THE CASE OF EQUALITY IN THE VON NEUMANN TRACE INEQUALITY

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Introduction

Recently the topics of matrix completion and robust Principal Component Analysis have been quite active. In order to fully understand these techniques, one must understand the subgradients of certain matrix norms, especially the so-called *nuclear norm*, defined to be the sum of the singular values of the matrix. The techniques in the beautiful paper of A. S. Lewis[7] allow one to find the subgradients of any unitarily invariant matrix norm, including the nuclear norm. A logical dependency of these techniques is von Neumann's inequality. There are some very short proofs of von Neumann's trace inequality, for instance those of Leon Mirsky[8] or Rolf Dieter Grigorieff[5], which we will review below. Short proofs that the case of equality occurs iff the two matrices possess a simultaneous singular value decomposition are harder to come by. We give two. The first proof, more or less, comes from a homework problem given in the book of Borwein and Lewis[2], and they attribute it to Fan and Theobald. The second proof is more historical. Adrian S. Lewis[7] encourages us to read de Sa[3], who encourages us to read von Neumann's original paper[9] and realize that he does actually prove the case of equality. We shorten the original proof up a bit via the theorem of Eckhart and Young[4], which we prove in a manner suggested by Horn and Johnson[6]. First, the statement of von Neumann's trace inequality:

Theorem 0.1. *For any $m \times n$ matrices A and B, $\mathrm{Re}\,\mathrm{tr}\, A^*B \leq \sigma(A)^T\sigma(B)$ where $\sigma_1(A) \geq \sigma_2(A) \geq \ldots \geq 0$ and $\sigma_1(B) \geq \sigma_2(B) \geq \ldots \geq 0$ are the descending singular values of A and B respectively. The case of equality occurs if and only if it is possible to find unitaries U and V that simultaneously singular value decompose A and B in the sense that*

$$A = U\Sigma_A V^* \quad \text{and} \quad B = U\Sigma_B V^*,$$

where Σ_A denotes the $m \times n$ matrix with the singular values $\sigma(A)$ descending down the diagonal, and Σ_B denotes the $m \times n$ matrix with the singular values $\sigma(B)$ descending down the diagonal.

Proofs of the inequality are found below. Assuming we have already demonstrated the inequality aspect, we deal with the case of equality:

The Case of Equality a la Borwein and Lewis

We would like to thank Ken Lange for insisting that the proof needed further shortening. We are following [2] p.17-21, upgraded to arbitrary rectangular matrices:

Suppose that we are in the case of equality, i.e. suppose that $\langle A, B\rangle := \mathrm{Re}\,\mathrm{tr}\, A^*B = \sigma(A)^T\sigma(B)$. Then we want to somehow prove that A and B have a simultaneous ordered singular value decomposition:

First, we take a singular value decomposition of $A+B$, i.e. there are unitary matrices U and V such that

$$A + B = U\Sigma_{A+B}V^*$$

Key words and phrases. von Neumann, trace, inequality, case of equality.

where Σ_{A+B} is the diagonal matrix with the descending singular values of $A+B$ down the diagonal.

It will turn out that these U and V will be the unitaries that accomplish the simultaneous S-V-D-ification of A and B:

First, notice that by von Neumann's inequality,

$$\langle U\Sigma_A V^*, B\rangle \leq \sigma(U\Sigma_A V^*)^T\sigma(B) = \sigma(A)^T\sigma(B).$$

Second, notice that

$$\langle U\Sigma_A V^*, A{+}B\rangle = \operatorname{Re}\operatorname{tr} V\Sigma_A^* U^*(A{+}B) = \operatorname{Re}\operatorname{tr} \Sigma_A^* U^*(A{+}B)V = \operatorname{Re}\operatorname{tr} \Sigma_A^*\Sigma_{A+B} = \sigma(A)^T\sigma(A{+}B).$$

