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Singular values, diagonal elements, and extreme matrices

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Abstract

For complex matrices A and B there are inequalities related to the diagonal elements of AB and the singular values of A and B. We study the conditions on the matrices for which those inequalities become equalities. In all cases, the conditions are both necessary and sufficient.
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Given an $n \times n$ complex matrix A, three sets of numbers are of particular interest: eigenvalues $\lambda_1, \ldots, \lambda_n (|\lambda_1| \geqslant \cdots \geqslant |\lambda_n|)$, singular values $a_1 \geqslant \cdots \geqslant a_n$, and diagonal elements $d_1, \ldots, d_n (|d_1| \geqslant \cdots \geqslant |d_n|)$. The relation between the eigenvalues and the singular values was obtained by Weyl [15] and Horn [5] and the relation between the diagonal elements and the singular values was obtained by Thompson [12] and Sing [9] independently. However, the relation between the eigenvalues and the diagonal elements is far from trivial, even for normal A [13].

Some inequalities for the singular values of the product $C = AB$ and the singular values of A and B are well-known, e.g. $\prod_{i=1}^{k} c_i \leqslant \prod_{i=1}^{k} a_i b_i$, $k = 1, \ldots, n-1$ and equality holds when $k = n$ [4]. This immediately yields its additive version and Lemma 4.

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So, if d_i, $i = 1, \dots, n$, denote the diagonal elements of *AB* their absolute values in nonincreasing order, then one has (part of Theorem 1)

$$|d_1| + \cdots + |d_k| \leqslant a_1 b_1 + \cdots + a_k b_k, \quad k = 1, \dots, n$$

and the inequality with a subtracted term

$$|d_1| + \cdots + |d_{n-1}| - |d_n| \leqslant a_1 b_1 + \cdots + a_{n-1} b_{n-1} - a_n b_n.$$

These inequalities completely describe the relation between the diagonal entries of a product *AB* and the singular values of *A* and *B*, respectively [8]. In recent years inequalities of subtracted term have appeared repeatedly and turn out to be closely related to the root system of some real simple Lie algebras. Here, we consider when these inequalities become equalities. The main results are Theorem 2 (for the weak majorization) and Theorem 3 (for the subtracted term inequality). The proofs rely on Lemma 3 and some work of Li [6] on the characterization of extremal matrices.

Let *A* and *B* be $n \times n$ complex matrices with singular values $a_1 \geqslant \cdots \geqslant a_n$ and $b_1 \geqslant \cdots \geqslant b_n$, respectively. Denote the set of $n \times n$ complex matrices by M_n.

The 1937 trace inequality of von Neumann [14] asserts that

$$\mathrm{Re}(\mathrm{tr}(AB)) \leqslant a_1 b_1 + \cdots + a_n b_n,$$

where Re denotes the real part, and tr the trace.

This inequality has commanded attention in more than 60 years since it was found and several applications of it in pure and applied mathematics are known. These include applications of group induced orderings to statistics [2], nonlinear elasticity [1], and applications to perturbation theory [10]. For more references, see [7].

A more detailed study of the theorem seems justified. Thus, in [8] we asked about the conditions satisfied by the individual diagonal elements of the product that sum to give the trace, and the answer was given in the following theorem.

Theorem 1. *Let A and B be in M_n with singular values $a_1 \geqslant \cdots \geqslant a_n$ and $b_1 \geqslant \cdots \geqslant b_n$, respectively. Then if $d_1, \dots, d_n$ denote the elements of the principal diagonal of AB numbered in order of decreasing absolute values, we have that*

$$|d_1| + \cdots + |d_k| \leqslant a_1 b_1 + \cdots + a_k b_k, \quad k = 1, \dots, n,$$

$$|d_1| + \cdots + |d_{n-1}| - |d_n| \leqslant a_1 b_1 + \cdots + a_{n-1} b_{n-1} - a_n b_n.$$

Conversely, if we have numbers satisfying the above inequalities, there exist matrices A and B with singular values $a_1 \geqslant \cdots \geqslant a_n$ and $b_1 \geqslant \cdots \geqslant b_n$, respectively, and $d_1, \dots, d_n$ the diagonal entries of AB.

