

ORDERING TREES BY THE MINIMAL ENTRIES OF THEIR DOUBLY STOCHASTIC GRAPH MATRICES*

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Abstract. Given an n -vertex graph G , the matrix $\Omega(G) = (I_n + L(G))^{-1} = (\omega_{ij})$ is called the doubly stochastic graph matrix of G , where I_n is the $n \times n$ identity matrix and $L(G)$ is the Laplacian matrix of G . Let $\underline{\omega}(G)$ be the smallest element of $\Omega(G)$. Zhang and Wu [X.D. Zhang and J.X. Wu. Doubly stochastic matrices of trees. *Appl. Math. Lett.*, 18:339–343, 2005.] determined the tree T with the minimum $\underline{\omega}(T)$ among all the n -vertex trees. In this paper, as a continuance of the Zhang and Wu's work, we determine the first $\lceil \frac{n-1}{2} \rceil$ trees $T_1, T_2, \dots, T_{\lceil \frac{n-1}{2} \rceil}$ such that $\underline{\omega}(T_1) < \underline{\omega}(T_2) < \dots < \underline{\omega}(T_{\lceil \frac{n-1}{2} \rceil}) \leq \underline{\omega}(T_{\lceil \frac{n-1}{2} \rceil}) < \underline{\omega}(T)$, where T_i is obtained by attaching a pendant vertex to v_i of path $P_{n-1} = v_1 v_2 \cdots v_i \cdots v_{n-1}$ and T is an n -vertex tree different from the trees $T_1, T_2, \dots, T_{\lceil \frac{n-1}{2} \rceil}$.

Key words. Tree, Doubly stochastic graph matrix, Pendant vertex.

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1. Introduction. Let $G = (V_G, E_G)$ be a simple graph with vertex set V_G and the edge set E_G . Let $\deg_G(v_i)$ or d_i be the degree of vertex v_i and $D(G) = \text{diag}(d_1, d_2, \dots, d_n)$. Let $A(G)$ be the $n \times n$ adjacency matrix whose (i, j) -entry is 1 if $v_i v_j \in E_G$ and 0 otherwise. The matrix $L(G) = D(G) - A(G)$ is called the Laplacian matrix of G , which may be dated back to Kirchhoff's Matrix-Tree Theorem and has been extensively studied for the past fifty years (e.g., see [15, 19] and the references therein). It is well known that $L(G)$ is positive semidefinite and singular. Thus, its eigenvalues can be arranged as $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{n-1} \geq \lambda_n = 0$. The second smallest eigenvalue λ_{n-1} , also denoted by $\alpha(G)$, is known as the algebraic connectivity of G ; see [10, 15]. It follows from Kirchhoff's Matrix-Tree Theorem that $\lambda_{n-1} > 0$ if and only if G is connected. Since the algebraic connectivity is relevant to important problems regarding the diameter of graphs, the expanding properties of graphs, the combinatorial optimization problems, and the theory of elasticity, etc. (for example, see [18, 19]), it has received much more attention. Recently, there is an excellent survey on algebraic connectivity of graphs written by de Abreu [1], which is referred to the reader for further information.

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In the study of chemical information processing, Golender et al. [11] introduced another important matrix: doubly stochastic graph matrix associated with a graph, which may be used to describe some properties of the topological structure of chemical molecules. Let I_n be the $n \times n$ identity matrix and $\Omega(G) = (I_n + L(G))^{-1} = (\omega_{ij})$. It can be verified that $\Omega(G)$ is a doubly stochastic matrix (see, for example, [11]). Thus, $\Omega(G)$ is called the *doubly stochastic graph matrix*. In [20] Pereira and Vali studied the spectra of doubly stochastic matrices. On the other hand, Chebotarev and Shamis [6] and Chebotarev [5] pointed out that the doubly stochastic graph matrix may be used to measure the proximity among vertices and evaluate the group cohesion in the construction of sociometric indices and represent a random walk. In particular, the diagonal entries ω_{ii} of $\Omega(G)$ measure the peripheralness (solitariness) of v_i [6]. An important result on the relationship between the entry of the doubly stochastic matrix of a graph and its number of spanning forests, which is called the matrix forest theorem (1995) (see Refs. [7, 8]), is due to Chebotarev and Shamis. Shamis presented the result at the 1995 International Linear Algebra Society (ILAS) Conference in Atlanta (see Ref. [9]), and a proof of an earlier version of this theorem can be found in [21]. Moreover, Merris [17] established the relationship between the entry ω_{ij} of $\Omega(G)$ and structure of the simple n -vertex graph G : If $\omega_{ij} < 4/(n^2 + 4n)$, then v_i is not adjacent to v_j . Moreover, ω_{ij} is also relative to the weights of routes of various lengths between v_i and v_j (see [6], Proposition 10). Zhang [23] determined a sharp lower bound for the smallest entries, among those corresponding to edges, of doubly stochastic matrices of trees. Zhang [24] also presented some relations between the diameter of a tree and the smallest entry $\underline{\omega}(G) = \min\{\omega_{ij} : 1 \leq i, j \leq n\}$. Recently, Zhang [25] studied the relationship between vertex degrees and entries of the doubly stochastic graph matrix.