Third, again by von Neumann's inequality

$$\langle A, A+B\rangle \leq \sigma(A)^T\sigma(A+B).$$

We now put all three of these together to prove that

$$\langle U\Sigma_A V^*, A\rangle \geq \langle A, A\rangle$$

as follows:

$$\begin{aligned}
&\langle U\Sigma_A V^*, A\rangle \\
&= \langle U\Sigma_A V^*, A+B\rangle - \langle U\Sigma_A V^*, B\rangle \\
&\overset{\text{first}}{\geq} \langle U\Sigma_A V^*, A+B\rangle - \sigma(A)^T\sigma(B) \\
&\overset{\text{second}}{=} \sigma(A)^T\sigma(A+B) - \sigma(A)^T\sigma(B) \\
&\overset{\text{third}}{\geq} \langle A, A+B\rangle - \sigma(A)^T\sigma(B) \\
&= \langle A, A\rangle + \langle A, B\rangle - \sigma(A)^T\sigma(B) \\
&\overset{\text{case of equality}}{=} \langle A, A\rangle
\end{aligned}$$

Since we have proved that

$$\langle U\Sigma_A V^*, A\rangle \geq \langle A, A\rangle,$$

we know that $A = U\Sigma_A V^*$ because the Frobenius length of $U\Sigma_A V^*$ is $\|A\|_F$, and the only vector of length $\|A\|_F$ that inner products with A to give the value $\langle A, A\rangle$ is A itself (the case of equality for Cauchy-Schwarz on real vector spaces).

Thus we have shown that $A = U\Sigma_A V^*$. As the hypotheses concerning A and B are symmetric, the same proof with A and B switching roles shows that $B = U\Sigma_B V^*$. Thus A and B have a simultaneous ordered singular value decomposition, and the case of equality is demonstrated.

Now we return to proving the inequality aspect of von Neumann's inequality. The remainder of this paper will speak only of square matrices, which is sufficient because:

The Case of Rectangular Matrices Follows from the case of Square Matrices

Suppose WLOG $m > n$ and suppose A has SVD $A = USV^*$, with U and V unitary. Then we can "square" the $m \times n$ matrix A by adding a block of zeros to get the $m \times m$ matrix

$$\begin{bmatrix} A & 0 \end{bmatrix} = U \begin{bmatrix} S & 0 \end{bmatrix} \begin{bmatrix} V^* & 0 \\ 0 & I \end{bmatrix}.$$

Notice that this is a SVD, so the singular values of A are unaltered by the squaring process. Similar truths hold for B being squared to $\begin{bmatrix} B & 0 \end{bmatrix}$. Also the trace value is unaffected by squaring:

$$\operatorname{tr} \begin{bmatrix} A & 0 \end{bmatrix}^* \begin{bmatrix} B & 0 \end{bmatrix} = \operatorname{tr} A^*B.$$

Thus it suffices to prove the inequality aspect of von Neumann's inequality for square matrices only.

In the case of equality for rectangular matrices, their squared versions will also have equality, and thus by the square version of the equality case of von Neumann, the squared versions have have a simultaneous SVD. Since the squared versions have at least $m-n$ nullity, their simultaneous SVDs can be written as

$$\begin{bmatrix} A & 0 \end{bmatrix} = U \begin{bmatrix} S & 0 \end{bmatrix} \begin{bmatrix} V^* & N^* \\ M^* & P^* \end{bmatrix} \text{ and } \begin{bmatrix} B & 0 \end{bmatrix} = U \begin{bmatrix} T & 0 \end{bmatrix} \begin{bmatrix} V^* & N^* \\ M^* & P^* \end{bmatrix},$$

from which we get simultaneous truths $A = USV^*$ and $B = UTV^*$. It is not at all clear that V is unitary; however, one of the things that is being said is $SN^* = 0$, and thus at least $rank(A)$ of the first rows of N^* are zeros, and therefore at least that many rows of V^* are orthonormal. Similarly $TN^* = 0$, so at least $rank(B)$ rows of V^* are orthonormal. Thus, let $\tilde{V}^*$ consist of $\max(rank(A), rank(B))$ rows of V^*, followed if necessary by more rows orthonormally extending it to an $n \times n$ matrix. Then

$$A = US\tilde{V}^* \text{ and } B = UT\tilde{V}^*$$

is a simultaneous singular value decomposition of A and B.