Here, we want to study the structure of the matrices in the case when the inequalities from Theorem 1 become equalities. In order to obtain an answer we need some results. Thompson [12] found the conditions satisfied by the diagonal elements and singular values of a complex matrix. Li [6] studied the extreme cases of these inequalities and found that:

Lemma 1. *Let $A \in M_n$ with singular values $a_1 \geqslant \cdots \geqslant a_n$, diagonal elements $d_1, \ldots, d_n$ such that $|d_1| \geqslant \cdots \geqslant |d_n|$. Let $1 \leqslant k \leqslant n$. Then*

$$|d_1| + \cdots + |d_k| = a_1 + \cdots + a_k$$

if and only if $A = A_1 \oplus A_2$ $(A_1 \in M_k)$ and there exists a diagonal matrix $D \in U(k)$ such that DA_1 is a positive semidefinite matrix with eigenvalues $a_1, \ldots, a_k$.

Lemma 2. *Let $A \in M_n$ with singular values $a_1 \geqslant \cdots \geqslant a_n$ diagonal elements $d_1, \ldots, d_n$ such that $|d_1| \geqslant \cdots \geqslant |d_n|$. Then*

$$|d_1| + \cdots + |d_{n-1}| - |d_n| = a_1 + \cdots + a_{n-1} - a_n$$

if and only if there exists a diagonal matrix $D \in U(n)$ such that DA is a hermitian matrix with diagonal elements $|d_1|, \ldots, |d_{n-1}|, -|d_n|$; and eigenvalues $a_1, \ldots, a_{n-1}$, $-a_n$.

Horn [4] proved that the vector of singular values of a product of two matrices is weakly majorized by the vector of the corresponding products of singular values of the factors, when they are ordered in decreasing order. The equality case is given in the next lemma.

Lemma 3. *Let $A, B \in M_n$ with singular values $a_1 \geqslant \cdots \geqslant a_n$, and $b_1 \geqslant \cdots \geqslant b_n$, respectively. Let $c_1 \geqslant \cdots \geqslant c_n$ denote the singular values of AB. Let $1 \leqslant k \leqslant n$. Then*

$$c_1 + \cdots + c_k = a_1 b_1 + \cdots + a_k b_k$$

if and only if there are $U, V, W \in U(n)$, the $n \times n$ unitary group, such that $U^* A V = \operatorname{diag}(a_1, \ldots, a_k) \oplus A_2$ and $V^* B W = \operatorname{diag}(b_1, \ldots, b_k) \oplus B_2$ for some $A_2, B_2 \in M_{n-k}$.

Proof. First assume that $k \leqslant \min\{\operatorname{rank} A, \operatorname{rank} B\}$, so $a_k b_k > 0$. The singular value decomposition ensures that there are $n \times n$ unitary matrices $X = [X_1 \quad X_2]$ and $Y = [Y_1 \quad Y_2]$ such that $X_1, Y_1 \in M_{n,k}$ and

$$X^* (AB) Y = \operatorname{diag}(c_1, \ldots, c_n) = \begin{bmatrix} X_1^* A B Y_1 & * \\ * & * \end{bmatrix}.$$

In particular, $\left(X_1^* A\right)(BY_1)$ is positive semidefinite.

Since

$$X^* A = \begin{bmatrix} X_1^* A \\ X_2^* A \end{bmatrix},$$

singular value interlacing ensures that $\sigma_i\left(X_1^* A\right) \leqslant \sigma_i\left(X^* A\right) = a_i$ for all $i = 1, \ldots, k$. If these inequalities are all equalities, then the k largest eigenvalues of

$$G = \left(X^* A\right)\left(X^* A\right)^* = \begin{bmatrix} X_1^* A A^* X_1 & * \\ X_2^* A A^* X_1 & * \end{bmatrix}$$

are exactly the k eigenvalues of its principal submatrix $H \equiv X_1^* A A^* X_1$, which means that the interlacing inequalities for H in G are all equalities; this forces $X_2^* A A^* X_1 = 0$ (the rows of $X_1^* A$ are orthogonal to the rows of $X_2^* A$). A similar conclusion holds for B.

Now compute

$$\begin{aligned}\sum_{i=1}^{k} c_i &= \operatorname{tr}\left(X_1^* A\right)(BY_1) = \operatorname{tr}(BY_1)\left(X_1^* A\right)\\ &\leqslant \sum_{i=1}^{k} \sigma_i\left(BY_1 X_1^* A\right) \qquad (1)\\ &\leqslant \sum_{i=1}^{k} \sigma_i(BY_1)\,\sigma_i\left(X_1^* A\right)\\ &\leqslant \sum_{i=1}^{k} \sigma_i(A)\,\sigma_i(B) \qquad (2)\\ &= \sum_{i=1}^{k} a_i b_i = \sum_{i=1}^{k} c_i .\end{aligned}$$

Thus, all these inequalities are equalities.

