OPTIMALITY OF THE TRACE OF A PRODUCT OF MATRICES

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Abstract

A simple and short proof of the optimality conditions in the John von Neumann trace inequality for singular values is shown. Possible generalizations and special cases are also considered.

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1. Introduction.

Let A and B be $n \times n$ real matrices, then

$$(0.1) \quad -\alpha_1\beta_1 - \dots - \alpha_n\beta_n \leq \text{tr}(AB^T) \leq \alpha_1\beta_1 + \dots + \alpha_n\beta_n$$

where $\alpha_1 \geq \dots \geq \alpha_n$ are the singular values of A , and $\beta_1 \geq \dots \geq \beta_n$ the singular values of B . Here, tr denotes trace of a matrix and T its transpose.

This inequality was first proved by John von Neumann [12] and has important applications in the study of certain equations of nonlinear elasticity [1, 4], numerical analysis [2, 3] and factor analysis [9].

2. Main result.

A short and straightforward proof of the case when the upper and lower bound in (1) are attained will be given. We will find that under this situation, both A and B have simultaneous singular decompositions.

Theorem 1. *Let $A, B \in M_n$. Then $\text{tr}(AB^T) = \alpha_1\beta_1 + \dots + \alpha_n\beta_n$ if and only if there exists $P, Q \in O(n)$ such that $A = PD_AQ$, $B = PD_BQ$, where $D_A = \text{diag}(\alpha_1, \dots, \alpha_n)$, $D_B = \text{diag}(\beta_1, \dots, \beta_n)$, and the singular values are arranged in weakly decreasing order. $O(n)$ denotes the group of $n \times n$ orthogonal matrices.*

Proof : The necessity of the conditions for equality is trivial. Suppose now that $\text{tr}(AB^T) = \alpha_1\beta_1 + \dots + \alpha_n\beta_n$, and let $R_{ij}(\theta)$ be a rotation matrix, that is, an identity matrix apart from elements $\cos\theta, \sin\theta, -\sin\theta, \cos\theta$ in positions (i, i) , (i, j) , (j, i) and (j, j) , respectively. Then, since $\sup_{R \in O(n)} \text{tr}(RAB^T) = \alpha_1\beta_1 + \dots + \alpha_n\beta_n$, $\text{tr}(R_{ij}(\theta)AB^T)$ achieves a maximum at $\theta = 0$.

$$\text{tr}(R_{ij}(\theta)AB^T) = c_{ii}\cos\theta - c_{ij}\sin\theta + c_{ji}\sin\theta + c_{jj}\cos\theta + \sum_{k \neq i, j} c_{kk}$$

where $C = AB^T = (c_{ij})$. Thus, its derivative with respect to θ vanishes at $\theta = 0$, and this implies that $c_{ij} = c_{ji}$. Consequently, AB^T is symmetric, and since $\text{tr}(AB^T) = \text{tr}(B^TA)$, B^TA is also symmetric. By the singular value decomposition for real matrices, there exist $P_1, Q_1 \in O(n)$ such that

$P_1 A Q_1 = \text{diag}(\alpha_1, \dots, \alpha_n) = D_A$. We may assume that the α_i are arranged in weakly decreasing order.

$$\text{tr}(AB^T) = \text{tr}(P_1 A Q_1 Q_1^T B^T P_1^T) = \text{tr}(D_A Q_1^T B^T P_1^T)$$

