\mathbf{v}_3,\mathbf{v}_2\rangle=\langle\mathbf{c},\mathbf{b}\rangle,\quad\langle\mathbf{v}_4,\mathbf{v}_1\rangle=\langle\mathbf{d},\mathbf{a}\rangle.$$

*Proof.* By choosing a suitable unitary (orthogonal if $\mathbb{F}=\mathbb{R}$) matrix $U\in M_4(\mathbb{F})$ and considering $U\mathbf{x}$ for $\mathbf{x}\in\{\mathbf{a},\mathbf{b},\mathbf{c},\mathbf{d}\}$, we may assume

$$\mathbf{a}=(a_1,0,0,0)^T,\quad\mathbf{b}=(b_1,b_2,0,0)^T,\quad\mathbf{c}=(c_1,c_2,c_3,0)^T,\quad\mathbf{d}=(d_1,d_2,d_3,d_4)^T.$$

The vectors

$$\mathbf{v}_1=(a_1,0,0)^T,\quad\mathbf{v}_2=(b_1,b_2,0)^T,\quad\mathbf{v}_3=(c_1,c_2,c_3)^T,\quad\mathbf{v}_4=(d_1,d_2,\sqrt{|d_3|^2+|d_4|^2})^T.$$

serve our purpose. ∎

The situation is different when $n=2$. Suppose we choose

$$\mathbf{a}=(1,0,0,0)^T,\quad\mathbf{b}=(0,1,0,0)^T,\quad\mathbf{c}=(0,0,1,0)^T,\quad\mathbf{d}=(1/\sqrt{2},0,0,1/\sqrt{2})^T.$$

Then

$$A=\langle\mathbf{a},\mathbf{c}\rangle=0,\quad B=\langle\mathbf{b},\mathbf{d}\rangle=0,\quad C=\langle\mathbf{c},\mathbf{b}\rangle=0,\quad D=\langle\mathbf{d},\mathbf{a}\rangle=1/\sqrt{2}.$$

However, for unit vectors $\mathbf{a},\mathbf{b},\mathbf{c},\mathbf{d}\in\mathbb{F}^2$,

$$A=\langle\mathbf{a},\mathbf{c}\rangle=0,\quad B=\langle\mathbf{b},\mathbf{d}\rangle=0,\quad C=\langle\mathbf{c},\mathbf{b}\rangle=0$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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imply $D = \langle \mathbf{d}, \mathbf{a} \rangle = 0$. Thus, we know that not all inner products $(A, B, C, D)$ that can be achieved by vectors in $\mathbb{F}^4$ can be achieved by vectors in $\mathbb{F}^2$. It is then not clear that $\mathcal{S}_2^{\mathbb{R}}$ is not a proper subset of $\mathcal{S}_4^{\mathbb{R}}$ $(= \mathcal{R})$, although numerical experiments strongly suggest $\mathcal{S}_2^{\mathbb{R}} = \mathcal{R}$ and the boundary of $\mathcal{R}$ can be achieved by $2 \times 2$ real matrices (see the proof of [7, Proposition 3.3]).

We will first show in Section 3 that the smaller freedom in order 2 does not change the result.

Theorem 1.2. *$\mathcal{S}_2^{\mathbb{R}} = \mathcal{R}$.*

This is not merely to give an alternative proof for $2 \times 2$ real matrices. The proof here also reveals that all the possible combinations of the singular values can be achieved by commutators having real eigenvalues and hence are orthogonally upper triangularizable. This fact is used in Section 4 for proving our main theorem.

Theorem 1.3. *$\mathcal{S}_2^{\mathbb{C}} = \mathcal{R}$.*

Our approach and proofs also give immediately interesting results relating the singular values, eigenvalues and diagonal elements of the commutators under consideration. Before going to the lengthy proofs of Theorems 1.2 and 1.3, we include below a discussion on the results.

**1.2. Singular values, eigenvalues and diagonal elements.** Suppose $X, Y \in \Sigma_2(\mathbb{F})$ and $[X, Y] = \left[\begin{smallmatrix} \lambda & \delta \\ 0 & -\lambda \end{smallmatrix}\right]$ has singular values $s_1$ and $s_2$, and eigenvalues $\pm\lambda$. It follows readily from the Böttcher-Wenzel inequality (e.g. [2, 6]) that $|\lambda| \le 1$ because

$$2|\lambda|^2 \le \|[X, Y]\|^2 \le 2\|X\|^2\|Y\|^2 = 2.$$

A simple proof of the inequality for $2 \times 2$ real matrix can be found in [1]. The proof there can easily be modified for $2 \times 2$ complex matrices. Our formulation leads us to consider the possible values of $|\delta|$ with $|\lambda|$ being fixed. The key result is that, for both the cases $\mathbb{F} = \mathbb{R}$ and $\mathbb{F} = \mathbb{C}$, $|\delta|$ can assume every value between 0 and a common maximum value $\delta_{|\lambda|}$ where $\delta_{|\lambda|}^2$ is given by

$$\delta_{|\lambda|}^2 = \begin{cases} 1 & \text{if } \ 0 \le |\lambda| \le 1/2, \\ 4|\lambda| - 4|\lambda|^2 & \text{if } \ 1/2 < |\lambda| \le 1. \end{cases} \tag{1.3}$$

The graph of $\delta_{|\lambda|}^2$ is given below.

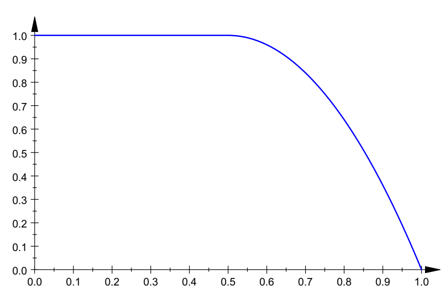


Figure 1.1. The graph of $\delta_{|\lambda|}^2$.

It is obvious that $\delta_{|\lambda|}^2$, and hence, $\delta_{|\lambda|}$ is non-increasing. This plain-looking fact will play a critical role in our later proof in Section 4.

When $X, Y \in \Sigma_2(\mathbb{C})$, $[X, Y]$ is unitarily triangularizable. Our key result asserts that when the complex commutator in triangular form has real eigenvalues and real $\delta$, it can also be achieved by $X, Y \in \Sigma_2(\mathbb{R})$. On

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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the other hand, it is easy to deduce that

$$|\delta| = s_1 - s_2. \tag{1.4}$$

Consequently, together with the obvious condition $|\lambda|^2 = s_1 s_2$, we can easily deduce the following two theorems. The first one gives the relation between the eigenvalues and singular values of the commutators, and the second one gives a simple characterization on the singular values of the commutators.

Theorem 1.4. *There exist $X, Y \in \Sigma_2(\mathbb{C})$ such that $[X,Y]$ has eigenvalues $\pm\lambda$ and singular values $s_1 \geq s_2$ if and only if $|\lambda| \leq 1$, $|\lambda|^2 = s_1 s_2$ and*

$$\begin{cases} s_1 - s_2 \leq 1 & \textit{if } \ 0 \leq |\lambda| \leq 1/2, \\ s_1 + s_2 \leq 2\sqrt{|\lambda|} & \textit{if } \ 1/2 < |\lambda| \leq 1. \end{cases}$$

*Moreover, $X$ and $Y$ can be taken to be real if $\lambda$ is real.*

Theorem 1.5. *There exist $X, Y \in \Sigma_2(\mathbb{C})$ such that $[X,Y]$ has singular values $s_1 \geq s_2$ if and only if $s_1 s_2 \leq 1$ and*

$$\begin{cases} s_1 - s_2 \leq 1 & \textit{if } \ 0 \leq \sqrt{s_1 s_2} \leq 1/2, \\ s_1 + s_2 \leq 2(s_1 s_2)^{1/4} & \textit{if } \ 1/2 < \sqrt{s_1 s_2} \leq 1. \end{cases}$$

*Moreover, the singular values can always be attained by real matrices.*

For $A \in M_n(\mathbb{C})$, the numerical range and numerical radius of $A$ are defined respectively by

$$W(A) = \{x^* A x : x \in \mathbb{C}^n, \|x\| = 1\} \quad \text{and} \quad w(A) = \max\{|z| : z \in W(A)\}.$$

The study of the numerical range and numerical radius has a long history and is extensive. One may refer to [5, Chapter 1] for more information. For $[X,Y] = \left[\begin{smallmatrix} \lambda & \delta \\ 0 & -\lambda \end{smallmatrix}\right]$, the Elliptical Range Theorem (e.g., [5, Theorem 1.3.6]) tells us that $W([X,Y])$ is an elliptical disk with foci $\pm\lambda$ and minor axis $|\delta|$. Thus, from the above discussion, we have the following theorem.

Theorem 1.6. *There exist $X, Y \in \Sigma_2(\mathbb{C})$ such that $W([X,Y])$ is an ellipse with foci $\pm\lambda$ ($\lambda \in \mathbb{C}$) and minor axis $\delta \geq 0$ if and only if*

$$0 \leq \delta \leq \begin{cases} 1 & \textit{if } \ 0 \leq |\lambda| \leq 1/2, \\ 2\sqrt{|\lambda| - |\lambda|^2} & \textit{if } \ 1/2 < |\lambda| \leq 1. \end{cases}$$

*Moreover, $X$ and $Y$ can be taken to be real if $\lambda$ is real.*

From Theorem 1.6, we have

Corollary 1.7. *There exist $X, Y \in \Sigma_2(\mathbb{C})$ such that $[X,Y]$ has eigenvalues $\pm\lambda$ and $w([X,Y]) = r$ if and only if $0 \leq |\lambda| \leq 1$ and*

$$|\lambda| \leq r \leq \begin{cases} \sqrt{|\lambda|^2 + 1/4} & \textit{if } \ 0 \leq |\lambda| \leq 1/2, \\ \sqrt{|\lambda|} & \textit{if } \ 1/2 < |\lambda| \leq 1. \end{cases}$$

*Moreover, $X$ and $Y$ can be taken to be real if $\lambda$ is real.*

The set $W(A)$ can be regarded as the collection of all values for the first diagonal entry of $U^*AU$ when $U$ varies over all unitary matrices. From Corollary 1.7, and replacing $|\lambda|$ there by $\sqrt{s_1 s_2}$, we have the following relation between the singular values and diagonal elements.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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COROLLARY 1.8. *There exist $X, Y \in \Sigma_2(\mathbb{C})$ such that $[X, Y]$ has singular values $s_1 \geq s_2$ and a diagonal element $d$ if and only if $s_1 s_2 \leq 1$ and*

$$|d| \leq \begin{cases} \sqrt{s_1 s_2 + 1/4} & \text{if } 0 \leq \sqrt{s_1 s_2} \leq 1/2, \\ (s_1 s_2)^{1/4} & \text{if } 1/2 < \sqrt{s_1 s_2} \leq 1. \end{cases}$$

*Moreover, $X$ and $Y$ can be taken to be real if $d$ is real.*

The elliptical disk with foci $\pm\lambda$ and minor axis $|\delta|$ is $\left\{z : |z - \lambda| + |z + \lambda| \leq 2\sqrt{|\lambda|^2 + |\delta|^2/4}\right\}$. From Theorem 1.4 and using (1.4), we can now have our ultimate result relating the singular values, eigenvalues and diagonal elements of the commutators under consideration.