Zhang and Wu [22] obtained sharp upper and lower bounds for the smallest entries of doubly stochastic matrices of trees and characterized all extreme graphs which attain the bounds. Motivated by these related results, we investigate the property of the smallest entries of doubly stochastic matrices of graphs. We identify the first $\lceil \frac{n-1}{2} \rceil$ n -vertex trees according to their smallest entries in the corresponding doubly stochastic matrices:

$$\underline{\omega}(T_1) < \underline{\omega}(T_2) < \cdots < \underline{\omega}\left(T_{\lfloor \frac{n-1}{2} \rfloor}\right) \leq \underline{\omega}\left(T_{\lceil \frac{n-1}{2} \rceil}\right) < \underline{\omega}(T),$$

where T_i is obtained by attaching a pendant vertex to v_i of path $P_{n-1} = v_1 v_2 \cdots v_i \cdots v_{n-1}$ and T is an n -vertex tree different from the trees $T_1, T_2, \dots, T_{\lceil \frac{n-1}{2} \rceil}$.

2. Preliminaries. We define $\varpi(G) = \max\{\omega_{ii} : 1 \leq i \leq n\}$. A *dominating vertex* of G is a vertex of degree $n - 1$, i.e., a vertex adjacent to every other vertex. We call v a *pendant vertex*, if $\deg_G(v) = 1$. For convenience, let $PV(G)$ be the set of all pendant vertices of G , and we set $\mathcal{T}_{n,k} = \{T : T \text{ is an } n\text{-vertex tree with } k \text{ pendant}$

vertices}. The *distance* between vertices u and v in G is denoted by $d_G(u, v)$. Let $N_G(v) = \{w \in V_G | vw \in E_G\}$. Clearly, $\deg_G(v) = |N_G(v)|$.

We first give some lemmas that will be used in the proofs of our main results.

LEMMA 2.1 ([17]). *Let G be a graph with doubly stochastic graph matrix $\Omega(G) = (\omega_{ij})$. If $r \neq s$, then $\omega_{rr} \geq 2\omega_{rs}$, with equality if v_r is a dominating vertex of the connected component of G that contains v_s , or if $\deg_G(v_s) = 1$ and $v_r v_s \in E_G$.*

LEMMA 2.2 ([25]). *Let G be a simple connected graph on n vertices with doubly stochastic graph matrix $\Omega(G) = (\omega_{ij})$. Then*

$$\overline{\omega}(G) \leq \frac{\phi^{2n-1} + \phi^{1-2n}}{\phi^{2n} - \phi^{-2n}}$$

with equality if and only if G is a path on n vertices, where $\phi = \frac{\sqrt{5}+1}{2}$.

LEMMA 2.3. *Let P_n be a path on n vertices with doubly stochastic matrix $\Omega(P_n) = (\omega_{ij})$. Then*

$$\omega_{11} > \omega_{22} > \cdots > \omega_{\lfloor \frac{n}{2} \rfloor \lfloor \frac{n}{2} \rfloor} \geq \omega_{\lceil \frac{n}{2} \rceil \lceil \frac{n}{2} \rceil},$$

the last equality holds if and only if n is even.