Thus, without loss of generality we can assume that A is diagonal. $D_A Q_1^T B^T P_1^T$ and $Q_1^T B^T P_1^T D_A$ are symmetric. We claim that $Q_1^T B^T P_1^T$ is diagonal. Call $X = (x_{ij}) = Q_1^T B^T P_1^T$. Then the symmetry of $D_A Q_1^T B^T P_1^T$ implies that $\alpha_i x_{ij} = \alpha_j x_{ji}$ and $x_{ij} \alpha_j = x_{ji} \alpha_i$ is obtained from the symmetry of $Q_1^T B^T P_1^T D_A$. Hence, $(\alpha_i^2 - \alpha_j^2) x_{ij} = 0$ for all i, j . If $\alpha_i^2 \neq \alpha_j^2$ for $i \neq j$, then $x_{ij} = 0$. So, if D_A^2 has distinct diagonal elements, then X must be diagonal. Because the diagonal elements of X are $\pm$ the singular values of B we conclude that $X = Q_1^T B^T P_1^T = \text{diag}(\pm \beta_{\pi(1)}, \dots, \pm \beta_{\pi(n)})$ with π a permutation of $1, \dots, n$. In the case where D_A^2 has nondistinct diagonal elements $X = Q_1^T B^T P_1^T$ splits as a direct sum of blocks $X = \text{diag}(X_1, \dots, X_k)$ corresponding to $D_A = \text{diag}(\alpha_1 I_1, \dots, \alpha_k I_k)$ with $\alpha_1 > \alpha_2 > \dots > \alpha_{k-1} > \alpha_k \geq 0$. Here, each I_i is an identity matrix. A simultaneous block diagonal similarity of D_A and X , with orthogonal diagonal blocks permits us to take $X_1, \dots, X_k$ to be diagonal. Thus, $\text{tr}(AB^T) = \text{tr}(D_A X) = \sum_1^n \alpha_i (\pm \beta_{\pi(i)})$, but $\text{tr}(AB^T) = \sum_1^n \alpha_i \beta_i$, therefore $A = P_1 D_A Q_1$ and $Q_1^T B^T P_1^T = D_B$, that is, $A = P_1 D_A Q_1$ and $B = P_1 D_B Q_1$.

The same proof with minor changes works for the lower bound. We have that a necessary and sufficient condition for equality is also a simultaneous singular value decomposition for A and B .

Theorem 2. *Let $A, B \in M_n$. Then $\text{tr}(AB^T) = -\alpha_1 \beta_1 - \dots - \alpha_n \beta_n$ if and only if there exists $P, Q \in O(n)$ such that $A = P D_A Q$, $B = P D_B Q$ where $D_A = \text{diag}(\alpha_1, \dots, \alpha_n)$, $D_B = \text{diag}(\beta_1, \dots, \beta_n)$, and the singular values are arranged in weakly decreasing order. $O(n)$ denotes the group of $n \times n$ orthogonal matrices.*

3. Comments.

3.1. If we replace $\text{tr}(AB^T)$ by $\text{tr}(AB)$ in the theorem we do not have a simultaneous singular decomposition for A and B , but we have from the proof of the theorem that AB and BA are symmetric.

3.2. Fan [6] extended the trace inequality to more than two matrices. The trace of a finite product of matrices is less than or equal to the sum of the products of the corresponding singular values of the factors when these are arranged in weakly decreasing order. It is not possible to extend the optimal result shown here to more than two matrices. As an example, consider the matrices

$$A = \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}, B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, C = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Then $\text{tr}(ABC) = 1$, and the sum of the products of the singular values is also 1, but AB and AC are not symmetric.

3.3. The optimality of (1) was studied by Kiers and Ten Berge [8] and their proof was strongly dependent on a result by Friedland [7]. According to de Sá [5] this optimality is hidden in the original von Neumann's proof of (1), but this is not that simple. Lewis [10] studied (1) under Lie theoretical terms.

3.4. In the case where the matrices are symmetric positive semidefinite, the singular values in (1) are replaced by eigenvalues. Theobald [11] used the structure of doubly stochastic matrices to give a proof of the optimality in this case. Our proof also works to produce:

Corollary 1. *If A and B are symmetric positive semidefinite matrices the inequality (1) becomes*

$$\text{tr}(AB) \leq \alpha_1\beta_1 + \dots + \alpha_n\beta_n$$

where the alpha and beta are now the eigenvalues of A and B respectively. In this case the upper bound is attained if and only if there exists $P \in O(n)$ such that $A = PD_AP^T$ and $B = PD_BP^T$, that is, A and B have simultaneous spectral decompositions.

3.5. It is not possible to extend the trace inequality in the real symmetric case to more than two matrices as Fan did it in the arbitrary case. For instance, consider the matrices

$$A = \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}, B = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}, C = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Then $\text{tr}(ABC) = -10$, but the sum of the product of the eigenvalues is -14 .

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