THEOREM 1.9. *There exist $X, Y \in \Sigma_2(\mathbb{C})$ such that $[X, Y]$ has singular values $s_1 \geq s_2$, eigenvalues $\pm\lambda$ and diagonal elements $\pm d$ if and only if, in addition to the necessary conditions in Theorem 1.4,*

$$|d + \lambda| + |d - \lambda| \leq s_1 + s_2.$$

*Moreover, $X$ and $Y$ can be taken to be real if $\lambda$ and $d$ are real.*

Finally, we mention here another consequence of our study. There is a close relation between the region $\mathcal{S}_n^{\mathbb{C}}$ and the determination of the best (smallest) constant $C_{p,1,1}$ such that

$$\|XY - YX\|_p \leq C_{p,1,1}\|X\|_1\|Y\|_1, \quad X, Y \text{ are } n \times n \text{ complex matrices,}$$

where $\|\cdot\|_p$ denotes the Schatten $p$-norm, $1 \leq p \leq \infty$. When $2 < p < \infty$, this is an unsolved situation of the general problem (see [8, 3]) of finding the best constant $C_{p,q,r}$ such that

$$\|XY - YX\|_p \leq C_{p,q,r}\|X\|_q\|Y\|_r, \quad X, Y \text{ are } n \times n \text{ complex matrices.}$$

For more information on commutator norm inequalities, see the surveys [2, 6]. In fact, we have $C_{p,1,1} = \max\{\|\mathbf{x}\|_p : \mathbf{x} \in \mathcal{S}_n^{\mathbb{C}}\}$ in which we also use $\|\cdot\|_p$ to denote the vector $p$-norm. In [4], the constant $C^{\mathbb{R}}_{p,1,1} = \max\{\|\mathbf{x}\|_p : \mathbf{x} \in \mathcal{S}_n^{\mathbb{R}}\}$ for real matrices is found via the determination of $C^{\mathbb{R}}_{\infty,q,1}$ for real matrices. Theorem 1.3 tells us that $\mathcal{S}_2^{\mathbb{C}} = \mathcal{S}_2^{\mathbb{R}}$ and consequently we can conclude that all the results obtained in [4] for real matrices are also true for $2 \times 2$ complex matrices.

**2. Transforming the problem geometrically.** Our approach is to consider, instead of the singular values $s_1([X, Y])$ and $s_2([X, Y])$ of the commutator $[X, Y]$, the characteristic polynomial of $[X, Y]^*[X, Y]$, i.e., the monic quadratic polynomial having $s_1^2([X, Y])$ and $s_2^2([X, Y])$ as roots. To this, we first consider

$$\{x^2 - (s_1^2 + s_2^2)x + s_1^2 s_2^2 : (s_1, s_2) \in \mathcal{R}\},$$

the set of monic quadratic polynomials having $s_1^2$ and $s_2^2$ as roots when $(s_1, s_2)$ varies over $\mathcal{R}$. To describe the set, it is equivalent to consider the set of the varying coefficients given by

$$\mathcal{Q} = \{(s_1^2 + s_2^2, s_1^2 s_2^2) : (s_1, s_2) \in \mathcal{R}\} \subset \mathbb{R}^2$$

and we have the following characterization.

PROPOSITION 2.1. *The set $\mathcal{Q}$ (see Figure 2.2) is the region bounded by the segment joining $(0, 0)$ and $(1, 0)$, the curve $x = 2\sqrt{y}$ for $0 \leq y \leq 1$, the curve $x = 1 + 2y^{1/2}$ for $0 \leq y \leq 1/16$, and the curve $x = 4y^{1/4} - 2y^{1/2}$ for $1/16 \leq y \leq 1$.*

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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*Proof.* Let $F : \mathcal{R} \to \mathbb{R}^2$ be defined by $F(s_1, s_2) = (s_1^2 + s_2^2, s_1^2 s_2^2)$ which clearly is injective. Then $\mathcal{Q} = F(\mathcal{R})$. For $0 \le \beta \le 1$, let $C_\beta = \{(s_1, s_2) : (s_1, s_2) \in \mathcal{R}, s_1^2 s_2^2 = \beta\}$. When $\beta = 0$, $C_0$ is the line segment joining $(0, 0)$ and $(1, 0)$; when $0 < \beta \le 1$, $C_\beta$ is the intersection of $\mathcal{R}$ and the hyperbola $s_1 s_2 = \sqrt{\beta}$, see Figure 2.1. [1]

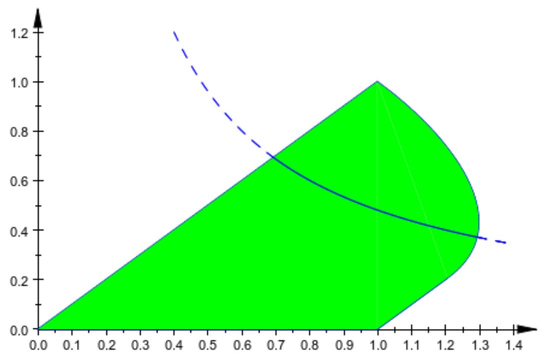


Figure 2.1. The region $\mathcal{R}$ (green) and the curve $s_1 s_2 = \sqrt{\beta}$ (blue).

$\xrightarrow{F}$

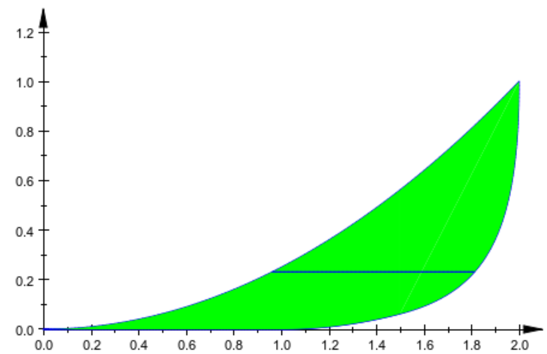


Figure 2.2. The region $\mathcal{Q}$ (green) and the segment $F(C_\beta)$ (blue).

Then

$$\bigcup_{0 \le \beta \le 1} C_\beta = \mathcal{R}, \qquad \text{and hence,} \qquad \mathcal{Q} = F(\mathcal{R}) = \bigcup_{0 \le \beta \le 1} F(C_\beta).$$

For each $\beta$, as $C_\beta$ is closed and connected, $F(C_\beta)$ is a horizontal segment in $\mathcal{Q}$ with height $\beta$ above the $x$-axis, see Figure 2.2. When $\beta$ increases from 0 to 1, the curve $C_\beta$ and the segment $F(C_\beta)$ sweep over the regions $\mathcal{R}$ and $\mathcal{Q}$, respectively. By clicking Figure 2.1 or 2.2, one can see the demonstration of the movement of the corresponding $C_\beta$ and $F(C_\beta)$ when $\beta$ increases.

Let $F(C_\beta) = \{(x, \beta) : x \in L_\beta\}$ where $L_\beta = \{s_1^2 + s_2^2 : (s_1, s_2) \in C_\beta\}$ is a closed interval. The result follows if we can show that

$$L_\beta = \begin{cases} \left[2\sqrt{\beta}, 1 + 2\sqrt{\beta}\right] & \text{if } \ 0 \le \beta \le 1/16, \\ \left[2\sqrt{\beta}, 4\beta^{1/4} - 2\sqrt{\beta}\right] & \text{if } \ 1/16 < \beta \le 1. \end{cases} \tag{2.1}$$

It remains to determine the two endpoints of $L_\beta$, i.e., to find the maximum and minimum of $L_\beta$.

When $\beta = 0$, $L_0 = [0, 1]$ obviously. We now suppose $\beta > 0$. When $\beta$ is fixed and $s_1^2 s_2^2 = \beta$, as $s_1 \ge s_2$, we see that the bigger is $s_1$, the bigger is $s_1^2 + s_2^2$. Hence, the minimum of $s_1^2 + s_2^2$ occurs when $s_1 = s_2 = \beta^{1/4}$, and thus, the minimum of $L_\beta$ is $2\sqrt{\beta}$. Similarly, the maximum of $s_1^2 + s_2^2$ occurs at a point $(s_1^*, s_2^*)$ which is on the right-hand boundary of the region $\mathcal{R}$, i.e., on the segment joining $(1, 0)$ and $\left(\frac{\sqrt{2}+1}{2}, \frac{\sqrt{2}-1}{2}\right)$, or on the curve (1.2).

When $0 < \beta \le 1/16$, the point $(s_1^*, s_2^*)$ is on the line segment joining $(1, 0)$ and $\left(\frac{\sqrt{2}+1}{2}, \frac{\sqrt{2}-1}{2}\right)$, i.e., $s_1^* - s_2^* = 1$, $s_1^* \in (1, (\sqrt{2} + 1)/2]$. Hence, we know that $(s_1^*)^2 + (s_2^*)^2 = (s_1^* - s_2^*)^2 + 2 s_1^* s_2^* = 1 + 2\sqrt{\beta}$.

When $1/16 \le \beta \le 1$, the point $(s_1^*, s_2^*)$ is on the curve (1.2), say with $\phi = \phi^*$. Let $\alpha = (s_1^*)^2 + (s_2^*)^2$ be

[1] A sketch of the region $\mathcal{R}$ is given in [4].