Proof. This result immediately follows from Theorem 1 in [5] and the main theorem in [2]. \square

LEMMA 2.4 ([24]). *Let T be a tree of order n with vertex set $V_T = \{v_1, v_2, \dots, v_n\}$. If $\underline{\omega}(T) = \min\{\omega_{ij} : 1 \leq i, j \leq n\} = \omega_{kl}$, then the following hold:*

- (i) v_k and v_l are two pendant vertices.
- (ii) *If the diameter d of T is no more than 4, then $d_G(v_k, v_l) = d$.*

LEMMA 2.5 ([23]). *Let T be a tree of order $n \geq 4$ with at least three pendant vertices, say, v_1, v_2, v_n . Suppose that $v_3 \in N_T(v_2)$ and $T' = T - v_2 v_3 + v_1 v_2$. Let $\Omega(T) = (\omega_{ij})$ and $\Omega(T') = (\omega'_{ij})$. Then $\omega_{1n} > \omega'_{2n}$.*

COROLLARY 2.6. *Let $T \in \mathcal{T}_{n,k}$ be a tree such that $\underline{\omega}(T)$ is as small as possible, where $n \geq 4$ and $k \geq 3$ are fixed. Suppose that $\underline{\omega}(T) = \omega_{1n}$, v_2 is a pendant vertex of T different from v_1, v_n and $v_3 \in N_T(v_2)$, then we have $\deg_T(v_3) > 2$.*

Proof. Suppose to the contrary that $\deg_T(v_3) = 2$. Since $\underline{\omega}(T) = \omega_{1n}$ by Lemma 2.4(i), we have that $v_1, v_n \in PV(T)$. Let

$$T' = T - v_2 v_3 + v_1 v_2.$$

Then $T' \in \mathcal{T}_{n,k}$ with doubly stochastic graph matrix $\Omega(T') = (\omega'_{ij})$. By Lemma 2.5,

we obtain

$$\underline{\omega}(T') \leq \omega'_{2n} < \omega_{1n} = \underline{\omega}(T).$$

A contradiction to the choice of T . \square

COROLLARY 2.7. *For any tree $T \in \mathcal{T}_{n,k+1}$, there exists a tree $T' \in \mathcal{T}_{n,k}$ such that $\underline{\omega}(T) > \underline{\omega}(T')$, where $n \geq 4$, $k \geq 2$.*

Proof. Choose $T \in \mathcal{T}_{n,k+1}$ such that $\underline{\omega}(T)$ is as small as possible. Assume that $\underline{\omega}(T) = \omega_{1n}$, then $v_1, v_n \in PV(T)$. Note that $k \geq 2$. Let v_2 be a pendant vertex of T different from v_1, v_n and $v_3 \in N_T(v_2)$. Then, by Corollary 2.6, we have $\deg_T(v_3) > 2$. Let

$$T' = T - v_2v_3 + v_1v_2.$$

Then $T' \in \mathcal{T}_{n,k}$ with doubly stochastic graph matrix $\Omega(T') = (\omega'_{ij})$. By Lemma 2.5, we obtain

$$\underline{\omega}(T') \leq \omega'_{2n} < \omega_{1n} = \underline{\omega}(T).$$

Thus, for any tree $T \in \mathcal{T}_{n,k+1}$, there exists a tree $T' \in \mathcal{T}_{n,k}$ such that $\underline{\omega}(T) > \underline{\omega}(T')$, as desired. \square

3. Main results. Let G be a simple graph obtained from graph G^* by attaching k pendant vertices to a vertex of G^* ; see Fig. 3.1. Then we characterize the $\underline{\omega}(G)$ by the entries of $\Omega(G^*)$.

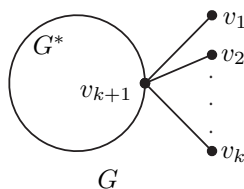


FIG. 3.1. Graph G .

THEOREM 3.1. *Let G be a graph of order n , which has $k \geq 1$ pendant vertices v_1, \dots, v_k attached to the same vertex v_{k+1} of G^* (see Fig. 3.1). Let $\Omega(G) = (\omega_{ij})$ for $1 \leq i, j \leq n$ and $\Omega(G^*) = (\omega^*_{ij})$ for $k+1 \leq i, j \leq n$. Then the smallest entry of $\Omega(G)$ satisfies*

$$\underline{\omega}(G) = \min \left\{ \omega^*_{ij} - \frac{k\omega^*_{i,k+1}\omega^*_{k+1,j}}{2 + k\omega^*_{k+1,k+1}}, \frac{\omega^*_{k+1,j}}{2 + k\omega^*_{k+1,k+1}} \right\}.$$

