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ON THE LARGEST EIGENVALUE OF THE DISTANCE MATRIX OF A TREE

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Abstract

The largest eigenvalue Λ_1 of the distance matrix of a tree has been proposed as a structure–descriptor. We provide upper and lower bounds for Λ_1 in terms of the number of vertices, the sum of the squares of the distances between all unordered pairs of vertices, or the Wiener index of the tree.

INTRODUCTION

Let G be a connected graph with vertex set $\{1, 2, \ldots, n\}$. The distance between vertices i and j of G, denoted by d_{ij}, is defined to be the length (i.e., the number of edges) of the shortest path from i to j. The distance matrix of G, denoted by $D(G)$ is the $n \times n$ matrix with its (i, j)-entry equal to d_{ij}, $i, j = 1, 2, \ldots, n$. Note that $d_{ii} = 0$, $i = 1, 2, \ldots, n$.

The Wiener index $W(G)$ of a connected graph G is the sum of distances between all unordered pairs of vertices in the graph [1]. The hyper–Wiener index $WW(G)$

can be written as $WW(G) = \frac{1}{2}W(G) + \frac{1}{2}S$, where S is the sum of the squares of the distances between all unordered pairs of vertices in the graph [2]. If T is a tree on n vertices, then [3]

$$(n-1)(2n-3) \leq S \leq \frac{1}{12}(n+1)n^2(n-1) \tag{1}$$

with left (right) equality if and only if T is the n-vertex star S_n (the n-vertex path P_n) .

Let T be a tree with $n \geq 2$ vertices and let $\Lambda_1, \Lambda_2, \ldots, \Lambda_n$ be the eigenvalues of $D = D(T)$ arranged in non-increasing order. Merris [4] obtained an interlacing inequality involving the distance and Laplacian eigenvalues of T :

$$0 > -\frac{2}{\mu_1} \geq \Lambda_2 \geq -\frac{2}{\mu_2} \geq \Lambda_3 \geq \cdots \geq -\frac{2}{\mu_{n-1}} \geq \Lambda_n\,,$$

where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > 0 = \mu_n$ are the Laplacian eigenvalues of T, while the Laplacian eigenvalues are connected with the Wiener index [5]:

$$W(T) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}\,.$$

Balaban *et al.* [6] proposed the use of Λ_1 as a structure–descriptor, and it was successfully used to make inferences about the extent of branching and boiling points of alkanes [6, 7].

Let T be a tree with $n \geq 3$ vertices. Gutman and Medeleanu [7] obtained the following bounds for Λ_1:

$$\sqrt{\frac{1}{2}S + n(n-1)\left(\frac{n-1}{4}\right)^{2/n}} < \Lambda_1 < \sqrt{\frac{n-1}{2}S + n\left(\frac{n-1}{4}\right)^{2/n}}\,. \tag{2}$$

We now provide new bounds for Λ_1 in terms of the number of vertices, the sum of the squares of the distances between all unordered pairs of vertices, or the Wiener index of the tree.

RESULTS

Let T be a tree with $n \geq 2$ vertices. The eigenvalues of D obey the following relations [7]:

$$\sum_{i=1}^{n} \Lambda_i = 0\,, \tag{3}$$

$$\sum_{i=1}^{n} \Lambda_i^2 = 2S\,. \tag{4}$$

In addition, from [8, 9], we have

$$\Lambda_1 > 0,\ \ \Lambda_i < 0 \text{ for } i = 2, \dots, n\,, \tag{5}$$

$$\det D = \Lambda_1 \Lambda_2 \cdots \Lambda_n = (-1)^{n-1}(n-1)2^{n-2}\,. \tag{6}$$

Note that (5) follows also from (3) and Merris' interlacing inequality.

We first present an upper bound for Λ_1.

Theorem 1. *Let T be a tree with $n \geq 3$ vertices. Then*

$$\Lambda_1 < \sqrt{\frac{2(n-1)}{n} S}\,. \tag{7}$$

Proof. By (3) and (5),

$$\Lambda_1 = \sum_{i=2}^{n} |\Lambda_i|\,.$$

By the Cauchy–Schwartz inequality and taking into account (4), we have

$$\left(\sum_{i=2}^{n} |\Lambda_i|\right)^2 \leq (n-1)\sum_{i=2}^{n} \Lambda_i^2 = (n-1)(2S - \Lambda_1^2)$$

with equality if and only if $|\Lambda_2| = \cdots = |\Lambda_n|$. Now it follows that

$$\Lambda_1^2 \leq (n-1)(2S - \Lambda_1^2)\,,$$

i.e.,

$$\Lambda_1 \leq \sqrt{\frac{2(n-1)}{n} S}\,.$$

Suppose equality holds in the inequality above. Then $|\Lambda_2| = \cdots = |\Lambda_n|$. By (3), (5) and (6),

$$\Lambda_1 = (n-1)2^{1-2/n},\ \ \Lambda_2 = \cdots = \Lambda_n = -2^{1-2/n}\,,$$

and so (4) becomes

$$2S = (n-1)^2 2^{2-4/n} + (n-1)2^{2-4/n} = (n-1)n2^{2-4/n}\,.$$

Note that $2S$ is an integer and $n \geq 3$. We have $n = 4$. There are two trees with 4 vertices: S_4 and P_4. By direct calculation, the eigenvalues of the distance matrix of S_4 are $2+\sqrt{7}, 2-\sqrt{7}, -2, -2$, and those of P_4 are $2+\sqrt{10}, 2-\sqrt{10}, -2+\sqrt{2}, -2-\sqrt{2}$. In either case, $\Lambda_1 \neq 3\sqrt{2}$, which is a contradiction. Hence (7) follows. $\square$