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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the required maximum, and write $z = \cos\phi^* \sin\phi^*$. Easily,

$$\sqrt{\alpha} = \sqrt{(s_1^*)^2 + (s_2^*)^2} = \frac{4\sqrt{\cos\phi^* \sin\phi^*}}{1 + 2\cos\phi^* \sin\phi^*} = \frac{4\sqrt{z}}{1+2z} \tag{2.2}$$

and

$$\sqrt{\beta} = s_1^* s_2^* = \frac{16\cos\phi^* \sin\phi^*}{(1 + 2\cos\phi^* \sin\phi^*)^2} \cos\phi^* \sin\phi^* = \alpha z. \tag{2.3}$$

Multiplying (2.2) by $\sqrt{\alpha}$, we get $2\alpha z - 4\sqrt{\alpha z} + \alpha = 0$ and hence, by (2.3), $\alpha = 4\beta^{1/4} - 2\sqrt{\beta}$ as required. □

**3. The real case.** In this section, we give a proof of Theorem 1.2.

*Proof of Theorem 1.2.* For $X, Y \in \Sigma_2(\mathbb{R})$, $\|[X,Y]\|^2 = s_1^2([X,Y]) + s_2^2([X,Y])$ and $(\det[X,Y])^2 = s_1^2([X,Y]) s_2^2([X,Y])$. The set of characteristic polynomials of $[X,Y]^*[X,Y]$ is

$$\{x^2 - \|[X,Y]\|^2 x + (\det[X,Y])^2 : X, Y \in \Sigma_2(\mathbb{R})\}$$

and, as before, we consider the set of varying coefficients

$$\mathcal{T}(\mathbb{R}) = \{\left(\|[X,Y]\|^2, (\det[X,Y])^2\right) : X, Y \in \Sigma_2(\mathbb{R})\} \subset \mathbb{R}^2.$$

It is then clear that $\mathcal{S}_2^{\mathbb{R}} = \mathcal{R}$ if and only if $\mathcal{T}(\mathbb{R}) = \mathcal{Q}$ (defined in Section 2), and we now show that the latter is true. We note that for $X, Y \in \Sigma_2(\mathbb{R})$, one has $0 \le |\det[X,Y]| \le 1$. To prove the result, it suffices to show that for each $0 \le \beta \le 1$,

$$\left\{\|[X,Y]\|^2 : X, Y \in \Sigma_2(\mathbb{R}), (\det[X,Y])^2 = \beta\right\} \text{ is as in the right-hand side of (2.1).} \tag{3.1}$$

The proof is divided into two parts, depending on whether the eigenvalues of $[X,Y]$ are real or not.

**3.1. Eigenvalues of $[\mathbf{X},\mathbf{Y}]$ are real.** Suppose the eigenvalues of $[X,Y]$ are real (and opposite), i.e., $\det[X,Y] = -\sqrt{\beta} \le 0$. Under suitable simultaneous orthogonal similarity on $X$ and $Y$, we may assume

$$[X,Y] = \begin{bmatrix} \lambda & \delta \\ 0 & -\lambda \end{bmatrix}, \tag{3.2}$$

where $\lambda \ge 0$ and $\delta \ge 0$. Of course $\lambda^2 = -\det[X,Y] = \sqrt{\beta}$, and

$$\|[X,Y]\|^2 = 2\lambda^2 + \delta^2 = 2\sqrt{\beta} + \delta^2.$$

Thus, to prove (3.1), we need to find the range of $\delta^2$. For each $0 \le \lambda \le 1$, suppose the maximum value of $\delta$ is $\delta_\lambda \ge 0$. We have to show that $\delta_\lambda^2$ is as given in (1.3) (note that as $\lambda \ge 0$ here, we drop the absolute value sign in $\delta_{|\lambda|}$) and that $\delta$ can attain every value between 0 and $\delta_\lambda$. The proof is divided into several steps.

*Step 1.* We give an alternative form of (3.2). As $X$ and $Y$ are of rank one, suppose

$$X = \begin{bmatrix} \cos a \\ \sin a \end{bmatrix} \begin{bmatrix} \cos b & \sin b \end{bmatrix} = \begin{bmatrix} \cos a \cos b & \cos a \sin b \\ \sin a \cos b & \sin a \sin b \end{bmatrix} \tag{3.3}$$

and

$$Y = \begin{bmatrix} \cos h \\ \sin h \end{bmatrix} \begin{bmatrix} \cos k & \sin k \end{bmatrix} = \begin{bmatrix} \cos h \cos k & \cos h \sin k \\ \sin h \cos k & \sin h \sin k \end{bmatrix},$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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where $a, b, h, k \in \mathbb{R}$. From (3.2), we have

$$\begin{aligned}\cos a \sin b \sin h \cos k - \cos h \sin k \sin a \cos b = \lambda,\\ \cos a \cos b \cos h \sin k + \cos a \sin b \sin h \sin k - \cos h \cos k \cos a \sin b - \cos h \sin k \sin a \sin b = \delta,\\ \sin a \cos b \cos h \cos k + \sin a \sin b \sin h \cos k - \sin h \cos k \cos a \cos b - \sin h \sin k \sin a \cos b = 0.\end{aligned}$$

The first equation can be rewritten as

$$\sin(a+b)\sin(h-k) - \sin(a-b)\sin(h+k) = 2\lambda,$$

while the second and third equations can be replaced by their sum and difference given by

$$\begin{aligned}\sin(a-b)\cos(h+k) - \sin(h-k)\cos(a+b) = \delta,\\ -\sin(a+b)\cos(h+k) + \sin(h+k)\cos(a+b) = \delta.\end{aligned}$$

Note that $a+b$ and $a-b$ can achieve any values independently, and so do $h+k$ and $h-k$. Thus, writing

$$a+b = A, \quad a-b = B, \quad h+k = H, \quad h-k = K, \tag{3.4}$$

the above three equations become, with independent variables $A$, $B$, $H$ and $K$,

$$\sin A \sin K - \sin B \sin H = 2\lambda, \tag{3.5}$$
$$\sin B \cos H - \sin K \cos A = \delta, \tag{3.6}$$
$$-\sin A \cos H + \sin H \cos A = \delta, \tag{3.7}$$

respectively.

We first show that $\delta$ can be 0. Take $A = H = \pi/2$, and $B$ and $K$ satisfy $\sin B = -\lambda$ and $\sin K = \lambda$. Then (3.5)–(3.7) are satisfied with $\delta = 0$.

*Step 2.* We further transform the problem. We now assume $\delta > 0$. Equation (3.7) gives

$$\delta = \sin(H - A). \tag{3.8}$$

Equations (3.5) and (3.6) give

$$\begin{bmatrix} -\sin H & \sin A \\ \cos H & -\cos A \end{bmatrix} \begin{bmatrix} \sin B \\ \sin K \end{bmatrix} = \begin{bmatrix} 2\lambda \\ \delta \end{bmatrix},$$

and hence, with (3.8) and using Cramer's rule, we obtain

$$\sin B = \frac{-2\lambda \cos A - \delta \sin A}{\sin H \cos A - \sin A \cos H} = -\frac{2\lambda}{\delta}\cos A - \sin A$$

and

$$\sin K = \frac{-2\lambda \cos H - \delta \sin H}{\sin H \cos A - \sin A \cos H} = -\frac{2\lambda}{\delta}\cos H - \sin H.$$

Thus, equivalently, we need to find the range of $\delta$ subject to (3.8),

$$\left|\frac{2\lambda}{\delta}\cos A + \sin A\right| \le 1 \quad \text{and} \quad \left|\frac{2\lambda}{\delta}\cos H + \sin H\right| \le 1. \tag{3.9}$$

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A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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*Step 3.* Suppose $0 \le 2\lambda \le 1$ (i.e., $0 \le \beta \le 1/16$). For any $0 < \delta \le 1$, choose $H = \pi/2$ and $A$ such that $\cos A = \delta$ and $\sin A = -\sqrt{1-\delta^2}$. Then $\sin(H - A) = \cos A = \delta$ and both inequalities in (3.9) are satisfied. Hence, $\delta$ can assume any value in $[0, 1]$ as required.

*Step 4.* We suppose $1 \le 2\lambda \le 2$ (i.e., $1/16 \le \beta \le 1$) and find the maximum value of $\delta$. Geometrically, (3.9) means that the inner products of the vector $(2\lambda/\delta, 1)^T$ with the two unit vectors $(\cos A, \sin A)^T$ and $(\cos H, \sin H)^T$ have absolute values not bigger than one.

Suppose the maximum value of $\delta$ is $\delta_\lambda = \sin(H_0 - A_0) > 0$ where $0 < H_0 - A_0 < \pi$. If $\sin(H_0 - A_0) = 1$, $\left\{(\cos A_0, \sin A_0)^T, (\cos H_0, \sin H_0)^T\right\}$ is an orthonormal basis of $\mathbb{R}^2$. Then, (3.9) implies $\|(2\lambda/\delta_\lambda, 1)^T\| \le \sqrt{2}$. This gives a contradiction as $2\lambda/\delta_\lambda > 1$. So $\sin(H_0 - A_0) < 1$. We claim that for $\delta = \delta_\lambda$, both inequalities in (3.9) must hold in equality. If both of them are strict inequalities, we can purturb $H_0$ and $A_0$ a bit to have a bigger value of $\delta$ without violating (3.9), and this gives a contradiction. If exactly one of them is equality, we may consider replacing $H_0$ and $A_0$ by $H_0 + \epsilon$ and $A_0 + \epsilon$ for small suitable $\epsilon$, resulting in both of them are strict inequalities and with $\delta = \sin((H_0 + \epsilon) - (A_0 + \epsilon)) = \delta_\lambda$. Thus, as in the previous case, we have a contradiction.

Now suppose both inequalities in (3.9) hold in equality. Geometrically, it is clear that there are 4 unit vectors $\mathbf{x} \in \mathbb{R}^2$ such that $|\langle \mathbf{x}, (2\lambda/\delta_\lambda, 1)^T\rangle| = 1$, namely, $\mathbf{u} = (0, 1)^T$, $\mathbf{v}$ and their negatives, where $\mathbf{v} = (\cos\theta, \sin\theta)^T$, $-\pi/2 < \theta < 0$, is the reflection of $\mathbf{u}$ across the vector $(2\lambda/\delta_\lambda, 1)^T$. See Figure 3.1 below.