Proof. Let

$$\mathbf{x} = \left(\overbrace{-\frac{1}{\sqrt{k}} \cdots -\frac{1}{\sqrt{k}}}^k \sqrt{k} \ 0 \ \cdots \ 0 \right)^T.$$

Then $\Omega(G) = (I_n + L(G))^{-1} = (F + \mathbf{x}\mathbf{x}^T)^{-1}$ with

$$F = \begin{pmatrix} K & \mathbf{0} \\ \mathbf{0} & I_{n-k} + L(G^*) \end{pmatrix},$$

where

$$K = \begin{pmatrix} \frac{2k-1}{k} & -\frac{1}{k} & \cdots & -\frac{1}{k} \\ -\frac{1}{k} & \frac{2k-1}{k} & \cdots & -\frac{1}{k} \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{k} & -\frac{1}{k} & \cdots & \frac{2k-1}{k} \end{pmatrix}.$$

Hence, we have

$$F^{-1} = \begin{pmatrix} K^{-1} & \mathbf{0} \\ \mathbf{0} & \Omega(G^*) \end{pmatrix} = \left(\begin{array}{cccc|cccc} \frac{k+1}{2k} & \frac{1}{2k} & \cdots & \frac{1}{2k} & & & & \\ \frac{1}{2k} & \frac{k+1}{2k} & \cdots & \frac{1}{2k} & & & & \\ \vdots & \vdots & \ddots & \vdots & & & & \\ \frac{1}{2k} & \frac{1}{2k} & \cdots & \frac{k+1}{2k} & & & & \\ \hline & & & & \omega_{k+1,k+1}^* & \cdots & \omega_{k+1,n}^* & \\ & & & & \vdots & \ddots & \vdots & \\ & & & & \omega_{n,k+1}^* & \cdots & \omega_{nn}^* & \end{array} \right).$$

By the Sherman–Morrison formula (see [13, p 19]), we have

$$\Omega(G) = F^{-1} - \frac{F^{-1}\mathbf{x}\mathbf{x}^T F^{-1}}{1 + \mathbf{x}^T F^{-1}\mathbf{x}}.$$

Note that $1 + \mathbf{x}^T F^{-1}\mathbf{x} = 2 + k\omega_{k+1,k+1}^*$ and

$$\begin{aligned} F^{-1}\mathbf{x}\mathbf{x}^T F^{-1} &= \left(\overbrace{-\frac{1}{\sqrt{k}} \cdots -\frac{1}{\sqrt{k}}}^k \sqrt{k}\omega_{k+1,k+1}^* \cdots \sqrt{k}\omega_{n,k+1}^* \right)^T \\ &\quad \times \left(\overbrace{-\frac{1}{\sqrt{k}} \cdots -\frac{1}{\sqrt{k}}}^k \sqrt{k}\omega_{k+1,k+1}^* \cdots \sqrt{k}\omega_{n,k+1}^* \right). \end{aligned}$$

Hence, we have

$$\omega_{ij} = \begin{cases} \frac{1}{2k} - \frac{1}{k(2+k\omega_{k+1,k+1}^*)}, & \text{if } i \neq j \leq k; \\ \omega_{ij}^* - \frac{k\omega_{i,k+1}^*\omega_{k+1,j}^*}{2+k\omega_{k+1,k+1}^*}, & \text{if } i \neq j \geq k+1; \\ \frac{\omega_{k+1,j}^*}{2+k\omega_{k+1,k+1}^*}, & \text{if } i \leq k < j \end{cases} \quad (3.1)$$

and

$$\omega_{ii} = \begin{cases} \frac{k+1}{2k} - \frac{1}{k(2+k\omega_{k+1,k+1}^*)}, & \text{if } i \leq k; \\ \omega_{ii}^* - \frac{k\omega_{i,k+1}^{*2}}{2+k\omega_{k+1,k+1}^*}, & \text{if } i \geq k+1. \end{cases} \quad (3.2)$$

By Lemma 2.1, it is straightforward to check that $\frac{1}{2k} - \frac{1}{k(2+k\omega_{k+1,k+1}^*)} > \frac{\omega_{k+1,j}^*}{2+k\omega_{k+1,k+1}^*}$ for $k \geq 1$, and hence

$$\underline{\omega}(G) = \min \left\{ \omega_{ij}^* - \frac{k\omega_{i,k+1}^*\omega_{k+1,j}^*}{2+k\omega_{k+1,k+1}^*}, \frac{\omega_{k+1,j}^*}{2+k\omega_{k+1,k+1}^*} \right\}.$$

This completes the proof. \square

COROLLARY 3.2. *Let G be a simple connected graph on n vertices with doubly stochastic graph matrix $\Omega(G) = (\omega_{ij})$. If v_1 is a pendant vertex of G and $v_1v_i \in E_G$, then*

$$\omega_{ii} \leq \frac{2\overline{\omega}(P_{n-1})}{2 + \overline{\omega}(P_{n-1})}$$

with equality if and only if G is a path on n vertices.

