



Note

The minimal Laplacian spectral radius of trees with diameter 4 [☆]

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ABSTRACT

We determine the trees with the minimal Laplacian spectral radius with diameter 4, which settles a conjecture posed by Liu et al. (2009) [5].

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1. Introduction

Throughout this paper all graphs considered are finite, connected and simple. Graph theoretical terms used but not defined can be found in [1].

Let $G = (V, E)$ be a graph with vertex set $V = \{v_1, \dots, v_n\}$ and edge set E . For $v \in V$, let $d(v)$ denote the degree of v and $N(v)$ denote the set of all neighbors of v . The diameter of G is the maximum distance between any two vertices of G . The Laplacian matrix of G is $L(G) = D(G) - A(G)$, where $D(G) = \text{diag}(d(v_1), \dots, d(v_n))$ is the degree diagonal matrix of G and $A(G)$ is the adjacency matrix of G . It is well known that $L(G)$ is positive semidefinite and singular. Its eigenvalues can be arranged as $\mu_1(G) \geq \dots \geq \mu_n(G) = 0$. The largest eigenvalue $\mu_1(G)$ is called the *Laplacian spectral radius* of G . Recent researches show that the Laplacian spectral radius of trees plays an important role in theoretical chemistry [2,3].

Let $\mathcal{T}_{n,d}$ be the set of trees on n vertices with diameter d . Guo [4] determined the first $\lfloor d/2 \rfloor + 1$ Laplacian spectral radii of trees in the set $\mathcal{T}_{n,d}$ for $3 \leq d \leq n - 3$. Liu et al. [5] characterized trees with the minimal Laplacian spectral radii in the set $\mathcal{T}_{n,d}$, where $d \in \{1, 2, 3, n - 3, n - 2, n - 1\}$, they also considered the case $d = 4$ and proposed *Conjecture 1* on the basis of a computer simulation.

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Fig. 1. $T^*(7, 2)$ and $T^*(7, 3)$.

For any tree $T \in \mathcal{T}_{n,4}$, T must be obtained from a path $P_5 : v_1 v_2 v_3 v_4 v_5$ by attaching some pendant edges to v_2, v_4 , and some pendant edges or some stars to v_3 , where the centers of stars are adjacent to v_3 . It is clear that the vertex v_3 is the center of the tree T .

Let n, k be integers with $2 \leq k \leq n - 3$. Let $T^*(n, k)$ be the tree on n vertices obtained from the star $K_{1,k}$ by attaching d_i pendant edges to the i th leaf u_i of $K_{1,k}$ for $i = 1, \dots, k$, where $\sum_{i=1}^k d_i = n - k - 1$ and $|d_i - d_j| \leq 1$ for all $1 \leq i < j \leq k$. Clearly, $T^*(n, k) \in \mathcal{T}_{n,4}$.

For $n \geq 2$, let

$$M_n = \frac{\sqrt{4(n-1)-1} + 1}{2}, N_n = \frac{\sqrt{4(n-1)+1} - 1}{2}.$$

Conjecture 1 ([5, Conjecture 11]). For any $T \in \mathcal{T}_{n,4}$, we have

$$\mu_1(T) \geq \mu_1(T^*(n, \lfloor M_n \rfloor)),$$

with the equality if and only if $T \cong T^*(n, \lfloor M_n \rfloor)$.

This conjecture is inaccurate in general. We give an example for the case $n = 7$, then $M_7 \approx 2.9$. However, trees $T^*(7, 2)$ and $T^*(7, 3)$, shown in Fig. 1, have the same Laplacian spectral radii: $\mu_1(T^*(7, 2)) = \mu_1(T^*(7, 3)) = 3 + \sqrt{2}$.

In this paper, we modify the conjecture above by replacing $\lfloor M_n \rfloor$ with $\lceil N_n \rceil$. (In fact, it is not difficult to verify that $\lfloor M_n \rfloor = \lceil N_n \rceil$.) Furthermore, we give a theoretical proof of the following theorem.

Theorem 2. For any $T \in \mathcal{T}_{n,4}$, we have

$$\mu_1(T) \geq \mu_1(T^*(n, \lceil N_n \rceil)).$$

The equality holds if and only if $T \cong T^*(n, \lceil N_n \rceil)$, or $T \cong T^*(n, \lceil N_n \rceil + 1)$ when $N_n \in \mathbb{N}$.

2. Proof of Theorem 2

To prove Theorem 2, we first review some relevant results. Let $X = (x_1, \dots, x_n)^T$ is an eigenvector of G corresponding to $\mu_1(G)$. For each vertex of G ,

$$(d(u) - \mu_1(G))x_u = \sum_{v \in N(u)} x_v, \tag{1}$$

where x_u denotes the component x_i of x if u stands for the vertex v_i of G .

Lemma 1 ([6, p. 220]). Let G be a bipartite graph. Then $Q(G)$ and $L(G)$ are unitarily similar, where $Q(G) = D(G) + A(G)$ is the signless Laplacian matrix of G . In particular, $\mu_1(G)$ is simple.

Lemma 2 ([7, p.149]). Let G be a graph with at least one edge, $\Delta(G)$ be its maximal degree, then $\mu_1(G) \geq \Delta(G) + 1$. Moreover, if G is connected, the equality holds if and only if $\Delta(G) = n - 1$.

Lemma 3 ([8, Lemma 2.9]). Let G be a graph and τ be an automorphism of G . If $\mu_1(G)$ is a simple eigenvalue of $L(G)$ and X is an eigenvector corresponding to $\mu_1(G)$, then $|x_v| = |x_{\tau(v)}|$ for every $v \in V(G)$.

The following result is direct but useful.

Lemma 4. Let $f(x)$ and $g(x)$ be two real polynomials with positive leading coefficients. If $f(x) > g(x)$ for $x \geq \mu_1(g(x))$, then $\mu_1(f(x)) < \mu_1(g(x))$, where $\mu_1(f(x)), \mu_1(g(x))$ is the largest real zero of $f(x), g(x)$, respectively.

In the tree $T^*(n, k)$, denote $a = \max_{1 \leq j \leq k} \{d_j\}$ and $i = |\{j | d_j = a, 1 \leq j \leq k\}|$. Clearly, $a = \lceil \frac{n-k-1}{k} \rceil$ and $n = 1 + ka + i$. We may assume that the vertex u_1, \dots, u_i and u_{i+1}, \dots, u_k has a and $a - 1$ pendant edges, respectively. Let $v_{j,1}, \dots, v_{j,a}$ be pendant vertices adjacent to the vertex $u_j, j = 1, \dots, i$, and $v_{j,1}, \dots, v_{j,a-1}$ adjacent to the vertex $u_j, j = i + 1, \dots, k$.

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