Equality at (2) means that all $\sigma_i\left(X_1^* A\right) = \sigma_i(A)$ and $\sigma_i(BY_1) = \sigma_i(B)$ since all the terms are positive (here's where we use the rank assumption).

Equality at (1) means that $(BY_1)\left(X_1^* A\right)$ is positive semidefinite. Since we already know that $\left(X_1^* A\right)(BY_1)$ is positive semidefinite, the simultaneous singular value decomposition [3] says there are $Z \in U(k)$ and $W \in U(n)$ such that $X_1^* A = Z\Sigma W^*$ and $BY = W\Lambda Z^*$, where $\Sigma = [D_A \;\; 0] \in M_{k,n}$ and $\Lambda^{\mathrm{T}} = [PD_B \;\; 0] \in M_{k,n}$, $D_A = \operatorname{diag}(a_1, \ldots, a_k)$, $D_B = \operatorname{diag}(b_1, \ldots, b_k)$, and P is some permutation matrix. The usual interchange argument using $\operatorname{tr}\left(X_1^* A\right)(BY_1) = \sum_{i=1}^{k} a_i b_i$ ensures that the b_i are in the correct position when the a_i are distinct, or that *they can be put into correct position* via a harmless permutation (which is then absorbed into W) when some a_i are repeated. The conclusion is that there are $Z \in U(k)$ and $W = [W_1 \;\; W_2] \in U(n)$ such that $W_1 \in M_{n,k}$, $X_1^* A = Z\Sigma W^* = ZD_A W_1^*$, and $BY = W\Lambda Z^* = W_1 D_B Z^*$. Compute

$$\begin{aligned}X^* A W &= \begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix} A \begin{bmatrix} W_1 & W_2 \end{bmatrix} = \begin{bmatrix} X_1^* A W_1 & X_1^* A W_2 \\ X_2^* A W_1 & * \end{bmatrix}\\ &= \begin{bmatrix} Z D_A W_1^* W_1 & Z D_A W_1^* W_2 \\ X_2^* A \left(A^* X_1 Z D_A^{-1}\right) & * \end{bmatrix} = \begin{bmatrix} Z D_A & 0 \\ 0 & * \end{bmatrix}\end{aligned}$$

since $W_1^* W_2 = 0$ and $X_2^* A A^* X_1 = 0$. Finally,

$$\left(Z^* \oplus I_{n-k}\right) X^*AW = \begin{bmatrix} D_A & 0 \\ 0 & * \end{bmatrix}$$

is a representation of the required form. A similar argument gives a representation of the desired form for B.

Now suppose that $k_1 = \operatorname{rank} A \leqslant \operatorname{rank} B$ and $k > k_1$. Then $\operatorname{rank} AB \leqslant k_1$, so $c_i = 0$ if $i > k_1$, and

$$\sum_{i=1}^{k_1} c_i = \sum_{i=1}^{k} c_i = \sum_{i=1}^{k} a_i b_i = \sum_{i=1}^{k_1} a_i b_i .$$

The preceding argument ensures that there are unitary U and V such that

$$U^*AV = \begin{bmatrix} D_A & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad U^*BV = \begin{bmatrix} D_B & 0 \\ 0 & B_2 \end{bmatrix},$$

where $D_A, D_B \in M_{k_1}$. Let $B_2 = V_3 \varDelta W_3^*$ be a singular value decomposition. Then

$$U_1 \left(I \oplus V_3^*\right) U^*AV\,(I \oplus W_3) = \begin{bmatrix} D_A & 0 \\ 0 & 0 \end{bmatrix}$$

and

$$\left(I \oplus V_3^*\right) U^*BV\,(I \oplus W_3) = \begin{bmatrix} D_B & 0 \\ 0 & \varDelta \end{bmatrix}$$

is a representation of the desired form for all $k \geqslant k_1$.

The converse is clear. $\square$

Let us prove now an inequality with subtracted term satisfied by the singular values of a product of matrices and the singular values of the factors.

Lemma 4. *Let $A, B \in M_n$ with singular values $a_1 \geqslant \cdots \geqslant a_n, b_1 \geqslant \cdots \geqslant b_n$, respectively. Denote by $c_1 \geqslant \cdots \geqslant c_n$ the singular values of AB. Then*

$$c_1 + \cdots + c_{n-1} - c_n \leqslant a_1 b_1 + \cdots + a_{n-1} b_{n-1} - a_n b_n .$$

Proof. We know that $c_1 \cdots c_k \leqslant a_1 b_1 \cdots a_k b_k,\ k = 1, \ldots, n,$ with equality when $k = n$.