Proof. Let $G^* = G - v_1v_i$ with doubly stochastic graph matrix $\Omega(G^*) = (\omega_{ij}^*)$ for $2 \leq i, j \leq n$. By Lemma 2.2, we have $\omega_{ii}^* \leq \overline{\omega}(P_{n-1})$ with equality if and only if G^* is a path on $n-1$ vertices and v_i is a pendant vertex of G^* . Therefore, by Eq. (3.2) in Theorem 3.1, we have

$$\omega_{ii} = \omega_{ii}^* - \frac{\omega_{ii}^{*2}}{2 + \omega_{ii}^*} = \frac{1}{\frac{1}{\omega_{ii}^*} + \frac{1}{2}} \leq \frac{1}{\frac{1}{\overline{\omega}(P_{n-1})} + \frac{1}{2}} = \frac{2\overline{\omega}(P_{n-1})}{2 + \overline{\omega}(P_{n-1})}$$

with equality if and only if G^* is a path on $n-1$ vertices and v_i is a pendant vertex of G^* , which is equivalent to that G is a path on n vertices. \square

COROLLARY 3.3. *For any P_i , we have*

- (i) $\underline{\omega}(P_{i+1}) = \frac{\underline{\omega}(P_i)}{2 + \overline{\omega}(P_i)}$ and $\overline{\omega}(P_{i+1}) = \frac{1 + \overline{\omega}(P_i)}{2 + \overline{\omega}(P_i)}$, where $i = 1, 2, \dots, n-1$.
- (ii) $\overline{\omega}^2(P_i) + \overline{\omega}(P_i) - \underline{\omega}^2(P_i) - 1 = 0$, where $i = 1, 2, \dots, n-1$.

Proof. By Theorem 1 in [5], $\underline{\omega}(P_i) = \Phi_{2i}^{-1}$ and $\overline{\omega}(P_i) = \frac{\Phi_{2i-1}}{\Phi_{2i}}$, where Φ_k are the Fibonacci numbers. This yields (i) and, using Cassini's identity, (ii). \square

Let T_i (see Fig. 3.2) be the tree on n vertices obtained from a path $P_{n-1} = v_1 v_2 \cdots v_i \cdots v_{n-1}$ by attaching a new pendant vertex v_n at v_i .

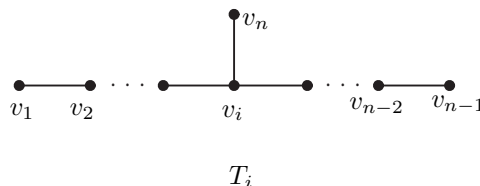


FIG. 3.2. Graph T_i .

THEOREM 3.4. Let T_i ($i = 1, 2, \dots, \lceil \frac{n-1}{2} \rceil$) be a tree of order n , which is depicted in Fig. 3.2, then we have

$$\underline{\omega}(T_1) < \underline{\omega}(T_2) < \cdots < \underline{\omega}(T_{\lfloor \frac{n-1}{2} \rfloor}) \leq \underline{\omega}(T_{\lceil \frac{n-1}{2} \rceil})$$

with equality if and only if n is odd.

Proof. Let \mathbf{x}_i be an n dimensional vector whose only nonzero component is 1 in the i th position and $\mathbf{x} = \mathbf{x}_n - \mathbf{x}_i$. Thus, $L(T_i) = L(F) + \mathbf{x}\mathbf{x}^T$. Let $\Omega(T_i) = (\omega_{ij})$ and $\Omega(P_{n-1}) = (\omega'_{ij})$. By the Sherman-Morrison formula (see, e.g. [13, p 19]), we have

$$\Omega(T_i) = \Omega(F) - \frac{\Omega(F)\mathbf{x}\mathbf{x}^T\Omega(F)}{1 + \mathbf{x}^T\Omega(F)\mathbf{x}}.$$

