Doubly stochastic matrices of trees

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Abstract

In this paper, we obtain sharp upper and lower bounds for the smallest entries of doubly stochastic matrices of trees and characterize all extreme graphs which attain the bounds. We also present a counterexample to Merris’ conjecture on relations between the smallest entry of the doubly stochastic matrix and the algebraic connectivity of a graph in [R. Merris, Doubly stochastic graph matrices II, Linear Multilinear Algebra. 45 (1998) 275–285].

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1. Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$ and edge set $E(G)$. Let $A(G)$ be the $n \times n$ adjacency matrix whose $(i, j)$-entry is 1 if $(v_i, v_j) \in E$ and 0 otherwise. Let $D(G)$ be the diagonal matrix whose $(i, i)$-entry is $d(v_i)$, the degree of the vertex $v_i$. The matrix $L(G) = D(G) - A(G)$ is called the Laplacian matrix of $G$. It is obvious that $L(G)$ is singular and semipositive. Thus, its eigenvalues can be arranged as $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G) = 0$. The second smallest eigenvalue $\lambda_{n-1}(G)$, also denoted $\alpha(G)$, is known as the algebraic connectivity of $G$ (see [2, 3]). It is well known that $\alpha(G) > 0$ if and only if $G$ is connected (see [4]). Let $I_n$ be the identity matrix.
The matrix $\Omega(G) = (I_n + L(G))^{-1}$ is called the doubly stochastic matrix of $G$, which was introduced in [5] (also see [1,6,7]). It is easy to see that $\Omega(G)$ is a doubly stochastic matrix (e.g., see [7]). Denote the smallest entry of $\Omega(G) = (\omega_{ij})$ by $\omega(G) = \min\{\omega_{ij}; 1 \leq i, j \leq n\}$. In the study of relations between the smallest entry of this doubly stochastic matrix and the algebraic connectivity, Merris in [1] proposed the following two conjectures.

**Conjecture 1.1.** Let $G$ be a graph on $n$ vertices. Then

$$\alpha(G) \geq 2(n + 1)\omega(G).$$

**Conjecture 1.2.** Let $E_n$ be the degree anti-regular graph, that is, the unique connected graph whose vertex degrees attain all values between $1$ and $n - 1$. Then

$$\omega(E_n) = \frac{1}{2(n + 1)}.$$

Berman and Zhang in [8] confirmed Conjecture 1.2. In this paper, we first give upper and lower bounds for the smallest entry of the doubly stochastic matrix of a tree. Furthermore, we characterize all extreme graphs that attain these bounds. Finally, we conclude this paper with a counterexample to Conjecture 1.1.

2. Main result

The main result of this paper is the following

**Theorem 2.1.** Let $T$ be a tree of order $n$ and $\omega(T)$ be the smallest entry of $\Omega(T)$. Then

$$\frac{\sqrt{5}}{\left(\frac{3 + \sqrt{5}}{2}\right)^n} \leq \omega(T) \leq \frac{1}{2(n + 1)}$$

with right equality if and only if $T$ is a star and left equality if and only if $T$ is a path.

In order to prove Theorem 2.1, we need a notion and some lemmas. A vertex of degree 1 is called a pendent vertex.

**Lemma 2.2.** Let $T'$ be a tree of order $n \geq 4$ with at least three pendent vertices, say, $v_1, v_2, v_n$. Let $v_3$ be the neighbor of $v_2$. Let $T''$ be the tree obtained from $T'$ by deleting the edge $(v_2, v_3)$ and adding an edge $(v_1, v_2)$. Let $\Omega(T') = (\omega'_{ij})$ and $\Omega(T'') = (\omega''_{ij})$. Then $v_2$ and $v_n$ are pendent vertices in $T''$ and

$$\omega'_{1n} > \omega''_{2n}.$$

**Proof.** Clearly, $v_2$ and $v_n$ are pendent vertices in $T''$. Let $F$ be the forest of order $n$ obtained from $T'$ by deleting the edge $(v_2, v_3)$. Let $\Omega(F) = (\omega_{ij})$ and $x_i$ be the $i$-th component. Let $x = x_2 - x_3$ and $y = x_2 - x_1$. Then (see, e.g. [1])

$$\Omega(T') = (I_n + L(T'))^{-1} = ((I_n + L(F)) + xx^T)^{-1} = \Omega(F) - \frac{\Omega(F)xx^T \Omega(F)}{1 + x^T \Omega(F)x}.$$