Thus for the remainder of the paper we can just prove von Neumann's inequality for square matrices A and B.

Leon Mirsky's proof

Mirsky's proof requires a celebrated result of Garrett Birkhoff: the convex hull of the permutation matrices is the set of doubly stochastic matrices. (Proof by greedy algorithm and Hall's Marriage Theorem) On top of being inherently beautiful, Birkhoff's theorem is often useful for matrix analysis. For instance, the entire topic of majorization is based on it, and it proves the famous Hoffman-Wielandt theorem[1]. Mirsky uses Birkhoff to prove this lemma:

Lemma 0.2. *Suppose that D is an $n \times n$ doubly stochastic matrix, i.e. all entries are nonnegative and each row and each column sum to one. Suppose that x and y are nonnegative nonincreasing column vectors of height n, i.e. $x_1 \geq x_2 \geq \ldots \geq x_n \geq 0$ and $y_1 \geq y_2 \geq \ldots \geq y_n \geq 0$. Then $x^T D y \leq x^T y$.*

Proof. It is not hard to see that the inequality holds for any permutation matrix D. Also the set of matrices D for which it holds is convex. Thus the inequality is true for all doubly stochastic matrices by Birkhoff's theorem. □

Mirsky uses this lemma to prove von Neumann's inequality:

Proof. Suppose we have the singular value decompositions

$$A = USV^* \text{ and } B = WTX^*.$$

Then $\operatorname{tr} A^*B = \operatorname{tr} VSU^*WTX^* = \operatorname{tr} X^*VSU^*WT = \operatorname{tr} Q^*SPT$ where $P \stackrel{\text{def}}{=} U^*W$ and $Q \stackrel{\text{def}}{=} V^*X$ are unitary, and thus the matrices $|p_{ij}|^2$ and $|q_{ij}|^2$ are doubly stochastic. For all $z, \zeta \in \mathbb{C}$, $|\bar{z}\zeta| \leq \frac{1}{2}(|z|^2 + |\zeta|^2)$. Thus

$$\begin{aligned}
|\operatorname{tr} A^*B| &= |\operatorname{tr} (SQ)^*PT| \\
&\leq \sum_{i=1}^{n}\sum_{j=1}^{n} s_i t_j |\bar{q}_{ij} p_{ij}| \\
&\leq \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} s_i t_j |q_{ij}|^2 + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} s_i t_j |p_{ij}|^2 \\
&\stackrel{\text{Lemma}}{\leq} \langle s, t\rangle.
\end{aligned}$$

Thus for any $n \times n$ complex matrices A and B, $\mathrm{Re}\,\mathrm{tr}\, A^*B \le |\mathrm{tr}\, A^*B| \le \langle s, t\rangle$. $\square$

Rolf Dieter Grigorieff's Proof

Proof. Again suppose we have the singular value decompositions

$$A = USV^* \text{ and } B = WTX^*.$$

By rescaling both sides, WLOG $1 \ge s_1 \ge s_2 \ge \ldots \ge s_n \ge 0$ and $1 \ge t_1 \ge t_2 \ge \ldots \ge t_n \ge 0$. Thinking of U, V, W, and X as fixed, we notice that $|\mathrm{tr}\, A^*B|$ is a convex function of s and t, as is $\langle s, t\rangle$. Define $e_k \stackrel{\text{def}}{=} (1, 1, 1, \ldots, 0, 0, \ldots)$ to be the vector of k ones followed by $n-k$ zeros. It suffices to prove the inequality for the finitely many cases where $s = e_I$ and $t = e_J$, because any s such that $1 \ge s_1 \ge s_2 \ge \ldots \ge s_n \ge 0$ is a convex combination of $e_1, \ldots, e_n$ and ditto for t. WLOG $I \le J$. $A = \sum_{i=1}^I u_i v_i^*$, so by Cauchy-Schwarz and the spectral norm of B is $t_1 \le 1$,

$$|\mathrm{tr}\, A^*B| = \left|\sum_{i=1}^I \mathrm{tr}\, v_i u_i^* B\right| = \left|\sum_{i=1}^I \mathrm{tr}\, u_i^* B v_i\right| \le \sum_{i=1}^I |u_i^* B v_i| \le \sum_{i=1}^I \|u_i\|\|Bv_i\| \le I = \langle e_I, e_J\rangle.$$