By Lemma 2.4(i), we have $\underline{\omega}(T_i) = \min\{\omega_{1,n-1}, \omega_{1n}, \omega_{n-1,n}\}$. Note that

$$\begin{aligned} \omega_{1n} &= \frac{\omega_{1i}\omega_{in}}{\omega_{ii}} = \frac{\omega_{1i}}{2} > \frac{\omega_{1i}\omega_{i,n-1}}{\omega_{ii}} = \omega_{1,n-1}, \\ \omega_{n-1,n} &= \frac{\omega_{n-1,i}\omega_{in}}{\omega_{ii}} = \frac{\omega_{n-1,i}}{2} > \frac{\omega_{1i}\omega_{i,n-1}}{\omega_{ii}} = \omega_{1,n-1}. \end{aligned}$$

Hence, we obtain

$$\underline{\omega}(T_i) = \omega_{1,n-1} = \omega'_{1,n-1} - \frac{\omega'_{1i}\omega'_{i,n-1}}{2 + \omega'_{ii}} = \omega'_{1,n-1} - \frac{\omega'_{1,n-1}\omega'_{ii}}{2 + \omega'_{ii}} = \frac{2\omega'_{1,n-1}}{2 + \omega'_{ii}} = \frac{2\underline{\omega}(P_{n-1})}{2 + \omega'_{ii}}.$$

By Lemma 2.3, we have $\underline{\omega}(T_1) < \underline{\omega}(T_2) < \cdots < \underline{\omega}(T_{\lfloor \frac{n-1}{2} \rfloor}) \leq \underline{\omega}(T_{\lceil \frac{n-1}{2} \rceil})$ with equality if and only if $n - 1$ is even, which is equivalent to that n is odd. \square

THEOREM 3.5. Let $T \in \mathcal{T}_{n,4}$ and $T_i \in \mathcal{T}_{n,3}$ where T_i ($i = 1, 2, \dots, \lceil \frac{n-1}{2} \rceil$) is depicted in Fig. 3.2, then we have $\underline{\omega}(T_i) < \underline{\omega}(T)$.

Proof. Let $T \in \mathcal{T}_{n,4}$ with doubly stochastic graph matrix $\Omega(T) = (\omega_{ij})$, such that $\underline{\omega}(T)$ is as small as possible. By Corollary 2.6, we obtain that $T \in \{\hat{T}_1, \hat{T}_2, \hat{T}_3\}$; see Fig. 3.3. In what follows, if two graphs, say G and H , are *isomorphic* graphs, then we write $G \cong H$.

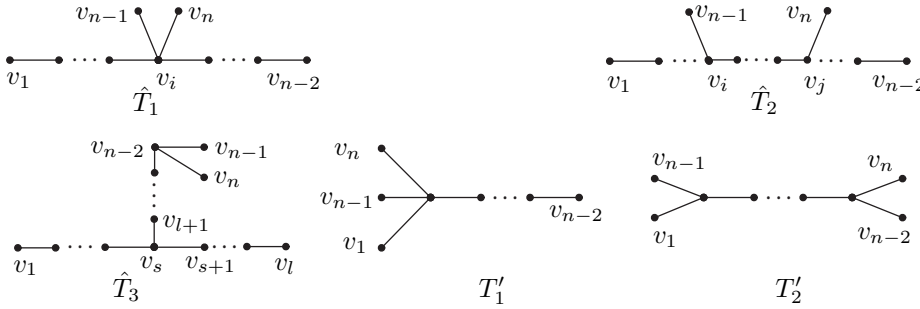


FIG. 3.3. Graphs $\hat{T}_1, \hat{T}_2, \hat{T}_3, T'_1$ and T'_2 .