Hence because $\Omega(F)$ is symmetric,

$$\omega'_{ij} = \omega_{ij} - \frac{(\omega_{i2} - \omega_{i3})(\omega_{j2} - \omega_{j3})}{1 + \omega_{22} - 2\omega_{23} + \omega_{33}}.$$
By an analogous argument, we have
\[
\omega''_i = \omega_{ij} - \frac{(\omega_{j2} - \omega_{j1})(\omega_{j2} - \omega_{j1})}{1 + \omega_{22} - 2\omega_{21} + \omega_{11}}.
\]

On the other hand, by the definition of \( \Omega(F) \), we have \( \omega_{21} = \omega_{23} = \omega_{31} = 0 \) and \( \omega_{22} = 1 \). Therefore
\[
\omega'_{1n} = \omega_{1n} - \frac{\omega_{13}\omega_{3n}}{2 + \omega_{33}}, \quad \omega'_{13} = \frac{2\omega_{13}}{2 + \omega_{33}},
\]
\[
\omega'_{2n} = \frac{2\omega_{2n}}{2 + \omega_{33}}, \quad \omega''_{2n} = \frac{\omega_{2n}}{2 + \omega_{11}}.
\]

Then by the above equations, we have
\[
\omega'_{1n} - \omega''_{2n} = \omega'_{1n} - \frac{\omega_{1n}}{2 + \omega_{11}}
\]
\[
= \omega'_{1n} - \frac{1}{2 + \omega_{11}} \left( \omega'_{1n} + \frac{\omega_{13}\omega_{3n}}{2 + \omega_{33}} \right)
\]
\[
= \omega'_{1n} - \frac{1}{2 + \omega_{11}} \left( \omega'_{1n} + \frac{\omega'_{13}\omega_{3n}}{2} \right)
\]
\[
= \frac{(1 + \omega_{11})\omega'_{1n} - \omega'_{13}\omega_{3n}}{2 + \omega_{11}}
\]
\[
= \frac{(1 + \omega_{11})\omega'_{1n} - \omega'_{13}\omega_{3n}(2 + \omega_{11})}{4(2 + \omega_{11})}.
\]

Let \( t \) be the first common vertex between the path \( P_{n1} \) from \( v_n \) to \( v_1 \) and the path \( P_{31} \) from \( v_3 \) to \( v_1 \) in \( T' \). If \( t = 3 \), then by Theorem 3.2 in [9], we have
\[
\omega'_{1n} = \frac{\omega'_{13}\omega_{3n}}{\omega_{33}}.
\]

Hence
\[
\omega'_{1n} - \omega''_{2n} = \frac{\omega'_{13}\omega_{3n}(4(1 + \omega_{11}) - \omega'_{33}(2 + \omega_{33}))}{4\omega_{33}'(2 + \omega_{11})} > 0,
\]
since \( \omega'_{33} < 1 \) and \( 4(1 + \omega_{11}) - \omega'_{33}(2 + \omega_{33}) > 4 - (2 + \omega_{33}) > 0 \). If \( t \neq 3 \), then by Theorem 3.2 in [9], we have
\[
\omega'_{1n} = \frac{\omega'_{13}\omega_{3n}}{\omega_{21}}, \quad \omega'_{3n} = \frac{\omega'_{3n}\omega_{1n}}{\omega_{1t}}, \quad \omega'_{13} = \frac{\omega'_{13}\omega_{13}}{\omega_{1t}}.
\]

Therefore
\[
\omega'_{1n} - \omega''_{2n} = \frac{\omega'_{1n}\omega_{1n}'[4\omega_{1n}'(1 + \omega_{11}) - (\omega'_{13})^2(2 + \omega_{33})]}{4(\omega_{1n})^2(2 + \omega_{11})} > 0,
\]
since \( 1 > \omega'_{1n} > \omega'_{13} \) by Theorem 2 in [1]. □

**Lemma 2.3.** Let \( T \) be a path of order \( n \). Then
\[
\omega(T) = \sqrt{3} \left( \frac{3 + \sqrt{5}}{2} \right)^n - \left( \frac{3 - \sqrt{5}}{2} \right)^n.
\]
Proof. Let $T$ be the path $v_1 \cdots v_n$. By Theorem 3.2 in [9] and Theorem 2 in [1], we have
\[ \omega_{1n} = \frac{\omega_{1i} \omega_{ij} \omega_{jn}}{\omega_{ij} \omega_{jj}} \leq \omega_{ij} \]
for $1 \leq i < j \leq n$. Hence $\omega(T) = \omega_{1n}$. Using the equality $\Omega(T)(I_n + L(T)) = I_n$ and some calculations, it is not difficult to see that the result holds. \qed

Lemma 2.4. Let $T$ be a tree of order $n \geq 3$. Then
\[ \omega(T) \leq \frac{1}{2(n + 1)} \]
with equality if and only if $T$ is a star $K_{1,n-1}$.