$c_n = 0$ implies $a_n b_n = 0$ and there is nothing to prove. So, assume $c_n \neq 0$. Thus,

$$c_n = \frac{a_1 b_1 \cdots a_n b_n}{c_1 \cdots c_{n-1}},$$

and

$$c_1 + \cdots + c_{n-1} - c_n = c_1 + \cdots + c_{n-1} - \frac{a_1 b_1 \cdots a_n b_n}{c_1 \cdots c_{n-1}}$$

$$\begin{aligned}&\leqslant c_1 + \cdots + c_{n-1} - a_n b_n\\ &\leqslant a_1 b_1 + \cdots + a_{n-1} b_{n-1} - a_n b_n,\end{aligned}$$

since

$$\frac{-1}{c_1 \cdots c_{n-1}} \leqslant \frac{-1}{a_1 b_1 \cdots a_{n-1} b_{n-1}}. \qquad \square$$

The equality case of the previous result is given now.

Lemma 5. *Let $A, B \in M_n$ with singular values $a_1 \geqslant \cdots \geqslant a_n, b_1 \geqslant \cdots \geqslant b_n$, respectively. Denote by $c_1 \geqslant \cdots \geqslant c_n$ the singular values of AB. Then*

$$c_1 + \cdots + c_{n-1} - c_n = a_1 b_1 + \cdots + a_{n-1} b_{n-1} - a_n b_n$$

if and only if, there are $U, V, W \in U(n)$ such that $U^* A V = \mathrm{diag}(a_1, \ldots, a_{n-1}) \oplus \mathrm{e}^{\mathrm{i}\theta} a_n$ and $V^* B W = \mathrm{diag}(b_1, \ldots, b_{n-1}) \oplus \mathrm{e}^{\mathrm{i}\delta} b_n$ for some real numbers θ and δ.

Proof. If $c_n \neq 0$, as in the proof of Lemma 4, we have

$$\begin{aligned}a_1 b_1 + \cdots + a_{n-1} b_{n-1} - a_n b_n &= c_1 + \cdots + c_{n-1} - c_n\\ &\leqslant c_1 + \cdots + c_{n-1} - a_n b_n.\end{aligned}$$

Therefore,

$$c_1 + \cdots + c_{n-1} = a_1 b_1 + \cdots + a_{n-1} b_{n-1},$$

and $c_n = a_n b_n$, and the result follows from Lemma 3. If $c_n = 0$, we do not have a subtracted term and again we can use Lemma 3.

For the converse, if $c_n = 0$ then $a_n b_n = 0$ and the result follows from Lemma 3. If $c_n \neq 0$, then

$$c_1 + \cdots + c_n \leqslant a_1 b_1 + \cdots + a_n b_n = c_1 + \cdots + c_{n-1} - c_n + 2 a_n b_n$$

and thus $c_n \leqslant a_n b_n$. Consequently,

$$\begin{aligned}a_1 b_1 + \cdots + a_{n-1} b_{n-1} - a_n b_n &= c_1 + \cdots + c_{n-1} - a_n b_n\\ &\leqslant c_1 + \cdots + c_{n-1} - c_n\end{aligned}$$

and we have equality from the previous lemma. $\square$

Now, we proceed with the main results.

Theorem 2. *Let A and B be in M_n with singular values $a_1 \geqslant \cdots \geqslant a_n$ and $b_1 \geqslant \cdots \geqslant b_n$, respectively. Let the diagonal elements of AB be denoted by $d_1, \ldots, d_n$ and numbered in order of decreasing absolute values. Let $1 \leqslant k \leqslant n$, then*

$$|d_1| + \cdots + |d_k| = a_1 b_1 + \cdots + a_k b_k$$

if and only if there are $U, V, W \in U(n)$ *such that* $U^*AV = \operatorname{diag}(a_1, \dots, a_k) \oplus A_2$ *and* $V^*BW = \operatorname{diag}(b_1, \dots, b_k) \oplus B_2$ *for some* $A_2, B_2 \in M_{n-k}$, *and* $AB = (AB)_1 \oplus (AB)_2$ *where* $(AB)_1 \in M_k$ *and there exists a diagonal matrix* $D \in U(k)$ *such that* $D(AB)_1$ *is a positive semidefinite matrix with eigenvalues* $a_1b_1, \dots, a_kb_k$.