$\square$

Now we recall some of the original method of von Neumann[9], and our own proof using the theorem of Eckhart and Young[4].

von Neumann's Lemmas

Lemma 0.3. *If tr $MH = 0$ for all Hermitian matrices H, then $M = 0$.*

Proof. If we could show that $\mathrm{tr}\, MM^* = 0$, we would be done since this is the sum of the squared absolute values of the entries of M. Recall that any complex matrix Z can be decomposed as $Z = X + iY$ where $X = \frac{1}{2}(Z + Z^*)$ and $Y = \frac{1}{2i}(Z - Z^*)$ are both Hermitian. Decomposing M^* as such we get that $\mathrm{tr}\, MM^* = \mathrm{tr}\, MX + i\mathrm{tr}\, MY = 0 + 0$ by assumption. $\square$

Lemma 0.4. *tr AH is real for all Hermitian H if and only if A is Hermitian.*

Proof. If A is Hermitian and H is Hermitian, then $AH + HA$ is Hermitian so it has real trace, and thus $\mathrm{tr}\, AH = \mathrm{tr}\, HA = \frac{1}{2}\mathrm{tr}\,(AH + HA)$ is real.

Suppose $\mathrm{tr}\, AH$ is real for all Hermitian matrices H. Then $\mathrm{tr}\, AH = \overline{\mathrm{tr}\, AH} = \mathrm{tr}\,(AH)^* = \mathrm{tr}\, H^*A^* = \mathrm{tr}\, A^*H^* = \mathrm{tr}\, A^*H$. Thus for all Hermitian H, $\mathrm{tr}\,(A^* - A)H = 0$. Thus by Lemma 0.3, $A^* = A$. $\square$

Lemma 0.5. *Suppose A is an $n \times n$ complex matrix, and suppose that for all $n \times n$ unitary matrices U*

$$\mathit{Re}\,\mathit{tr}\, A \ge \mathit{Re}\,\mathit{tr}\, AU.$$

Then A is Hermitian. Said in words: any matrix whose real trace cannot be increased by multiplying by a unitary is Hermitian.

Proof. Let H be any Hermitian matrix. For all ε of small enough absolute value, $I + i\varepsilon H$ is invertible because it does not have zero as an eigenvalue since its eigenvalues are one plue $i\varepsilon$ times the eigenvalues of H. For such small enough ε define

$$U_\varepsilon = (I + i\varepsilon H)(I - i\varepsilon H)^{-1} = (I - i\varepsilon H)^{-1}(I + i\varepsilon H).$$

Notice that

$$U_\varepsilon^* = (I + i\varepsilon H)^{-1}(I - i\varepsilon H) = (I - i\varepsilon H)(I + i\varepsilon H)^{-1}.$$

Thus $U_\varepsilon^* U_\varepsilon = U_\varepsilon U_\varepsilon^* = I$, i.e. U_ε is unitary. Also $U_\varepsilon = I + 2i\varepsilon H + O(\varepsilon^2)$ since

$$(I - i\varepsilon H)^{-1} = 1 + i\varepsilon H + (i\varepsilon H)^2 + (i\varepsilon H)^3 + \ldots$$

Thus for small enough ε,

$$\mathrm{Re}\,\mathrm{tr}\,AU_\varepsilon = \mathrm{Re}\,\mathrm{tr}\,A + 2\varepsilon \mathrm{Re}\,(i \cdot \mathrm{tr}\,AH) + O(\varepsilon^2).$$

In order for this to not violate that

$$\mathrm{Re}\,\mathrm{tr}\,A \geq \mathrm{Re}\,\mathrm{tr}\,AU,$$

it must be that

$$\mathrm{Re}\,(i \cdot \mathrm{tr}\,AH) = 0,$$

i.e. $\mathrm{tr}\,AH \in \mathbb{R}$. So we have proven that for all Hermitian H, $\mathrm{tr}\,AH \in \mathbb{R}$. By Lemma 0.4 this shows that A is Hermitian. □

Lemma 0.6. *Suppose that for all $n \times n$ unitaries U and V*

$$\mathit{Re}\,\mathit{tr}\,AB \geq \mathit{Re}\,\mathit{tr}\,AUBV.$$

Then both AB and BA are Hermitian.

