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# A trace bound for integer-diagonal positive semidefinite matrices

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**Abstract:** We prove that an $n$-by-$n$ complex positive semidefinite matrix of rank $r$ whose graph is connected, whose diagonal entries are integers, and whose non-zero off-diagonal entries have modulus at least one, has trace at least $n + r - 1$.

**Keywords:** positive semidefinite matrices, integer-diagonal, trace

**MSC:** 15B48, 15A15, 05C50

## 1 Introduction

The graph of an $n$-by-$n$ Hermitian matrix $M = (m_{ij})$ has vertex set $\{1, 2, \dots, n\}$ and edge set $\{ij \mid i < j, m_{ij} \neq 0\}$. As part of their work on the Schur-Siegel-Smyth problem for totally positive algebraic integers, James McKee and Pavlo Yatsyna [3] proved that an $n$-by-$n$ positive definite matrix $S$ whose entries are integers and whose graph is connected must have trace at least $2n - 1$. As a consequence, 2 is the smallest limit point of the absolute trace (which for an $n$-by-$n$ matrix is the trace divided by $n$) of such matrices.

The integer entries are important to McKee and Yatsyna's proof: since $S$ is positive definite, it can be factored as $S = B^{\mathrm{T}}B$, and thus viewed as the Gram matrix of the columns $x_1, x_2, \dots, x_n$ of $B$. In a minimal-trace connected counterexample, we can assume without loss of generality that $x_1$ is a unit vector. Then the Gram matrix of $x_1, x_2', x_3, \dots, x_n$, where $x_2' = x_2 - (x_1^{\mathrm{T}}x_2)x_1$, still has integer entries and eventually provides a contradiction.

Are the integer entries necessary? In this note, we prove a generalization for complex positive semidefinite matrices and show that while the diagonal entries must be integers, the off-diagonal non-zero entries need only have modulus at least 1. A generalization of McKee and Yatsyna's absolute trace result follows as a corollary.

In addition to standard tools and definitions from matrix analysis [2] and graph theory [1], one fact we will use repeatedly is that, because the sum of a positive definite matrix and a positive semidefinite matrix is still positive definite, adding a positive number to a diagonal entry of a positive definite matrix results in another positive definite matrix. Also note that an empty graph on a single vertex is connected.

## 2 New Results

**Lemma 1.** An $n$-by-$n$ complex positive definite matrix whose graph is a tree, whose diagonal entries are integers, and whose non-zero off-diagonal entries have modulus at least one, has trace at least $2n - 1$.

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*Proof.* Proceed by induction on $n$, noting the result is true for $n = 1$. Assume that the result is true for all $k$-by-$k$ matrices where $1 \le k < n$, and let $M = (m_{ij})$ be an $n$-by-$n$ positive definite matrix whose graph is a tree with vertices labeled $v_1, v_2, \dots, v_n$ corresponding to the rows of $M$. Assume for the sake of eventual contradiction that the trace of $M$, $\operatorname{tr} M$, is less than $2n - 1$.

Since the graph $G$ of $M$ is a tree, it has a pendant vertex (a vertex of degree one). Without loss of generality, we can assume vertex $v_1$ has unique neighbor $v_2$. If the diagonal element $m_{11}$ of $M$ is greater than 1, then applying the induction hypothesis to $M_{11}$, the matrix obtained from $M$ by deleting the first row and column, yields $\operatorname{tr} M \ge 2 + \operatorname{tr} M_{11} \ge 2 + 2(n-1) - 1 = 2n - 1$, a contradiction. So we may assume $m_{11} = 1$. Since $v_1$ is pendant,

$$M = \begin{bmatrix} 1 & \overline{\alpha} e_1^* \\ \alpha e_1 & M_{11} \end{bmatrix},$$

where $\alpha$ is a complex number with $|\alpha| \ge 1$ and $e_1$ is the standard basis vector.

Consider next the Schur complement $M' = M_{11} - |\alpha|^2 e_1 e_1^{\mathrm{T}}$, which is an $(n-1)$-by-$(n-1)$ positive definite matrix. All off-diagonal elements of $M'$ remain unchanged from the corresponding entries of $M$, so the graph of $M'$ is a tree. All main-diagonal elements of $M'$ also remain unchanged with the exception of $m'_{11} = m_{22} - |\alpha|^2 \le m_{22} - 1$.

Since $m'_{11}$ may not be an integer, let $M''$ be the matrix obtained from $M'$ by replacing $m'_{11}$ with $m''_{11} = m_{22} - 1$. Since $m''_{11} \ge m'_{11}$, $M''$ is also positive definite. Further, its graph is a tree, its diagonal entries are integers, and its non-zero off-diagonal entries have modulus at least one. Finally, $\operatorname{tr} M'' = \operatorname{tr} M - 2 < 2n - 3$, a contradiction of the induction hypothesis. Thus $\operatorname{tr} M \ge 2n - 1$. □

**Theorem 1.** An $n$-by-$n$ complex positive definite matrix whose graph is connected, whose diagonal entries are integers, and whose non-zero off-diagonal entries have modulus at least one, has trace at least $2n - 1$.