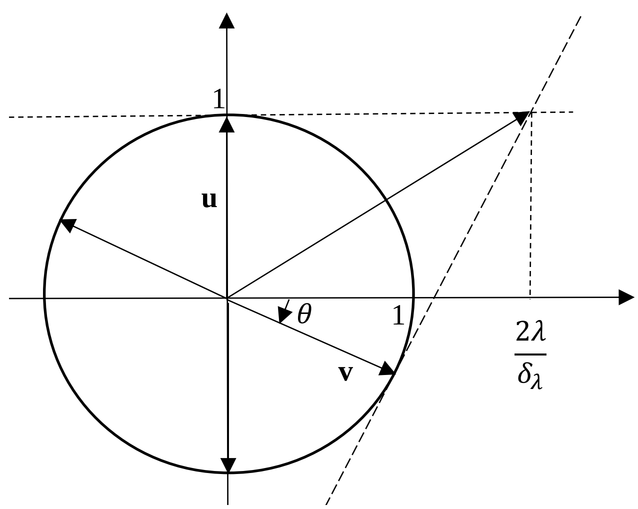


Figure 3.1. The vectors $\mathbf{u}$ and $\mathbf{v}$.

In other words, when restricting $-\pi < H_0, A_0 \le \pi$, we have $H_0, A_0 \in \{\pm\pi/2, \theta, \theta+\pi\}$. Since $\sin(H_0 - A_0) > 0$, the possible choices for $(H_0, A_0)$ are $(\pi/2, \theta)$, $(\theta, -\pi/2)$, $(-\pi/2, \theta + \pi)$ and $(\theta + \pi, \pi/2)$.

We may take $(H_0, A_0) = (\pi/2, \theta)$. The other choices of $(H_0, A_0)$ will always lead to this case. For example, if $(H_0, A_0) = (\theta, -\pi/2)$, (3.9) becomes

$$\left|\frac{2\lambda}{\sin(\theta - (-\pi/2))}\cos\left(-\frac{\pi}{2}\right) + \sin\left(-\frac{\pi}{2}\right)\right| = 1 \quad \text{and} \quad \left|\frac{2\lambda}{\sin(\theta - (-\pi/2))}\cos\theta + \sin\theta\right| = 1,$$

which is equivalent to

$$\left|\frac{2\lambda}{\sin(\pi/2 - \theta)}\cos\left(\frac{\pi}{2}\right) + \sin\left(\frac{\pi}{2}\right)\right| = 1 \quad \text{and} \quad \left|\frac{2\lambda}{\sin(\pi/2 - \theta)}\cos\theta + \sin\theta\right| = 1,$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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and these two new conditions exactly mean taking $(H_0, A_0) = (\pi/2, \theta)$.

So, fix now $(H_0, A_0) = (\pi/2, \theta)$. It is easy to check that the triangle with vertices $(0,0)$, $(0,1)$ and $(2\lambda/\delta_\lambda, 1)$ and the triangle with vertices $(0,0)$, $(\cos\theta, \sin\theta)$ and $(2\lambda/\delta_\lambda, 1)$ are congruent (see Figure 3.1). Consequently, in the triangle with vertices $(0,0)$, $(0,1)$ and $(2\lambda/\delta_\lambda, 1)$, the angle at $(0,0)$ is $\frac{\pi/2-\theta}{2}$ (remember $\theta < 0$). Hence,

$$\sqrt{1+\left(\frac{2\lambda}{\delta_\lambda}\right)^2}\cos\left(\frac{\pi/2-\theta}{2}\right) = 1,$$

which gives, with $\delta_\lambda = \sin(\pi/2-\theta)$,

$$\left(1+\frac{\lambda^2}{\sin^2((\pi/2-\theta)/2)\cos^2((\pi/2-\theta)/2)}\right)\cos^2\left(\frac{\pi/2-\theta}{2}\right) = 1.$$

Thus,

$$\lambda = \sin^2\left(\frac{\pi/2-\theta}{2}\right),$$

and hence,

$$\delta_\lambda^2 = \sin^2(\pi/2-\theta) = 4\sin^2\left(\frac{\pi/2-\theta}{2}\right)\cos^2\left(\frac{\pi/2-\theta}{2}\right) = 4\lambda(1-\lambda).$$

*Step 5.* Finally, we show that any value between 0 and $\delta_\lambda$ can be achieved by $\delta$. For any $0 < \delta < \delta_\lambda$, take $H = \pi/2$ and $A$ such that

$$(\cos A, \sin A) = \left(\delta, -\sqrt{1-\delta^2}\right). \tag{3.10}$$

Then $\delta = \cos A = \sin(H - A)$ and the second part of (3.9) is satisfied. It remains to show that the first part of (3.9) is also satisfied. With (3.10), it suffices to show $\left|2\lambda - \sqrt{1-\delta^2}\right| \le 1$ for all $\delta$ where $0 < \delta < \delta_\lambda$. Note that

$$\left|2\lambda - \sqrt{1-\delta^2}\right| \le 1 \quad\Leftrightarrow\quad 4\lambda^2 - \delta^2 \le 4\lambda\sqrt{1-\delta^2}.$$

If $4\lambda^2 - \delta^2 \le 0$, we are done. Now suppose $4\lambda^2 - \delta^2 > 0$. Then

$$4\lambda^2 - \delta^2 \le 4\lambda\sqrt{1-\delta^2} \quad\Leftrightarrow\quad 16\lambda^4 + 8\lambda^2\delta^2 + \delta^4 - 16\lambda^2 \le 0.$$

Since $0 < \delta < \delta_\lambda$, it suffices to show that $16\lambda^4 + 8\lambda^2\delta_\lambda^2 + \delta_\lambda^4 - 16\lambda^2 \le 0$. With $\delta_\lambda^2 = 4\lambda - 4\lambda^2$, the result follows from $16\lambda^4 + 8\lambda^2\delta_\lambda^2 + \delta_\lambda^4 - 16\lambda^2 = 0$.

**3.2. Eigenvalues of $[\mathbf{X}, \mathbf{Y}]$ are purely imaginary.** We now suppose the two eigenvalues of $[X, Y]$ are purely imaginary, i.e., $\det[X, Y] = \sqrt{\beta} > 0$. We claim that

$$\sqrt{\beta} \le 1/4. \tag{3.11}$$

We don't have the upper triangular form as in (3.2). Under suitable simultaneous orthogonal similarity on $X$ and $Y$ we may assume

$$X = \begin{bmatrix} p & q \\ 0 & 0 \end{bmatrix} \quad \text{where } p^2 + q^2 = 1, \quad Y = \begin{bmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{bmatrix}.$$

Then

$$[X, Y] = \begin{bmatrix} qy_{21} & py_{12} + q(y_{22} - y_{11}) \\ -py_{21} & -qy_{21} \end{bmatrix}.$$

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A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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Taking the determinant on both sides,

$$\sqrt{\beta} = -q^2y_{21}^2 + py_{21}[py_{12} + q(y_{22} - y_{11})]. \tag{3.12}$$

As $y_{11}y_{22} = y_{21}y_{12}$ (i.e., $\det Y = 0$), we get

$$(qy_{21})^2 - p(y_{22} - y_{11})(qy_{21}) + (\sqrt{\beta} - p^2y_{11}y_{22}) = 0.$$

Regarding this as a quadratic equation in $qy_{21}$ with real coefficients, it has (one and hence) two real roots. Its discriminant must be non-negative, i.e.,

$$0 \le [p(y_{22} - y_{11})]^2 - 4(\sqrt{\beta} - p^2y_{11}y_{22}) = [p(y_{22} + y_{11})]^2 - 4\sqrt{\beta}.$$

Thus, $\sqrt{\beta} \le p^2(y_{22} + y_{11})^2/4 \le 1/4$ as claimed.

To complete the proof, as $0 < \beta \le 1/16$, it suffices to show that $\|[X,Y]\|^2 \le 1 + 2\sqrt{\beta}$. Note that, using (3.12),

$$\begin{aligned}
&\|[X,Y]\|^2 \le 1 + 2\sqrt{\beta}\\
\Leftrightarrow\ & 2q^2y_{21}^2 + 2\sqrt{\beta} + p^2y_{21}^2 + [py_{12} + q(y_{22} - y_{11})]^2 \le 1 + 2\sqrt{\beta} + 2\sqrt{\beta}\\
\Leftrightarrow\ & 2\{py_{21}[py_{12} + q(y_{22} - y_{11})]\} + p^2y_{21}^2 + [py_{12} + q(y_{22} - y_{11})]^2 \le 1 + 4\sqrt{\beta}\\
\Leftrightarrow\ & \{py_{21} + [py_{12} + q(y_{22} - y_{11})]\}^2 \le 1 + 4\sqrt{\beta}.
\end{aligned}$$

That is, subject to (3.12), we have to show that

$$[p(y_{21} + y_{12}) + q(y_{22} - y_{11})]^2 \le 1 + 4\sqrt{\beta}.$$

From $y_{11}^2 + y_{22}^2 + y_{12}^2 + y_{21}^2 = 1$ and $y_{11}y_{22} - y_{12}y_{21} = 0$, we get $(y_{21} + y_{12})^2 + (y_{22} - y_{11})^2 = 1$. The result is now clear as both $(y_{21} + y_{12}, y_{22} - y_{11})^T$ and $(p, q)^T$ are unit vectors. □

## 4. The complex case.

**4.1. Complex vs. real.** There are fundamental differences between the real and complex problems and we tried in vain to modify the proof of Theorem 1.2 to prove the complex case. As an illustration, suppose

$$X = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \begin{bmatrix} \bar{b}_1 & \bar{b}_2 \end{bmatrix} = \begin{bmatrix} a_1\bar{b}_1 & a_1\bar{b}_2 \\ a_2\bar{b}_1 & a_2\bar{b}_2 \end{bmatrix}$$

where $(a_1, a_2)^T$ and $(b_1, b_2)^T$ are unit vectors in $\mathbb{C}^2$. When the two vectors are real, in the proof of Theorem 1.2, we have

$$a_1\bar{b}_1 - a_2\bar{b}_2 = \cos a \cos b - \sin a \sin b = \cos(a + b) = \cos A$$

and

$$a_2\bar{b}_1 + a_1\bar{b}_2 = \sin a \cos b + \cos a \sin b = \sin(a + b) = \sin A.$$

In the real case, $|\cos A| \le 1$, $|\sin A| \le 1$ and $\|(\cos A, \sin A)^T\| = 1$. In the complex case, though we have

$$|a_1\bar{b}_1 - a_2\bar{b}_2| \le 1 \quad \text{and} \quad |a_2\bar{b}_1 + a_1\bar{b}_2| \le 1,$$

the norm of $(a_1\bar{b}_1 - a_2\bar{b}_2, a_2\bar{b}_1 + a_1\bar{b}_2)^T$ ranges from 0 to 2. For example, the matrices $\frac{1}{2}\left[\begin{smallmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{smallmatrix}\right]$ and $\frac{1}{2}\left[\begin{smallmatrix} 1 & \mathrm{i} \\ \mathrm{i} & -1 \end{smallmatrix}\right]$ give the norms of the corresponding vectors 0 and 2, respectively. Consequently, there are several places in the proof of Theorem 1.2 where the geometric argument cannot be adopted directly to prove the complex problem.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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**4.2. Some lemmas.** When $[X,Y]$ is not in triangular form, we may use $\|[X,Y]\|^2 - 2|\det[X,Y]|$ to represent $\delta^2$ in our formulation. The following proposition tells us that if we can reduce one of the matrices $X$ and $Y$ to have zero trace then we are done.