Let T be a tree with $n \geq 3$ vertices. By Theorem 1 and the upper bound for S in (1), we have

$$\Lambda_1 < \sqrt{\frac{(n-1)^2 n(n+1)}{6}} < \frac{(n-1)n}{2}\,. \tag{8}$$

Now we give a lower bound for Λ_1.

Theorem 2. *Let T be a tree with at least 3 vertices. Then*

$$\Lambda_1 > \sqrt{S}\,. \tag{9}$$

Proof. From (3), (4) and (5), we have

$$\sum_{1\le i<j\le n} |\Lambda_i||\Lambda_j| > |\sum_{1\le i<j\le n} \Lambda_i \Lambda_j| = S\,.$$

From (3) and (5), we have $2\Lambda_1 = \sum_{i=1}^{n} |\Lambda_i|$, and so

$$4\Lambda_1^2 = \sum_{i=1}^{n} |\Lambda_i|^2 + 2 \sum_{1\le i<j\le n} |\Lambda_i||\Lambda_j| > 4S\,,$$

i.e., $\Lambda_1 > \sqrt{S}$. $\square$

The upper bound (7) is always better than that in (2) when $n \ge 4$, while the lower bound (9) is better than that in (2) if $S > 2n(n-1)\left(\frac{n-1}{4}\right)^{2/n}$.

In the following, more lower bounds for Λ_1 are given.

Theorem 3. *Let T be a tree on $n \ge 3$ vertices. Then*

$$\Lambda_1 > (n-1)2^{1-2/n}\,. \tag{10}$$

Proof By the arithmetic–geometric–mean inequality, we have

$$\frac{\sum_{i=2}^{n} |\Lambda_i|}{n-1} \ge \left(\prod_{i=2}^{n} |\Lambda_i|\right)^{1/(n-1)}$$

with equality only if $|\Lambda_2| = \cdots = |\Lambda_n|$. From $\Lambda_1 = \sum_{i=2}^{n} |\Lambda_i|$ and (6), we have

$$\frac{\Lambda_1}{n-1} \ge \left[\frac{(n-1)2^{n-2}}{\Lambda_1}\right]^{1/(n-1)}.$$

Therefore

$$\Lambda_1 \ge (n-1)2^{1-2/n}\,.$$

Using the same arguments as those in the proof of Theorem 1, equality in the inequality above cannot hold. $\square$

Theorem 4. *Let T be a tree on $n \ge 3$ vertices. Then*

$$\Lambda_1 > \frac{2}{n} W(T)\,. \tag{11}$$

Proof. Note that

$$\Lambda_1 = \sup\left\{\frac{\mathbf{v}^T D\mathbf{v}}{\mathbf{v}^T\mathbf{v}} : \mathbf{v} \neq 0\right\},$$

where $\mathbf{v}$ is a column vector and $\mathbf{v}^T$ is the transpose of $\mathbf{v}$. By setting $\mathbf{v} = \mathbf{1}$, the all 1's vector, we have

$$\Lambda_1 \geq \frac{2}{n}W(T)$$

and equality does not hold since $D\mathbf{1} \neq \Lambda_1\mathbf{1}$ for a tree on $n \geq 3$ vertices. $\square$

There is another way to prove Theorem 4. By Merris' interlacing inequality and the expression for the Wiener index in terms of the Laplacian eigenvalues, we have

$$\sum_{i=2}^{n} |\Lambda_i| \geq 2\sum_{i=2}^{n} \frac{1}{\mu_{i-1}} = \frac{2}{n}W(T).$$

So $\Lambda_1 \geq \frac{2}{n}W(T)$. Suppose that $\Lambda_1 = \frac{2}{n}W(T)$. Then $\Lambda_i = -\frac{2}{\mu_{i-1}}$ for $i = 2, \ldots, n$. Note [10, p. 39] that $\prod\limits_{i=1}^{n-1} \mu_i = n$. In view of (6), we have $\Lambda_1 = \frac{1}{2}n(n-1)$, a contradiction to (8) for $n \geq 3$. Hence (11) follows.

Since $W(T) \geq (n-1)^2$, we have from Theorem 4 that $\Lambda_1 > 2(n-1)\left(1 - \frac{1}{n}\right)$ for $n \geq 3$.

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