Proof. We have $|d_1| + \cdots + |d_k| = c_1 + \cdots + c_k = a_1b_1 + \cdots + a_kb_k$. Lemma 3 gives us the structure for *A* and *B*, and Lemma 1 decomposes *AB* as $(AB)_1 \oplus (AB)_2$ and produces $D \in U(k)$ so that $D(AB)_1$ has eigenvalues $c_1, \dots, c_k$. Multiplying *A* and *B* gives us

$$AB = (AB)_1 \oplus (AB)_2 = U(D_A D_B \oplus A_2B_2)W^*$$

where

$$D_A = \operatorname{diag}(a_1, \dots, a_k), \quad \text{and} \quad D_B = \operatorname{diag}(b_1, \dots, b_k).$$

Consequently, the eigenvalues of $D(AB)_1$ are $a_1b_1, \dots, a_kb_k$.

The converse is clear. □

Theorem 3. *Let A and B be in* M_n *with singular values* $a_1 \geqslant \cdots \geqslant a_n$ *and* $b_1 \geqslant \cdots \geqslant b_n$, *respectively. Let the diagonal elements of AB be denoted by* $d_1, \dots, d_n$ *and numbered in order of decreasing absolute values. Then*

$$|d_1| + \cdots + |d_{n-1}| - |d_n| = a_1b_1 + \cdots + a_{n-1}b_{n-1} - a_nb_n$$

if and only if there are $U, V, W \in U(n)$ *such that* $U^*AV = \operatorname{diag}(a_1, \dots, a_{n-1}) \oplus \mathrm{e}^{\mathrm{i}\theta}a_n$ *and* $V^*BW = \operatorname{diag}(b_1, \dots, b_{n-1}) \oplus \mathrm{e}^{\mathrm{i}\delta}b_n$ *for some real numbers* θ *and* δ, *and there exists a diagonal matrix* $D \in U(n)$ *such that* $D(AB)$ *is hermitian with diagonal elements* $|d_1|, \dots, |d_{n-1}|, -|d_n|$ *and eigenvalues* $a_1b_1, \dots, a_{n-1}b_{n-1}, -a_nb_n$.

Proof. We have

$$\begin{aligned} |d_1| + \cdots + |d_{n-1}| - |d_n| &= c_1 + \cdots + c_{n-1} - c_n \\ &= a_1b_1 + \cdots + a_{n-1}b_{n-1} - a_nb_n. \end{aligned}$$

Lemma 5 gives us the structure for *A* and *B*, and Lemma 2 produces a unitary diagonal matrix *D* such that $D(AB)$ is hermitian with diagonal entries $|d_1|, \dots, |d_{n-1}|$, $-|d_n|$ and eigenvalues $c_1, \dots, c_{n-1}, -c_n$. The eigenvalues of $D(AB)$ are $a_1b_1, \dots, a_{n-1}b_{n-1}, -a_nb_n$. This follows from the proof of Lemma 5.

The converse is trivial. □

Comments.

1. The theorems remain valid when *A* and *B* are real matrices. This is because the real version of the diagonal elements–singular values relation is proved in [12].
2. These results can be extended to more than two matrices since Theorem 1 was be generalized by Tam [11].

3. The trace of a matrix can be viewed as the sum of the eigenvalues. This is one of the reasons why Miranda and Thompson [8] proved Theorem 2 to study the inequalities satisfied by the eigenvalues of the product of two matrices in terms of the singular values of the factors. It would be interesting to study the equality cases in this context.
4. It would also be of interest to consider the diagonal elements $d_1, \ldots, d_n$ of the sum $A + B$. It is clear that
$$\sum_{i=1}^{k} |d_i| \leqslant \sum_{i=1}^{k} (a_i + b_i), \quad k = 1, \ldots, n.$$
What is the complete characterization of the diagonal elements of $UAV + WBX$ where U, V, W, X run over the unitary group independently? What happens with the extremal characterization in this case? Finally, one can also consider the extremal characterization for the real parts of the diagonal elements of the sum of two matrices since we have
$$\sum_{i=1}^{k} |\mathrm{Re}\, d_i| \leqslant \sum_{i=1}^{k} (a_i + b_i), \quad k = 1, \ldots, n.$$
5. Another possibility to explore in the future, instead of the additive equality which appears in Lemma 3, is to study equality cases in product inequalities like in the case $\prod_{i=1}^{k} c_i = \prod_{i=1}^{k} a_i b_i$. It is important to note that the same characterization does not work since the additive inequality does not imply the multiplicative one. A sufficient condition is given by the decomposition $A = A_1 \oplus A_2$ and $B = B_1 \oplus B_2$, where A_1 and $B_1 \in M_k$ have $a_1, \ldots, a_k$ and $b_1, \ldots, b_k$, respectively, as their singular values.

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