PROPOSITION 4.1. *For $0 \le |\lambda| \le 1$ and $\delta^2_{|\lambda|}$ as given in (1.3),*

$$\max\{\|[X,Y]\|^2 - 2|\det[X,Y]| : X,Y \in \Sigma_2(\mathbb{C}), |\det[X,Y]| = |\lambda|^2, \operatorname{tr} X = 0\} \le \delta^2_{|\lambda|}.$$

*Proof.* Under suitable unitary similarity, we may assume $X = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$. With $Y = (y_{ij})$,

$$XY - YX = \begin{bmatrix} y_{21} & y_{22} - y_{11} \\ 0 & -y_{21} \end{bmatrix}$$

and so $|y_{21}| = \sqrt{|\det[X,Y]|} = |\lambda|$. Hence,

$$\begin{aligned} \|[X,Y]\|^2 &= 2|\lambda|^2 + |y_{22} - y_{11}|^2 \le 2|\lambda|^2 + (|y_{22}| + |y_{11}|)^2 && (4.1)\\ &\le 2|\lambda|^2 + (s_1(Y) + s_2(Y))^2 && (4.2)\\ &= 2|\lambda|^2 + 1. \end{aligned}$$

Inequality (4.2) follows from the relation between the singular values and diagonal elements of a matrix, e.g. see [5, (3.1.10a)]. Consequently, for $0 \le |\lambda| \le 1/2$, we get as desired the maximum to be bounded by $\delta^2_{|\lambda|} = 1$.

When $1/2 < |\lambda| \le 1$, we can have a smaller upper bound for $(|y_{22}| + |y_{11}|)^2$ instead of 1. The conditions $|y_{11}|^2 + |y_{22}|^2 + |\lambda|^2 + |y_{12}|^2 = 1$ (i.e., $\|Y\|^2 = 1$) and $|y_{11}||y_{22}| = |\lambda||y_{12}|$ (i.e., $\det Y = 0$) give

$$(|y_{11}| + |y_{22}|)^2 + (|\lambda| - |y_{12}|)^2 = 1.$$

Replacing $|y_{12}|$ by $|y_{11}||y_{22}|/|\lambda|$, and using $|y_{11}||y_{22}| \le \left(\frac{|y_{11}|+|y_{22}|}{2}\right)^2 \le 1/4 < |\lambda|^2$, we get

$$(|y_{11}| + |y_{22}|)^2 + \frac{\left(|\lambda|^2 - \left(\frac{|y_{11}|+|y_{22}|}{2}\right)^2\right)^2}{|\lambda|^2} \le 1$$

which, by direct calculation, gives

$$\left(|\lambda| + \frac{\left(\frac{|y_{11}|+|y_{22}|}{2}\right)^2}{|\lambda|}\right)^2 \le 1.$$

Consequently, after taking square root on both sides, we easily get

$$(|y_{11}| + |y_{22}|)^2 \le 4|\lambda| - 4|\lambda|^2.$$

Thus, from (4.1), the result follows. □

In the following lemma, we modify the proof of Theorem 1.2 to handle a particular case of the complex problem.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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LEMMA 4.2. *Suppose* $X \in \Sigma_2(\mathbb{R})$ *and*

$$Y = \begin{bmatrix} c + d\mathbf{i} & y_{12} \\ y_{21} & -c + d\mathbf{i} \end{bmatrix} \in \Sigma_2(\mathbb{C}), \quad c, d, y_{12}, y_{21} \in \mathbb{R},\ d \neq 0,$$

*such that* $XY - YX = \begin{bmatrix} \lambda & \delta \\ 0 & -\lambda \end{bmatrix}$. *Then, with* $\delta_{|\lambda|}$ *as given in (1.3),*

*(i)* $|\delta| \leq \delta_{|\lambda|}$ *; or*

*(ii) there exist* $\tilde{X}, \tilde{Y} \in \Sigma_2(\mathbb{C})$ *such that* $\tilde{X}\tilde{Y} - \tilde{Y}\tilde{X} = \begin{bmatrix} \lambda & \tilde{\delta} \\ 0 & -\lambda \end{bmatrix}$ *with* $|\tilde{\delta}| > |\delta|$.

*Proof.* We remark that $\|Y\| = 1$ and $\det Y = 0$ read $2(c^2+d^2)+y_{12}^2+y_{21}^2 = 1$ and $-(c^2+d^2)-y_{12}y_{21} = 0$, respectively. So, $\begin{bmatrix} \sqrt{c^2+d^2} & y_{12} \\ y_{21} & -\sqrt{c^2+d^2} \end{bmatrix} \in \Sigma_2(\mathbb{R})$. Let

$$\begin{bmatrix} \sqrt{c^2+d^2} & y_{12} \\ y_{21} & -\sqrt{c^2+d^2} \end{bmatrix} = \begin{bmatrix} \cos h \\ \sin h \end{bmatrix} \begin{bmatrix} \cos k & \sin k \end{bmatrix} = \begin{bmatrix} \cos h \cos k & \cos h \sin k \\ \sin h \cos k & \sin h \sin k \end{bmatrix}.$$

The matrix on the left has zero trace and so the condition

$$0 = \cos h \cos k + \sin h \sin k = \cos(h - k)$$

grants $h - k \in \{\pi/2 + l\pi : l \text{ is an integer}\}$. Set $t = c/\sqrt{c^2+d^2}$, so that we can rewrite $Y$ as

$$Y = \begin{bmatrix} t\cos h \cos k & \cos h \sin k \\ \sin h \cos k & t \sin h \sin k \end{bmatrix} + dI_2\mathbf{i}, \quad -1 < t < 1. \tag{4.3}$$

Suppose $X$ is as in (3.3). We divide the proof into several steps.

*Step 1.* Parallel to Step 1 in Section 3.1, by replacing the terms $\cos h \cos k$ and $\sin h \sin k$ there by $t \cos h \cos k$ and $t \sin h \sin k$, we obtain (parallel to (3.5)–(3.7))

$$\sin K \sin A - \sin B \sin H = 2\lambda, \tag{4.4}$$

$$t \sin B \cos H - \sin K \cos A = \delta, \tag{4.5}$$

$$-t \sin A \cos H + \sin H \cos A = \delta, \tag{4.6}$$

where $A$, $B$, $H$ and $K$ (defined in (3.4)) are independent variables with $K \in \{\pi/2 + l\pi : l \text{ is an integer}\}$. From (4.6), in which the left-hand side can be regarded as the inner product of $(-\sin A, \cos A)^T$ and $(t \cos H, \sin H)^T$, we know that $|\delta| \leq 1$. Thus, we have (i) if $|\lambda| \leq 1/2$.

*Step 2.* Suppose $|\lambda| > 1/2$. Following the calculation in Step 2 in Section 3.1, we see that the solvability of (4.4)–(4.6) is equivalent to the solvability of (4.6),

$$\left| \frac{2\lambda}{\delta} \cos A + \sin A \right| = |\sin B| \leq 1 \quad \text{and} \quad \left| \frac{2\lambda}{\delta} t \cos H + \sin H \right| = |\sin K| = 1. \tag{4.7}$$

Note that as $B$ and $K$ are independent of the other variables, we may focus on $t$, $\delta$ $A$ and $H$. If we want to show that there are matrices satisfying the assertion in (ii), it suffices to show that there are $t_1$, $\delta_1$, $A_1$ and $H_1$ such that, with the terms $|\sin B|$ and $|\sin K|$ dropped, (4.6) and (4.7) are satisfied and $|\delta_1| > |\delta|$. The values of $B$ and $K$ can then be chosen suitably.

We use a perturbation argument, assuming that there are $t$, $\delta$, $A$ and $H$ satisfying (4.6) and (4.7). Let us outline our steps first.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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*Step 2.1.* Perturb $t$ in (4.6) to $t_1$ to have $\delta_1$ such that $|\delta_1| > |\delta|$. With the values $t_1$, $\delta_1$ and $H$, the second part of (4.7) will probably be violated.
*Step 2.2.* Adjust $H$ to $H_1$ so that $t_1$, $\delta_1$ and $H_1$ satisfy the second part of (4.7). With the values $t_1$, $\delta_1$ and $H_1$, (4.6) will probably be violated.
*Step 2.3.* Adjust $A$ to $A_1$ so that $t_1$, $\delta_1$, $H_1$ and $A_1$ satisfy (4.6) .

During the steps, we also have to ensure that the first part of (4.7) is always satisfied. Before we carry out our plan, we first note the following points.

*Point 1.* We now eliminate the situation that $\sin A \cos H = 0$, so that we can perturb $t$ in (4.6) to have a bigger value of $|\delta|$. If $\sin A = 0$, we have $-\sin B \sin H = 2\lambda$ from (4.4) and this contradicts $2\lambda > 1$. If $\cos H = 0$, then (4.5) and (4.6) are independent of $t$. Take $t = 1$ in (4.3) to have

$$\hat{Y} = \begin{bmatrix} \cos h \cos k & \cos h \sin k \\ \sin h \cos k & \sin h \sin k \end{bmatrix} \in \Sigma_2(\mathbb{R}).$$

Readily, the pair $X, \hat{Y} \in \Sigma_2(\mathbb{R})$ satisfies (4.4)–(4.6). Thus, $|\delta| \leq \delta_{|\lambda|}$ and we are done.

*Point 2.* We refer to the first part of (4.7). If equality holds, then $|\sin B| = 1$, and hence, $\operatorname{tr} X = \cos B = 0$. By Proposition 4.1, we have (i) and we are done. We now assume

$$\left| \frac{2\lambda}{\delta} \cos A + \sin A \right| < 1.$$

With this assumption, we know that the first part of (4.7) will not be violated if we perturb $t$, $\delta$, $H$ and $A$ small enough. This ensures the first part of (4.7) will be satisfied throughout the perturbations.

