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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 $1 \leq k < n$, 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 $\operatorname{tr} M \geq 2 + \operatorname{tr} M_{11} \geq 2 + 2(n-1) - 1 = 2n - 1$, 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 α is a complex number with $|\alpha| \geq 1$ 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 $m'_{11} = m_{22} - |\alpha|^2 \leq m_{22} - 1$.

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 $m''_{11} \geq m'_{11}$, 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 $\operatorname{tr} M \geq 2n - 1$. □

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 $1 \leq k \leq n - 1$, 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

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

Thus we must have that $m_v \leq c(v)$ 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 $d_T(v) \geq c(v) \geq m_v$ 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 $x_1, x_2, \ldots, x_n$ 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 $x_1, x_2, \ldots, x_{l-1}, x_l + y, x_{l+1}, \ldots, x_n$ 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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