Proof. Particularizing to $U = I$, we get that for all unitary V

$$\mathrm{Re}\,\mathrm{tr}\,AB \geq \mathrm{Re}\,\mathrm{tr}\,ABV.$$

By Lemma 0.5, AB is Hermitian. Particularizing to $V = I$ instead, we get that for all unitary U

$$\mathrm{Re}\,\mathrm{tr}\,BA = \mathrm{Re}\,\mathrm{tr}\,AB \geq \mathrm{Re}\,\mathrm{tr}\,AUB = \mathrm{Re}\,\mathrm{tr}\,BAU,$$

so again by Lemma 0.5, BA is Hermitian. □

Finishing the equality case via Eckhart and Young

The following theorem is due to Eckhart and Young[4]:

Theorem 0.7. *Let A and B be $n \times n$ matrices. Then both A^*B and BA^* are Hermitian if and only if A and B have an "Eckhart-Young-style simultaneous singular value decomposition," i.e. there exist S, T, W, and X such that:*

- *W and X are $n \times n$ unitaries*
- *S is a nonnegative nonincreasing diagonal $n \times n$ matrix*
- *T is a real diagonal $n \times n$ matrix (some entries may be negative)*
- *$A = WSX^*$ and $B = WTX^*$.*

We prove the theorem of Eckhart and Young below. First, let us see how their result finishes the case of equality:

Proof. Suppose we have equality in von Neumann's trace inequality, i.e. suppose

$$\mathrm{Re}\,\mathrm{tr}\,A^*B = \langle \sigma(A), \sigma(B) \rangle.$$

For all unitary U and V, $\sigma(UBV) = \sigma(B)$. Thus, by the inequality part of von Neumann's trace inequality, for all unitary U and V

$$\mathrm{Re}\,\mathrm{tr}\,A^*B = \langle \sigma(A), \sigma(B) \rangle = \langle \sigma(A), \sigma(UBV) \rangle \geq \mathrm{Re}\,\mathrm{tr}\,A^*UBV.$$

Thus by von Neumann's Lemma 8 it must be that both A^*B and BA^* are Hermitian. Thus by Eckhart and Young, A and B have a "simultaneous singular value decomposition" in the sense above. Thus $\mathrm{tr}\,A^*B = \mathrm{tr}\,S^*T$. Seeing as the absolute values of T's diagonal elements are the singular values of B, and seeing as T is real, T must be all nonnegative and nonincreasing, else $\mathrm{Re}\,\mathrm{tr}\,A^*B = \mathrm{Re}\,\mathrm{tr}\,S^*T$ could not be as large as $\langle \sigma(A), \sigma(B) \rangle$. Thus A and B possess a "true" simultaneous singular value decomposition in the sense that both S and T are nonnegative nonincreasing down the diagonal. □

Proof of the Eckhart and Young Theorem, as suggested by Horn and Johnson

Suppose A and B are $n \times n$ complex matrices such that both A^*B and BA^* are Hermitian. Let $A = USV^*$ be a singular value decomposition of A so that U and V are unitary and S is diagonal nonnegative nonincreasing, so in particular $S^* = S$. Define $M = U^*BV$. Notice that $V^*A^*BV = SM$ and $U^*BA^*U = MS$. Also notice both SM and MS are Hermitian.

We will construct a unitary X and a real diagonal T such that $S = XSX^*$, $M = XTX^*$, and then we will be done since $A = USV^* = (UX)S(VX)^*$ and $B = UMV^* = (UX)T(VX)^*$ give an "Eckhart-Young-style simultaneous SVD" for A and B since UX and VX are unitary.