*Point 3.* We show that

$$|\delta| < \sqrt{t^2 \cos H^2 + \sin^2 H}. \tag{4.8}$$

The main purpose of showing this is to guarantee that after we perturb $t$, $\delta$ and $H$ to $t_1$, $\delta_1$ and $H_1$, respectively, we still have

$$|\delta_1| < \sqrt{t_1^2 \cos H_1^2 + \sin^2 H_1}. \tag{4.9}$$

Consequently, we can perturb $A$ to $A_1$ as required in Step 2.3. (Note: Geometrically, the left-hand side of (4.6) is the inner product of the vectors $(t \cos H, \sin H)^T$ and $(-\sin A, \cos A)^T$. To have $A_1$ in Step 2.3, we need $|\delta_1| < \|(t_1 \cos H_1, \sin H_1)^T\|$.)

We now prove (4.8). By the Cauchy-Schwarz inequality, we know from (4.6) that (4.8) is true when "$\leq$" is written. If equality holds, then the two vectors $(-\sin A, \cos A)^T$ and $(t \cos H, \sin H)^T$ are linearly dependent and $\|(t \cos H, \sin H)^T\| = |\delta|$. So, we can rewrite the second part of (4.7) as

$$\left| \frac{2\lambda}{\delta}(-\sin A) + \cos A \right| = \frac{1}{|\delta|}. \tag{4.10}$$

The two vectors $(-\sin A, \cos A)^T$ and $(\cos A, \sin A)^T$ form an orthonormal basis of $\mathbb{R}^2$. Using (4.10) and the first part of (4.7) we get

$$\left(\frac{2\lambda}{|\delta|}\right)^2 + 1 = \left\| \left(\frac{2\lambda}{\delta}, 1\right)^T \right\|^2 = \left| \frac{2\lambda}{\delta}(-\sin A) + \cos A \right|^2 + \left| \frac{2\lambda}{\delta} \cos A + \sin A \right|^2 \leq \frac{1}{|\delta|^2} + 1,$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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and this contradicts the assumption $2\lambda > 1$. Hence, we have (4.8).

We are ready to carry out the Steps 2.1–2.3.

- For Step 2.1, by Point 1, we may assume $\sin A \cos H \neq 0$. By a small perturbation of $t$ to $t_1$ in (4.6), we get
$$-t_1 \sin A \cos H + \sin H \cos A = \delta_1, \qquad \text{where} \quad |\delta_1| > |\delta|.$$
- For Step 2.2, with $t_1$ and $\delta_1$ obtained, we adjust $H$ to $H_1$ (with $|H - H_1|$ small) so that the second part of (4.7) is satisfied with $t_1$, $\delta_1$ and $H_1$. This is possible because of the second part of (4.7), $\left\|\left(\frac{2\lambda t_1}{\delta_1}, 1\right)^T\right\| > 1$, and that $t_1$ and $\delta_1$ are small perturbations of $t$ and $\delta$, respectively.
- For Step 2.3, with (4.9), we can adjust $A$ suitably to $A_1$ (again with $|A_1 - A|$ small) so that $t_1$, $\delta_1$, $H_1$ and $A_1$ satisfy (4.6).

Summing up, with reference to Point 2, we have found $t_1$, $\delta_1$, $H_1$ and $A_1$ such that (4.6) and (4.7) are satisfied and $|\delta_1| > |\delta|$. Assertion (ii) follows. ∎

**4.3. The main proof.** We now give the proof of Theorem 1.3.

*Proof of Theorem 1.3.* Similar to $\mathcal{T}(\mathbb{R})$ in the proof of Theorem 1.2, let

$$\mathcal{T}(\mathbb{C}) = \{(\|[X,Y]\|^2, |\det[X,Y]|^2) : X, Y \in \Sigma_2(\mathbb{C})\} \subset \mathbb{R}^2.$$

To prove the theorem, it suffices to show that $\mathcal{T}(\mathbb{C}) = \mathcal{Q}$. As $\mathcal{Q} = \mathcal{T}(\mathbb{R}) \subseteq \mathcal{T}(\mathbb{C})$, it suffices to consider the right boundary of $\mathcal{T}(\mathbb{C})$ and show that

$$\max\left\{\|[X,Y]\|^2 : X, Y \in \Sigma_2(\mathbb{C}), |\det[X,Y]|^2 = \beta\right\} = \max\left\{\|[X,Y]\|^2 : X, Y \in \Sigma_2(\mathbb{R}), |\det[X,Y]|^2 = \beta\right\}.$$

The left boundary (which corresponds to diagonal $[X,Y]$) and the bottom boundary of $\mathcal{T}(\mathbb{R})$ and $\mathcal{T}(\mathbb{C})$ are obviously the same.

**4.3.1. A transformation of the problem.** Suppose

$$X = \tilde{X} + \frac{\operatorname{tr} X}{2} I_2$$

in which $\operatorname{tr} \tilde{X} = 0$, and similarily for $\tilde{Y}$. Then $XY - YX = \tilde{X}\tilde{Y} - \tilde{Y}\tilde{X}$ which allows us to work with zero trace matrices. As $X$ is of rank one, its non-trivial eigenvalue is $\operatorname{tr} X$. On the other hand, suppose the eigenvalues of $\tilde{X}$ (which has zero trace) are $\pm\mu$. Then $\tilde{X} + \frac{\operatorname{tr} X}{2} I_2$ is of rank one if and only if $\frac{1}{2}\operatorname{tr} X = \pm\mu$. When $\mathbb{F} = \mathbb{R}$, the latter is possible only if $\tilde{X}$ has real eigenvalues, equivalently, $\det \tilde{X} \leq 0$. Note that

$$\|X\|^2 = \|\tilde{X}\|^2 + 2\left|\frac{1}{2}\operatorname{tr} X\right|^2 = \|\tilde{X}\|^2 + 2|\mu|^2 = \|\tilde{X}\|^2 + 2|\det \tilde{X}|.$$

Thus, instead of matrices from $\Sigma_2(\mathbb{F})$, we may assume, if $\mathbb{F} = \mathbb{R}$, the matrices are chosen from

$$\Phi(\mathbb{R}) = \{H : H \in M_2(\mathbb{R}), \operatorname{tr} H = 0, \|H\|^2 + 2|\det H| = 1, \det H \leq 0\}$$

that and, if $\mathbb{F} = \mathbb{C}$, the matrices are chosen from

$$\Phi(\mathbb{C}) = \{H : H \in M_2(\mathbb{C}), \operatorname{tr} H = 0, \|H\|^2 + 2|\det H| = 1\}.$$

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A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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We also note that

$$\|H\|^2 + 2|\det H| = s_1^2(H) + s_2^2(H) + 2s_1(H)s_2(H) = \big(s_1(H) + s_2(H)\big)^2 = \|H\|_1^2.$$

The condition $\|H\|^2 + 2|\det H| = 1$ in the definitions of $\Phi(\mathbb{F})$ above is equivalent to $\|H\|_1 = 1$.

We now work with matrices in $\Phi(\mathbb{F})$. We see from the proof of Theorem 1.2 that the region $\mathcal{T}(\mathbb{R})$ (i.e., $\mathcal{Q}$) can be fully filled by commutators that are orthogonally upper triangularizable. Thus, under simultaneous unitary (orthogonal if $\mathbb{F} = \mathbb{R}$) similarity, we may assume

$$H = \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & -h_{11} \end{bmatrix},\ K = \begin{bmatrix} k_{11} & k_{12} \\ k_{21} & -k_{11} \end{bmatrix} \in \Phi(\mathbb{F})$$

are chosen such that

$$\begin{bmatrix} \lambda & \delta \\ 0 & -\lambda \end{bmatrix} = HK - KH = \begin{bmatrix} h_{12}k_{21} - k_{12}h_{21} & 2h_{11}k_{12} - 2h_{12}k_{11} \\ 2h_{21}k_{11} - 2h_{11}k_{21} & h_{21}k_{12} - k_{21}h_{12} \end{bmatrix}. \tag{4.11}$$

Though we may assume $\lambda, \delta \geq 0$ under diagonal unitary (orthogonal if $\mathbb{F} = \mathbb{R}$) similarity and multiplication with a unit scalar, we do not do so here. Such actions will be used later.

Without assuming $\delta, \lambda \geq 0$, we need to amend our problem. Our original formulation has $|\det([X, Y])|^2 = \beta$ with $\beta$ being fixed and so $|\lambda|$ is fixed, and we need to determine the maximum of $|\delta|$. Thus, referring to (4.11), the equivalent problem is to find, for $0 \leq |\lambda| \leq 1$,

$$\delta_{|\lambda|}^{\mathbb{F}} = \max\{2|h_{11}k_{12} - k_{11}h_{12}| : |h_{12}k_{21} - k_{12}h_{21}| = |\lambda|, h_{11}k_{21} - k_{11}h_{21} = 0, H, K \in \Phi(\mathbb{F})\}. \tag{4.12}$$

The value of $\delta_{|\lambda|}^{\mathbb{R}}$ is exactly the $\delta_{|\lambda|}$ as given in (1.3). Here, we need to prove $\delta_{|\lambda|}^{\mathbb{R}} = \delta_{|\lambda|}^{\mathbb{C}}$.