*Proof.* Proceed by induction on $n$, noting the result is true for $n = 1$. Assume that the result is true for all $k$-by-$k$ matrices where $1 \le k \le n - 1$, and let $M$ be an $n$-by-$n$ positive definite matrix whose diagonal entries are integers, whose graph is connected, and whose non-zero off-diagonal entries have modulus at least one.

Assume for the sake of eventual contradiction that $\operatorname{tr} M < 2n - 1$. By adding to a diagonal entry if needed, we can assume that we have a matrix $M$ with the above-mentioned properties and with $\operatorname{tr} M = 2n - 2$.

Let $G$ be the graph of $M$ and let $m_v$ be the diagonal entry of $M$ corresponding to vertex $v$ in $G$. For each vertex $v$ of $G$, let $c(v)$ be the number of connected components of $G \setminus v$.

Suppose first that there is a vertex $v$ of $G$ such that $m_v > c(v)$. Consider $M(v)$, the matrix obtained from $M$ by removing the row and column corresponding to $v$. Applying the induction hypothesis to the principal submatrices $M_1, M_2, \dots, M_{c(v)}$ of $M(v)$ corresponding to the connected components $C_1, C_2, \dots, C_{c(v)}$ of $G \setminus v$, we find that

$$\begin{aligned} \operatorname{tr} M = m_v + \operatorname{tr} M(v) &= m_v + \sum_{i=1}^{c(v)} \operatorname{tr} M_i \\ &\ge m_v + \sum_{i=1}^{c(v)} (2|C_i| - 1) = m_v - c(v) + 2(n-1) \ge 2n - 1. \end{aligned}$$

Thus we must have that $m_v \le c(v)$ for each vertex $v$.

Let $T$ be a spanning tree of $G$. Since $T$ is a tree on $n$ vertices, it has $n - 1$ edges, and so

$$\sum_{v \in G} d_T(v) = 2(n-1)$$

where $d_T(v)$ is the degree of the vertex $v$ in $T$. Since $d_T(v) \ge c(v) \ge m_v$ for each $v$ but

$$\sum_{v \in G} d_T(v) = 2(n-1) = \operatorname{tr} M = \sum_{v \in G} m_v,$$

we must have $d_T(v) = c(v) = m_v$ for each $v$.

For any vertex $v$ of $G$, because $d_T(v) = c(v)$, there is a bijective correspondence between the neighbors of $v$ in $T$ and the connected components of $G \setminus v$. Thus, if vertices $v_i$ and $v_j$ are not adjacent in $T$, then they belong to different connected components of $G \setminus w$ for any vertex $w$ on a path between them in $T$, and so are not adjacent in $G$ either. So, in fact, $G = T$, and Lemma 1 requires $\operatorname{tr} M \geq 2n - 1$, contradicting our earlier assumption. Thus $\operatorname{tr} M \geq 2n - 1$. □

**Corollary 1.** The smallest limit point of the set of absolute traces of matrices satisfying the conditions of Theorem 1 is 2.

**Remark.** The matrices $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, $\begin{bmatrix} 1.0 & 0.5 \\ 0.5 & 1.0 \end{bmatrix}$, and $\begin{bmatrix} 1.1 & 1.0 \\ 1.0 & 1.1 \end{bmatrix}$ show that none of the conditions of Theorem 1 can be removed.

**Theorem 2.** An $n$-by-$n$ complex positive semidefinite matrix of rank $r$ whose graph is connected, whose diagonal entries are integers, and whose non-zero off-diagonal entries have modulus at least one, has trace at least $n + r - 1$.

*Proof.* Proceed by induction on the nullity. The nullity zero case is Theorem 1. Assume the result is true for all nullities less than some $k > 0$. Let $M$ be an $n$-by-$n$ complex positive semidefinite matrix of nullity $k = n - r$ whose graph is connected, whose diagonal entries are integers, and whose non-zero off-diagonal entries have modulus at least one.

Consider $M$ as the Gram matrix of linearly dependent vectors $x_1, x_2, \dots, x_n$ in $\mathbb{C}^n$. Let $l$ be such that $x_l$ is in the span of the other vectors, and let $y$ be a unit vector in $\mathbb{C}^n$ orthogonal to each $x_i$. Then the Gram matrix $M'$ of $x_1, x_2, \dots, x_{l-1}, x_l + y, x_{l+1}, \dots, x_n$ is equal to $M$ except for an increase of 1 in the $m_{ll}$ main-diagonal element, so its graph is connected, its diagonal entries are integers, and the non-zero off-diagonal entries have modulus at least one. The nullity of $M'$ is $k - 1$, so by the induction hypothesis and by construction, $\operatorname{tr} M = \operatorname{tr} M' - 1 \geq (n + (r + 1) - 1) - 1 = n + r - 1$. □

**Corollary 2.** An $n$-by-$n$ complex positive semidefinite matrix of rank $r$ whose graph has $s$ connected components, whose diagonal entries are integers, and whose non-zero off-diagonal entries have modulus at least one, has trace at least $n + r - s$.

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