If $T \cong \hat{T}_1$, then $T - v_i v_{n-1} - v_i v_n \cong P_{n-2}$. Let $\Omega(P_{n-2}) = (\omega'_{pq})$. By Theorem 3.1, [14, Theorem 3.2], and Lemma 2.3, we have

$$\begin{aligned} \underline{\omega}(T) &= \omega_{1,n-2} = \omega'_{1,n-2} - \frac{2\omega'_{1i}\omega'_{i,n-2}}{2 + 2\omega'_{ii}} = \omega'_{1,n-2} - \frac{\omega'_{ii}\omega'_{1,n-2}}{1 + \omega'_{ii}} \\ &= \frac{\omega'_{1,n-2}}{1 + \omega'_{ii}} \geq \frac{\omega'_{1,n-2}}{1 + \omega'_{22}} = \underline{\omega}(T'_1). \end{aligned}$$

If $T \cong \hat{T}_2$, then $T - v_j v_n \cong T_i$. Let $\Omega(T_i) = (\omega''_{ij})$. By Theorem 3.1 and [14, Theorem 3.2], we have

$$\underline{\omega}(T) = \omega_{1,n-2} = \omega''_{1,n-2} - \frac{\omega''_{1i}\omega''_{i,n-2}}{2 + \omega''_{ii}} = \omega''_{1,n-2} - \frac{\omega''_{ii}\omega''_{1,n-2}}{2 + \omega''_{ii}} = \frac{2\omega''_{1,n-2}}{2 + \omega''_{ii}}.$$

Since $\omega''_{ii} = \omega'_{ii} - \frac{\omega'^2_{ij}}{2 + \omega'_{jj}}$, $\omega''_{1,n-2} = \frac{2\omega'_{1,n-2}}{2 + \omega'_{jj}}$ and $\omega'_{ij} = \frac{\omega'_{ii}\omega'_{jj}\omega'_{1,n-2}}{\omega'_{1i}\omega'_{j,n-2}}$, together with Lemma 2.1, [14, Theorem 3.2], and Lemma 2.3, we obtain

$$\begin{aligned} \underline{\omega}(T) &= \frac{4\omega'_{1,n-2}}{4 + 2\omega'_{ii} + 2\omega'_{jj} + \omega'_{ii}\omega'_{jj} - \omega'^2_{ij}} = \frac{4\omega'_{1,n-2}}{4 + 2\omega'_{ii} + 2\omega'_{jj} + \omega'_{ii}\omega'_{jj} - \left(\frac{\omega'_{ii}\omega'_{jj}\omega'_{1,n-2}}{\omega'_{1i}\omega'_{j,n-2}}\right)^2} \\ &\geq \frac{4\omega'_{1,n-2}}{4 + 2\omega'_{ii} + 2\omega'_{jj} + \omega'_{ii}\omega'_{jj} - \left(\frac{4\omega'_{1i}\omega'_{j,n-2}\omega'_{1,n-2}}{\omega'_{1i}\omega'_{j,n-2}}\right)^2} \\ &= \frac{4\omega'_{1,n-2}}{4 + 2\omega'_{ii} + 2\omega'_{jj} + \omega'_{ii}\omega'_{jj} - 16\omega'^2_{1,n-2}} \\ &\geq \frac{4\omega'_{1,n-2}}{4 + 2\omega'_{22} + 2\omega'_{n-3,n-3} + \omega'_{22}\omega'_{n-3,n-3} - 16\omega'^2_{1,n-2}} = \underline{\omega}(T'_2). \end{aligned}$$

If $T \cong \hat{T}_3$, let $T_s^* = T - v_i v_{n-1} - v_i v_n$ and $\Omega(T_s^*) = (\omega_{pq}^*)$. Then $T_s^* \in \mathcal{T}_{n-2,3}$ and $\underline{\omega}(P_{n-2}) < \omega_{pq}^* \leq 1$ for $1 \leq p, q \leq n-2$. By Theorem 3.1, [14, Theorem 3.2], Lemma 2.1, and Corollary 3.2, we have

$$\begin{aligned} \underline{\omega}(T) &= \omega_{1l} = \omega_{1l}^* - \frac{2\omega_{1,n-2}^* \omega_{n-2,l}^*}{2 + 2\omega_{n-2,n-2}^*} \\ &= \omega_{1l}^* - \frac{\frac{\omega_{1s}^* \omega_{s,n-2}^*}{\omega_{ss}^*} \frac{\omega_{s,n-2}^* \omega_{sl}^*}{\omega_{ss}^*}}{1 + \omega_{n-2,n-2}^*} = \omega_{1l}^* \left[1 - \frac{\omega_{s,n-2}^{*2}}{(1 + \omega_{n-2,n-2}^*) \omega_{ss}^*} \right] \\ &\geq \omega_{1l}^* \left[1 - \frac{\omega_{s,n-2}^*}{2(1 + \omega_{n-2,n-2}^*)} \right] > \omega_{1l}^* \left(1 - \frac{\omega_{n-2,n-2}^*}{1 + \omega_{n-2,n-2}^*} \right) = \frac{\omega_{1l}^*}{1 + \omega_{n-2,n-2}^*} \\ &> \frac{\underline{\omega}(P_{n-2})}{1 + \omega_{n-2,n-2}^*} \geq \frac{\underline{\omega}(P_{n-2})}{2}. \end{aligned}$$