How to construct such an X? It turns out that S being diagonal nonnegative nonincreasing and SM and MS being Hermitian force M to be block diagonal subordinate to the runs of equality on the diagonal of S. We prove this later. Once that is demonstrated, we unitarily diagonalize block by block to get a diagonal T filled with the eigenvalues of each block (which are necessarily real since each block is Hermitian, but might be negative). For example, suppose that S has two runs of equality, i.e. there are $s_1 \geq s_2 \geq 0$ such that

$$S = \begin{bmatrix} \underset{k\times k}{s_1 I} & 0 \\ 0 & \underset{(n-k)\times(n-k)}{s_2 I} \end{bmatrix},$$

and suppose that M has block structure subordinate to the lengths of those runs, i.e.

$$M = \begin{bmatrix} \underset{k\times k}{B_1} & 0 \\ 0 & \underset{(n-k)\times(n-k)}{B_2} \end{bmatrix},$$

then we can unitarily diagonalize block-by-block to get T

$$\begin{bmatrix} X_1^* & 0 \\ 0 & X_2^* \end{bmatrix} \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix} \begin{bmatrix} X_1 & 0 \\ 0 & X_2 \end{bmatrix} = \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix} = T$$

and notice that since scalar multiples of the identity commute with all matrices,

$$\begin{bmatrix} X_1^* & 0 \\ 0 & X_2^* \end{bmatrix} \begin{bmatrix} s_1 I & 0 \\ 0 & s_2 I \end{bmatrix} \begin{bmatrix} X_1 & 0 \\ 0 & X_2 \end{bmatrix} = \begin{bmatrix} s_1 I & 0 \\ 0 & s_2 I \end{bmatrix} = S.$$

Thus

$$X = \begin{bmatrix} X_1 & 0 \\ 0 & X_2 \end{bmatrix}$$

is the unitary we wanted. Thus we have proven the result of Eckhart and Young, in the manner suggested by [6][page 426].

We owe a proof that S being diagonal nonnegative nonincreasing and SM and MS being Hermitian force M to be block diagonal subordinate to the runs of equality on the diagonal of S.

Proving that M is block diagonal subordinate to equality runs in S

Suppose that SM and MS are both Hermitian, and S is a nonnegative nonincreasing diagonal square matrix, and M is a same size square matrix. We claim that M must be block diagonal subordinate to runs of equality in S's diagonal.

Proof. Suppose that $n \times n$ is the smallest size for which the claim has not yet been demonstrated (begin induction). If S is a multiple of the identity, then there is only one run of equality, so we are already done. Otherwise, for some $s > 0$, we can write

$$S = \begin{bmatrix} sI & 0 \\ 0 & E \end{bmatrix} \quad \text{and} \quad M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

where E is a square diagonal matrix with nonnegative nonincreasing diagonal entries all strictly smaller than s, and where the sizes of the blocks make SM and MS compatible block multiplies. Then we get that both

$$SM = \begin{bmatrix} sA & sB \\ EC & ED \end{bmatrix} \quad \text{and} \quad MS = \begin{bmatrix} sA & BE \\ sC & DE \end{bmatrix}$$

are Hermitian. Thus DE and ED are Hermitian with E a square diagonal matrix with nonnegative nonincreasing diagonal entries, so by induction D is block diagonal subordinate to the runs of equality in E. Also, $sB^* = EC$ and $sC^* = BE$, so $s^2C = s(sC^*)^* = s(BE)^* = E^*(sB^*) = E^*EC$, i.e. $(s^2I - E^*E)C = 0$, and $(s^2I - E^*E)$ is diagonal with all positive entries, so it is invertible and thus $C = 0$. Similarly $s^2B = s(sB^*)^* = s(EC)^* = (sC^*)E^* = BEE^*$, i.e. $B(s^2I - EE^*) = 0$ and $s^2I - EE^*$ is invertible so $B = 0$. Thus M is block diagonal subordinate to the runs of equality in S. □

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