For $\mathbb{F} = \mathbb{R}$, $\mathbb{C}$ and $0 \leq |\lambda| \leq 1$, we consider the following problem which has the constraint $|h_{12}k_{21} - k_{12}h_{21}| = |\lambda|$ in (4.12) relaxed:

$$\begin{aligned} &\max && F(H,K) = 2|h_{11}k_{12} - k_{11}h_{12}| \\ &\text{subject to} && |h_{12}k_{21} - k_{12}h_{21}| \geq |\lambda| && (4.13) \\ &&& h_{11}k_{21} - k_{11}h_{21} = 0 && (4.14) \\ &&& H, K \in \Phi(\mathbb{F}). && (4.15) \end{aligned}$$

Let us denote the maximum value of the above problem by $\Delta_{|\lambda|}^{\mathbb{F}}$. Obviously we have

$$\delta_{|\lambda|}^{\mathbb{R}} \leq \left\{ \begin{matrix} \Delta_{|\lambda|}^{\mathbb{R}} \\ \\ \delta_{|\lambda|}^{\mathbb{C}} \end{matrix} \right\} \leq \Delta_{|\lambda|}^{\mathbb{C}}.$$

It is easy to see that $\Delta_{|\lambda|}^{\mathbb{F}} = \max\{\delta_t^{\mathbb{F}} : |\lambda| \leq t \leq 1\}$. From (1.3), we know that $\delta_{|\lambda|}^{\mathbb{R}}$ is non-increasing in $|\lambda|$ (see Figure 1.1 for $\big(\delta_{|\lambda|}^{\mathbb{R}}\big)^2$), and so

$$\delta_{|\lambda|}^{\mathbb{R}} = \Delta_{|\lambda|}^{\mathbb{R}}.$$

Hence, if we can show $\Delta_{|\lambda|}^{\mathbb{R}} = \Delta_{|\lambda|}^{\mathbb{C}}$, we get $\delta_{|\lambda|}^{\mathbb{R}} = \delta_{|\lambda|}^{\mathbb{C}}$ as required.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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**4.3.2. Proof of $\boldsymbol{\Delta}^{\mathbb{R}}_{|\lambda|} = \boldsymbol{\Delta}^{\mathbb{C}}_{|\lambda|}$.** We now regard $\mathbb{F} = \mathbb{C}$. Suppose the maximum is attained with matrices $H$ and $K$, i.e.,

$$0 < \Delta^{\mathbb{C}}_{|\lambda|} = F(H,K) = 2|h_{11}k_{12} - k_{11}h_{12}|.$$

We will show that, under different assumptions, either $\Delta^{\mathbb{C}}_{|\lambda|} \le \delta^{\mathbb{R}}_{|\lambda|}$ or else there is a contradiction.

*Step 1.* Firstly, we handle the situations that $H$ or $K$ has a zero entry. Note that if $|h_{12}| = 1$, then $H \in \Sigma_2(\mathbb{C})$ and has zero trace. By Proposition 4.1, we get $\Delta^{\mathbb{C}}_{|\lambda|} \le \delta^{\mathbb{R}}_{|\lambda|}$ and we are done. The same is true for $K$. We have the following three situations:

(I) $h_{11} = 0$. Then (4.14) implies $k_{11}h_{21} = 0$. If $k_{11} = 0$ then $\Delta^{\mathbb{C}}_{|\lambda|} = 0$ and we have a contradiction. If $h_{21} = 0$ then $|h_{12}| = 1$ and we are done.

(II) $h_{21} = 0$. Then $h_{11}k_{21} = 0$ by (4.14). If $h_{11} = 0$ we are back to (I). If $k_{21} = 0$ then $\lambda = 0$ by (4.13). Moreover, $\|H\|_1 = \|K\|_1 = 1$ implies $(2h_{11}, -h_{12})^T$ and $(\overline{k_{12}}, 2\overline{k_{11}})^T$ are unit vectors. Thus, $\Delta^{\mathbb{C}}_0 \le 1 = \delta^{\mathbb{R}}_0$ and we are done.

(III) $h_{12} = 0$. If $k_{12} = 0$ then $\Delta^{\mathbb{C}}_{|\lambda|} = 0$ and hence a contradiction. If $|k_{12}| = 1$, again, we are done. Suppose $0 < |k_{12}| < 1$. Then

$$|h_{21}| \ge |\lambda|/|k_{12}| \quad \text{and} \quad 2|h_{11}| = \Delta^{\mathbb{C}}_{|\lambda|}/|k_{12}|.$$

With $4|h_{11}|^2 + |h_{21}|^2 = \|H\|_1^2 = 1$, we get back to $\left(\Delta^{\mathbb{C}}_{|\lambda|}\right)^2 + |\lambda|^2 \le |k_{12}|^2 < 1$, which implies (as $1 + |\lambda| < 4|\lambda|$ for $|\lambda| > 1/3$)

$$\left(\Delta^{\mathbb{C}}_{|\lambda|}\right)^2 < 1 - |\lambda|^2 \le \left\{ \begin{array}{ll} 1 & \text{if } \ 0 \le |\lambda| \le 1/2 \\ 4|\lambda|(1-|\lambda|) & \text{if } \ 1/2 < |\lambda| \le 1 \end{array} \right\} = \left(\delta^{\mathbb{R}}_{|\lambda|}\right)^2,$$

which gives a contradiction.

*Step 2.* We derive some necessary conditions on $H$ and $K$. From now on, we can assume all the entries of $H$ and $K$ nonzero. If $\det H = 0$, then $H \in \Sigma_2(\mathbb{C})$ with zero trace. By Proposition 4.1, we have $\Delta^{\mathbb{C}}_{|\lambda|} \le \delta^{\mathbb{R}}_{|\lambda|}$ and we are done. The same is true for $K$. We now further assume

$$\det H \ne 0 \quad \text{and} \quad \det K \ne 0. \tag{4.16}$$

Via multiplication by suitable unit scalars on $H$ and $K$, we assume $h_{11} > 0$ and $k_{11} > 0$.

Write

$$H = \begin{bmatrix} h_{11} & |h_{12}|e^{\mathbf{i}\theta_{12}} \\ |h_{21}|e^{\mathbf{i}\theta_{21}} & -h_{11} \end{bmatrix} \quad \text{and} \quad K = \begin{bmatrix} k_{11} & |k_{12}|e^{\mathbf{i}\mu_{12}} \\ |k_{21}|e^{\mathbf{i}\mu_{21}} & -k_{11} \end{bmatrix},$$

where $\theta_{12}, \theta_{21}, \mu_{12}, \mu_{21} \in [0, 2\pi)$. Define

$$H_1(\theta) = \begin{bmatrix} h_{11} & h_{12}e^{\mathbf{i}\theta} \\ h_{21} & -h_{11} \end{bmatrix} \quad \text{and} \quad K_1(\theta) = \begin{bmatrix} k_{11} & k_{12}e^{\mathbf{i}\theta} \\ k_{21} & -k_{11} \end{bmatrix}, \quad \theta \in J,$$

where $J$ is an open interval containing 0 such that $\det H_1(\theta)$ and $\det K_1(\theta)$ are nonzero on $J$. Such an interval exists because $H_1(0) = H$, $K_1(0) = K$ and (4.16). We see that for any $\theta \in J$, $H_1(\theta)$ and $K_1(\theta)$ satisfy (4.13) and (4.14), though they may not belong to $\Phi(\mathbb{C})$ because their trace norms may not be 1. If there exists a $\theta_0 \in J$ such that $\|H_1(\theta_0)\|_1^2 \cdot \|K_1(\theta_0)\|_1^2 < 1$, then for $\alpha = 1/\|H_1(\theta_0)\|_1$ and $\beta = 1/\|K_1(\theta_0)\|_1$, $\alpha\beta > 1$, $\|\alpha H_1(\theta_0)\|_1 = 1$ and $\|\beta K_1(\theta_0)\|_1 = 1$. It is easy to check that $\alpha H_1(\theta_0)$ and $\beta K_1(\theta_0)$ satisfy (4.13)–(4.15) and

$$F(\alpha H_1(\theta_0), \beta K_1(\theta_0)) = \left|\alpha\beta e^{\mathbf{i}\theta_0}(2h_{11}k_{12} - 2k_{11}h_{12})\right| = \alpha\beta\Delta^{\mathbb{C}}_{|\lambda|} > \Delta^{\mathbb{C}}_{|\lambda|}.$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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This gives a contradiction. Thus, the function $G(\theta) = \|H_1(\theta)\|_1^2 \cdot \|K_1(\theta)\|_1^2$ has a global minimum value 1 attained at $\theta = 0$ and, consequently, $G'(0) = 0$ and $G''(0) \geq 0$. As $\|H_1(0)\|_1 = \|K_1(0)\|_1 = 1$, we get

$$\left(\|H_1(\theta)\|_1^2\right)'\Big|_{\theta=0} + \left(\|K_1(\theta)\|_1^2\right)'\Big|_{\theta=0} = G'(0) = 0, \tag{4.17}$$

and

$$\left(\|H_1(\theta)\|_1^2\right)''\Big|_{\theta=0} + 2\left(\|H_1(\theta)\|_1^2\right)'\Big|_{\theta=0} \cdot \left(\|K_1(\theta)\|_1^2\right)'\Big|_{\theta=0} + \left(\|K_1(\theta)\|_1^2\right)''\Big|_{\theta=0} = G''(0) \geq 0. \tag{4.18}$$

From (4.17), we have $\left(\|H_1(\theta)\|_1^2\right)'\Big|_{\theta=0} \cdot \left(\|K_1(\theta)\|_1^2\right)'\Big|_{\theta=0} \leq 0$, and thus, (4.18) implies

$$\left(\|H_1(\theta)\|_1^2\right)''\Big|_{\theta=0} + \left(\|K_1(\theta)\|_1^2\right)''\Big|_{\theta=0} \geq 0. \tag{4.19}$$

We now obtain the explicit expressions for (4.17) and (4.19). From (4.14), since $h_{11}k_{21} \neq 0$, we have

$$\theta_{21} = \mu_{21}. \tag{4.20}$$

Then

$$\begin{aligned}\|H_1(\theta)\|_1^2 &= 2h_{11}^2 + |h_{12}|^2 + |h_{21}|^2 + 2\left|h_{11}^2 + |h_{12}||h_{21}|e^{\mathrm{i}(\theta_{12}+\theta_{21}+\theta)}\right| \\ &= 2h_{11}^2 + |h_{12}|^2 + |h_{21}|^2 + 2\sqrt{h_{11}^4 + 2h_{11}^2|h_{12}||h_{21}|\cos(\theta_{12}+\theta_{21}+\theta) + |h_{12}|^2|h_{21}|^2}.\end{aligned}$$

Thus,

$$\left(\|H_1(\theta)\|_1^2\right)' = \frac{-2h_{11}^2|h_{12}||h_{21}|\sin(\theta_{12}+\theta_{21}+\theta)}{\sqrt{h_{11}^4 + 2h_{11}^2|h_{12}||h_{21}|\cos(\theta_{12}+\theta_{21}+\theta) + |h_{12}|^2|h_{21}|^2}},$$

and hence,

$$\left(\|H_1(\theta)\|_1^2\right)'\Big|_{\theta=0} = \frac{-2h_{11}^2|h_{12}||h_{21}|\sin(\theta_{12}+\theta_{21})}{|\det H|}. \tag{4.21}$$