For $1 \leq i \leq \lceil \frac{n-1}{2} \rceil$, by Theorem 3.1 and Corollary 3.3, we get

$$\underline{\omega}(T_i) = \frac{2\omega'_{1,n-1}}{2 + \omega'_{ii}} = \frac{2\underline{\omega}(P_{n-1})}{2 + \omega'_{ii}} = \frac{2}{2 + \omega'_{ii}} \frac{\underline{\omega}(P_{n-2})}{2 + \overline{\omega}(P_{n-2})} < \frac{\underline{\omega}(P_{n-2})}{2}.$$

Therefore, $\underline{\omega}(T_i) < \underline{\omega}(T)$ for any tree $T \cong \hat{T}_3$. Furthermore, note that

$$\begin{aligned} \underline{\omega}(T_i) &= \frac{2}{2 + \omega'_{ii}} \frac{\underline{\omega}(P_{n-2})}{2 + \overline{\omega}(P_{n-2})} = \frac{2}{2 + \omega'_{ii}} \frac{\underline{\omega}(P_{n-3})}{5 + 3\overline{\omega}(P_{n-3})} \\ &= \frac{2}{2 + \omega'_{ii}} \frac{\underline{\omega}(P_{n-4})}{13 + 8\overline{\omega}(P_{n-4})}, \\ \underline{\omega}(T'_1) &= \frac{\omega'_{2,n-2}}{2 + 3\omega'_{22}} = \frac{\underline{\omega}(P_{n-3})}{2 + 3\overline{\omega}(P_{n-3})} = \frac{\underline{\omega}(P_{n-4})}{7 + 5\overline{\omega}(P_{n-4})}, \\ \underline{\omega}(T'_2) &= \frac{\omega'_{2,n-2}}{2 + 2\omega'_{22}} = \frac{\frac{\underline{\omega}(P_{n-4})}{2 + 2\overline{\omega}(P_{n-4})}}{2 + 2 \left[\overline{\omega}(P_{n-4}) - \frac{2\underline{\omega}^2(P_{n-4})}{2 + 2\overline{\omega}(P_{n-4})} \right]} \\ &= \frac{\underline{\omega}(P_{n-4})}{4[\overline{\omega}(P_{n-4}) + \underline{\omega}(P_{n-4}) + 1][\overline{\omega}(P_{n-4}) - \underline{\omega}(P_{n-4}) + 1]} \\ &= \frac{\underline{\omega}(P_{n-4})}{8 + 4\overline{\omega}(P_{n-4})}, \end{aligned}$$

and hence it is easy to obtain $\underline{\omega}(T_i) < \underline{\omega}(T'_2) < \underline{\omega}(T'_1)$ for $\underline{\omega}(P_{n-4}) < \overline{\omega}(P_{n-4}) < 1$. Thus, $\underline{\omega}(T_i) < \underline{\omega}(T)$, where $T \in \mathcal{T}_{n,4}$ and $i = 1, 2, \dots, \lceil \frac{n-1}{2} \rceil$. \square

Our last main result of this paper is to generalize [22, Theorem 2.1]. We identify the first $\lceil \frac{n-1}{2} \rceil$ trees on n vertices according to their smallest entries in the corresponding doubly stochastic matrices.

THEOREM 3.6. *Let T be a tree of order n . If $T \not\cong T_i$, where T_i ($i = 1, 2, \dots$),*

$\lceil \frac{n-1}{2} \rceil$) is depicted in Fig. 3.2, then we have

$$\underline{\omega}(T_1) < \underline{\omega}(T_2) < \cdots < \underline{\omega}\left(T_{\lfloor \frac{n-1}{2} \rfloor}\right) \leq \underline{\omega}\left(T_{\lceil \frac{n-1}{2} \rceil}\right) < \underline{\omega}(T)$$

with equality if and only n is odd.

Proof. Theorem 3.6 follows directly from Corollary 2.7, Theorem 3.4, and Theorem 3.5. This completes the proof. \square

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