Proof. If $n \leq 5$, by a simple calculation, it is easy to see that the result holds. Hence we assume that $n \geq 6$. If $T$ is not a star, then by Corollary 4.5 in [10], the algebraic connectivity $\alpha(T)$ of $T$, $\alpha(T) < 0.49$. Further by equation (11) in [1], we have
\[ n\omega(T) \leq \frac{\alpha(T)}{1 + \alpha(T)} < \frac{0.49}{1 + 0.49}. \]
Hence $\omega(T) < \frac{1}{2n+1}$. On the other hand, by [8], $\omega(K_{1,n-1}) = \frac{1}{2(n+1)}$. \qed

Now we are ready to present a proof of Theorem 2.1.

Proof of Theorem 2.1. Let $T$ be a tree of order $n$. If $T$ has only two pendent vertices, then $T$ must be a path. Hence we may assume that $T$ has at least three pendent vertices and $\omega_{1n} = \min\{\omega_{ij}, 1 \leq i, j \leq n\}$. Then $v_1$ and $v_n$ must be two pendent vertices. In fact, suppose that $v_1$ is not a pendent vertex, then there exists a pendent vertex $v_i$, $1 < i < n$ such that there is a path $P_{ni}$ from $v_n$ to $v_i$ throughout vertex $v_1$. By Theorem 3.2 in [9], $\omega_{ni} = \frac{\omega_{1n}}{\omega_{ij}} < \omega_{1n}$. Since $\omega_{11} > \omega_{ii}$ and $\Omega(T)$ is symmetric, this is impossible. Therefore $v_1$ is a pendent vertex. By a similar argument, $v_n$ is also a pendent vertex. Moreover, there exists another pendent vertex, say, $v_2$ and $(v_2, v_3) \in E(T)$. Let $T'$ be the tree obtained from $T$ by deleting the edge $(v_2, v_3)$ and adding an edge $(v_1, v_2)$. Let $\Omega(T') = (\omega'_{ij})$. By Lemma 2.2, $\omega_{1n} > \omega'_{2n}$. Moreover, $v_2$ and $v_n$ are pendent vertices in $T'$. Further, by repeated use of Lemma 2.2, we can get a tree $T''$ with exactly two pendent vertices $v_2, v_{n-1}$, that is, $T''$ is a path, which satisfies $\omega_{1n} > \omega'_{2n} > \cdots > \omega''_{n-1,n}$. Hence left inequality holds in Theorem 2.1. The right inequality in Theorem 2.1 follows from Lemma 2.4. So we finish the proof of Theorem 2.1. \qed

At the end of this paper, we present an example to illustrate that Conjecture 1.1 is not true.

Example 2.5. Let $T$ be the tree of order 7 as in Fig. 1.
Then the eigenvalues of $L(T)$ are 5.2618, 3.3399, 1, 1, 1, 0.3983, 0. Moreover,

$$\Omega(T) = \begin{bmatrix}
0.5789 & 0.0789 & 0.0789 & 0.1579 & 0.0526 & 0.0263 & 0.0263 \\
0.0789 & 0.5789 & 0.0789 & 0.1579 & 0.0526 & 0.0263 & 0.0263 \\
0.0789 & 0.0789 & 0.5789 & 0.1579 & 0.0526 & 0.0263 & 0.0263 \\
0.1579 & 0.0789 & 0.1579 & 0.3158 & 0.1053 & 0.0526 & 0.0526 \\
0.0526 & 0.0526 & 0.0526 & 0.1053 & 0.3684 & 0.1842 & 0.1842 \\
0.0263 & 0.0263 & 0.0263 & 0.0526 & 0.1482 & 0.5921 & 0.0921 \\
0.0263 & 0.0263 & 0.0263 & 0.0526 & 0.1482 & 0.0921 & 0.5921 \\
0.0263 & 0.0263 & 0.0263 & 0.0526 & 0.1482 & 0.0921 & 0.5921
\end{bmatrix}.$$ 

Hence $\alpha(T) = 0.3983 < 2 \times (7 + 1) \times 0.0263 = 2(n + 1)\omega(T)$.

References