With a similar expression for $\left(\|K_1(\theta)\|_1\right)'\Big|_{\theta=0}$, condition (4.17) implies

$$\frac{h_{11}^2|h_{12}||h_{21}|\sin(\theta_{12}+\theta_{21})}{|\det H|} + \frac{k_{11}^2|k_{12}||k_{21}|\sin(\mu_{12}+\mu_{21})}{|\det K|} = 0. \tag{4.22}$$

Also, by direct calculation,

$$(\|H_1(\theta)\|_1^2)''\Big|_{\theta=0} = \frac{-2|h_{11}|^2|h_{12}||h_{21}|\cos(\theta_{12}+\theta_{21})}{|\det H|} - \frac{2|h_{11}|^4|h_{12}|^2|h_{21}|^2\sin^2(\theta_{12}+\theta_{21})}{|\det H|^3}.$$

Thus, with a similar expression for $\left(\|K_1(\theta)\|_1\right)''\Big|_{\theta=0}$, (4.19) implies

$$\begin{aligned}&\frac{h_{11}^2|h_{12}||h_{21}|\cos(\theta_{12}+\theta_{21})}{|\det H|} + \frac{h_{11}^4|h_{12}|^2|h_{21}|^2\sin^2(\theta_{12}+\theta_{21})}{|\det H|^3} \\ &+ \frac{k_{11}^2|k_{12}||k_{21}|\cos(\mu_{12}+\mu_{21})}{|\det K|} + \frac{k_{11}^4|k_{12}|^2|k_{21}|^2\sin^2(\mu_{12}+\mu_{21})}{|\det K|^3} \leq 0\end{aligned} \tag{4.23}$$

*Step 3.* We now come to the final argument. We refer to (4.22) and divide the proof into two cases, depending on whether $\sin(\theta_{12}+\theta_{21})$ is zero or not.

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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*Case 1.* $\sin(\theta_{12}+\theta_{21}) = 0$. By (4.22), $\sin(\mu_{12}+\mu_{21}) = 0$ and so both $\theta_{12}+\theta_{21}$ and $\mu_{12}+\mu_{21}$ are multiples of $\pi$. With (4.20), we can easily deduce that $H$ and $K$ are of the form

$$H = \begin{bmatrix} h_{11} & \tau_H|h_{12}|e^{-\theta_{21}\mathbf{i}} \\ |h_{21}|e^{\theta_{21}\mathbf{i}} & -h_{11} \end{bmatrix} \quad \text{and} \quad K = \begin{bmatrix} k_{11} & \tau_K|k_{12}|e^{-\theta_{21}\mathbf{i}} \\ |k_{21}|e^{\theta_{21}\mathbf{i}} & -k_{11} \end{bmatrix},$$

where $\tau_H, \tau_K \in \{1, -1\}$. Let $D = \operatorname{diag}(1, e^{\mathbf{i}\theta_{21}})$, which is unitary. Then $D^*HD$ and $D^*KD$ are real matrices. For notation simplicity, instead of using $D^*HD$ and $D^*KD$, we now just assume $H$ and $K$ are real. We have three subcases.

*Subcase 1.1.* $\det H < 0$ and $\det K < 0$. Here, both $H$ and $K$ belong to $\Phi(\mathbb{R})$. Consequently, we have $\Delta^{\mathbb{R}}_{|\lambda|} \geq \Delta^{\mathbb{C}}_{|\lambda|}$ and the result follows.

*Subcase 1.2.* $\det H > 0$ and $\det K > 0$. The condition $\det H > 0$ implies $h_{11}^2 + h_{12}h_{21} < 0$ and consequently the condition $\|H\|_1^2 = 1$ becomes $(h_{12} - h_{21})^2 = 1$, which is independent of $h_{11}$. It means that as long as the condition $h_{11}^2 + h_{12}h_{21} < 0$ is satisfied, we may vary $h_{11}$ freely. The same is true for $k_{11}$ when $\det K > 0$. Thus, for $\epsilon > 0$ but small enough, the pair

$$\hat{H} = \begin{bmatrix} (1+\epsilon)h_{11} & h_{12} \\ h_{21} & -(1+\epsilon)h_{11} \end{bmatrix} \quad \text{and} \quad \hat{K} = \begin{bmatrix} (1+\epsilon)k_{11} & h_{12} \\ k_{21} & -(1+\epsilon)k_{11} \end{bmatrix}$$

satisfies (4.13)–(4.15) and $F(\hat{H}, \hat{K}) = (1+\epsilon)F(H,K) > F(H,K) = \Delta^{\mathbb{C}}_{|\lambda|}$. This gives a contradiction.

*Subcase 1.3.* $\det H < 0$ and $\det K > 0$ (the other case $\det H > 0$ and $\det K < 0$ is the same). We check that $X = H + \sqrt{|\det H|}I_2 \in \Sigma_2(\mathbb{R})$ and $Y = K + \sqrt{|\det K|}I_2\mathbf{i} \in \Sigma_2(\mathbb{C})$. By Lemma 4.2, we conclude that either $\Delta^{\mathbb{C}}_{|\lambda|} \leq \delta^{\mathbb{R}}_{|\lambda|}$ or there is another pair that gives a larger value of $F$. The latter contradicts the maximality of $F(H,K)$. The result follows.

*Case 2.* $\sin(\theta_{12}+\theta_{21}) \neq 0$. Suppose $\sin(\theta_{12}+\theta_{21}) > 0$ (the case $\sin(\theta_{12}+\theta_{21}) < 0$ is similar). Then $\sin(\mu_{12}+\mu_{21}) < 0$ by (4.22) and we have from (4.21)

$$\left(\|H_1(\theta)\|_1^2\right)'\big|_{\theta=0} < 0 \quad \text{and} \quad \left(\|K_1(\theta)\|_1^2\right)'\big|_{\theta=0} > 0.$$

*Subcase 2.1.* $\cos((\theta_{12}+\theta_{21}) - (\mu_{12}+\mu_{21})) \neq -1$. We can find an $\epsilon \in J$ (with $|\epsilon|$ small enough, to be determined later) such that

$$\cos((\theta_{12}+\theta_{21}) - (\mu_{12}+\mu_{21})) > \cos((\theta_{12}+\theta_{21}) - (\mu_{12}+\mu_{21}) + \epsilon).$$

Then, using (4.20),

$$\begin{aligned} \Delta^{\mathbb{C}}_{|\lambda|} &= 2\left|h_{11}|k_{12}| - k_{11}|h_{12}|e^{\mathbf{i}((\theta_{12}+\theta_{21})-(\mu_{12}+\mu_{21}))}\right| \\ &< 2\sqrt{h_{11}^2|k_{12}|^2 - 2h_{11}k_{11}|h_{12}||k_{12}|\cos((\theta_{12}+\theta_{21}) - (\mu_{12}+\mu_{21}) + \epsilon) + k_{11}^2|h_{12}|^2} := p \end{aligned}$$

and at the same time, again using (4.20),

$$\begin{aligned} |\lambda| \leq |h_{12}k_{21} - k_{12}h_{21}| &= \left||h_{12}||k_{21}|e^{\mathbf{i}(\theta_{12}+\mu_{21}-\mu_{12}-\theta_{21})} - |k_{12}||h_{21}|\right| \\ &< \sqrt{|h_{12}|^2|k_{21}|^2 - 2|h_{12}||k_{21}||h_{21}||k_{12}|\cos((\theta_{12}+\theta_{21}) - (\mu_{12}+\mu_{21}) + \epsilon) + |k_{12}|^2|h_{21}|^2} := q. \end{aligned}$$

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 36, pp. 1-20, January 2020.
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Suppose $\epsilon > 0$. Since $\left(\|H_1(\theta)\|_1^2\right)'\big|_{\theta=0} < 0$, we know that $\left(\|H_1(\theta)\|_1^2\right)'$, being continuous on $J$, is negative on a neighborhood $N$ of 0. Thus, $\|H_1(\theta)\|_1^2$ is decreasing on $N$. We can assume $\epsilon$ small enough so that $\|H_1(\epsilon)\|_1^2 < \|H_1(0)\|_1^2 = 1$. Note that

$$H_1(\epsilon)K - KH_1(\epsilon) = \begin{bmatrix} h_{12}e^{\mathbf{i}\epsilon}k_{21} - k_{12}h_{21} & 2h_{11}k_{12} - 2k_{11}h_{12}e^{\mathbf{i}\epsilon} \\ 0 & -(h_{12}e^{\mathbf{i}\epsilon}k_{21} - k_{12}h_{21}) \end{bmatrix}$$

with $|2h_{11}k_{12} - 2k_{11}h_{12}e^{\mathbf{i}\epsilon}| = p > \Delta^{\mathbb{C}}_{|\lambda|}$ and $|h_{12}e^{\mathbf{i}\epsilon}k_{21} - k_{12}h_{21}| = q > |\lambda|$. We now have a contradiction because $H_1(\epsilon)/\|H_1(\epsilon)\|_1$ and $K$ satisfy (4.13)–(4.15) and

$$F(H_1(\epsilon)/\|H_1(\epsilon)\|_1, K) = p/\|H_1(\epsilon)\|_1 > \Delta^{\mathbb{C}}_{|\lambda|}/\|H_1(\epsilon)\|_1 > \Delta^{\mathbb{C}}_{|\lambda|}.$$

If $\epsilon < 0$, we use $\left(\|K_1(\theta)\|_1^2\right)'\big|_{\theta=0} > 0$, and we have a contradiction similarly.

*Subcase 2.2.* $\cos((\theta_{12} + \theta_{21}) - (\mu_{12} + \mu_{21})) = -1$. We have

$$(\theta_{12} + \theta_{21}) = (\mu_{12} + \mu_{21}) + (2k + 1)\pi \quad \text{for some integer } k.$$

This implies

$$(0 \neq)\ \sin(\theta_{12} + \theta_{21}) = -\sin(\mu_{12} + \mu_{21}) \quad \text{and} \quad \cos(\theta_{12} + \theta_{21}) = -\cos(\mu_{12} + \mu_{21}). \tag{4.24}$$

Then, (4.22) and the first part of (4.24) give

$$\frac{h_{11}^2|h_{12}||h_{21}|}{|\det H|} = \frac{k_{11}^2|k_{12}||k_{21}|}{|\det K|}. \tag{4.25}$$

We now refer to (4.23). Using (4.24), (4.25) and the assumption that all the entries of $H$ and $K$ are nonzero, we get a contradiction. ∎

**Acknowledgments.** The authors would like to thank Prof. D. Wenzel for his valuable discussion on this topic, and the referee for his/her constructive suggestions which greatly improved the readability of the paper.

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