

# Maximizing Spectral Radius of Trees with Given Maximal Degree

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**Abstract** In this paper, we characterize the trees with the largest Laplacian and adjacency spectral radii among all trees with fixed number of vertices and fixed maximal degree, respectively.

**Keywords** trees; maximal degree; Laplacian eigenvalue; adjacency eigenvalue; spectral radius.

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## 1. Introduction

Let  $G = (V, E)$  be a simple graph on vertices  $v_1, v_2, \dots, v_n$ . For each vertex  $v$  of  $G$ , the degree of  $v$ , denoted by  $d_G(v)$  or simply  $d(v)$ , is the number of edges incident with  $v$ . The *adjacency matrix* of the graph  $G$  is defined as  $A(G) = [a_{ij}]$  of order  $n$ , where  $a_{ij} = 1$  if  $v_i$  is adjacent to  $v_j$  and  $a_{ij} = 0$  otherwise. The eigenvalues of  $A(G)$  can be ordered as:

$$\mu_n(G) \leq \mu_{n-1}(G) \leq \dots \leq \mu_1(G).$$

Let  $D(G)$  be the diagonal matrix of vertex degrees of  $G$ , i.e.,  $D(G) = \text{diag}\{d(v_1), d(v_2), \dots, d(v_n)\}$ . The Laplacian matrix of  $G$  is  $L(G) = D(G) - A(G)$ . One can find that  $L(G)$  is a symmetric, positive semidefinite, singular matrix, so that its eigenvalues can be arranged as follows:

$$0 = \lambda_n(G) \leq \lambda_{n-1}(G) \leq \dots \leq \lambda_1(G).$$

We call  $\mu_1(G)$  and  $\lambda_1(G)$  the adjacency spectral radius and Laplacian spectral radius of  $G$ , respectively.

Recently, much attention is focused on the work of ordering trees by some extremely Laplacian or adjacency eigenvalues. Let  $\mathcal{T}(n, d)$  be the set of trees on  $n$  vertices with diameter  $d$ . Kirkland and Neumann<sup>[10]</sup> provided a lower bound on the algebraic connectivity over all such

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trees. Furthermore, Fallat and Kirkland<sup>[2]</sup> determined the trees with the maximum and minimum algebraic connectivity in the set  $\mathcal{T}(n, d)$ , respectively. Guo and Shao<sup>[8]</sup> gave the first  $\lfloor \frac{d}{2} + 1 \rfloor$  adjacency spectral radii of trees in the set  $\mathcal{T}(n, d)$  ( $3 \leq d \leq n - 4$ ); Guo<sup>[9]</sup> gave the first  $\lfloor \frac{d}{2} + 1 \rfloor$  Laplacian spectral radii of trees in the set  $\mathcal{T}(n, d)$  ( $3 \leq d \leq n - 3$ ).

Let  $\mathcal{T}(n, \Delta)$  be the set of trees on  $n$  vertices with given maximal degree  $\Delta$ . Among all trees in  $\mathcal{T}(n, \Delta)$ , Lin and Guo<sup>[11]</sup> characterized the tree which minimizes the adjacency spectral radius, and the tree which maximizes the adjacency spectral radius when  $\Delta \geq \lceil \frac{n-2}{2} \rceil$ . They extend the order of trees on  $n$  vertices by adjacency spectral radius to the 13th tree. With respect to the Laplacian spectral radius, Zhang, Li<sup>[14]</sup> and Guo<sup>[7]</sup> gave the first four trees on  $n$  vertices. Yu et.al.<sup>[13]</sup> determined the fifth to eighth trees in the above ordering.

In this paper, by using vertex valuation and comparing the quadratic form of the adjacency or Laplacian matrix, we give a simple method to determine the trees which maximize the Laplacian (and adjacency) spectral radius among all trees in  $\mathcal{T}(n, \Delta)$ . On maximizing the adjacency spectral radius of trees in  $\mathcal{T}(n, \Delta)$ , our result has no limitation on  $\Delta$ , which extends the result of Lin and Guo<sup>[11]</sup>.

On the other hand, the idea of this paper is different from some known work on ordering trees subject to certain graphic invariant, which usually applies the relation between the characteristic polynomials of the adjacency (Laplacian) matrix of a graph  $G$  and that of some subgraph of  $G$  (or a graph obtained from  $G$  by some operations) to obtain the desired results.

## 2. Lemmas and results

**Lemma 2.1**<sup>[5]</sup> *Let  $G$  be a bipartite graph. Then there exists a diagonal matrix  $D$  such that  $D^{-1}L(G)D = D(G) + A(G)$ .*

The matrix  $D(G) + A(G) =: \bar{L}(G)$  is also called the unoriented Laplacian matrix of  $G$ <sup>[6]</sup>. Since a tree  $T$  is one of bipartite graphs, by Lemma 2.1, the spectral radius of  $L(T)$  equals that of  $\bar{L}(T)$ . So we consider the matrix  $\bar{L}(T)$  instead of  $L(T)$ .

Let  $G = (V, E)$  be a connected graph with  $V = \{v_1, v_2, \dots, v_n\}$  and let  $x = (x_1, x_2, \dots, x_n)^T \in \mathbb{R}^n$  be a nonzero vector. It will be convenient to adopt the following terminology from [4]:  $x$  is said to give a valuation of the vertices of  $V$ , that is, for each vertex  $v_i$  of  $V$ , we associate the value  $x_i$ , i.e.,  $x(v_i) = x_i$ . Then

$$x^T A(G)x = 2 \sum_{v_i v_j \in E} x(v_i)x(v_j), \tag{2.1}$$

$$x^T \bar{L}(G)x = \sum_{v_i v_j \in E} [x(v_i) + x(v_j)]^2. \tag{2.2}$$

As  $A(G)$  is nonnegative, irreducible and symmetric, by the Perron-Frobenius theory,  $\mu_1(G)$  is exactly the spectral radius of  $A(G)$ , and there exists a unique (up to multiples) positive eigenvector, referred to as Perron vector of  $A(G)$ , corresponding to the eigenvalue  $\mu_1(G)$ . In addition,

$$\mu_1(G) = \max_{x, \|x\|=1} 2 \sum_{v_i v_j \in E} x(v_i)x(v_j). \tag{2.3}$$

Similarly,  $\bar{L}(G)$  has a Perron vector corresponding to  $\lambda_1(G)$ , and

$$\lambda_1(G) = \max_{x, \|x\|=1} \sum_{v_i v_j \in E} [x(v_i) + x(v_j)]^2. \quad (2.4)$$

Denote by  $N_G(v)$  or simply  $N(v)$  the set of neighbors of the vertex  $v$  in a graph  $G$ . One can find that  $\mu$  is an eigenvalue of  $A(G)$  corresponding to the eigenvector  $x$  if and only if

$$\mu x(v_i) = \sum_{v_j \in N(v_i)} x(v_j), \quad i = 1, 2, \dots, n; \quad (2.5)$$

and  $\lambda$  is an eigenvalue of  $\bar{L}(G)$  corresponding to the eigenvector  $x$  if and only if

$$[\lambda - d(v_i)]x(v_i) = \sum_{v_j \in N(v_i)} x(v_j), \quad i = 1, 2, \dots, n. \quad (2.6)$$

**Lemma 2.2** *Let  $G$  be a graph on vertices  $v_1, v_2, \dots, v_n$ , with  $x$  as a unit Perron vector of  $\bar{L}(G)$ .*

(i) *If  $x(v_i) \geq x(v_j)$ ,  $v_t v_j \in E(G)$  and  $v_t v_i \notin E(G)$ , let  $G' = G - v_t v_j + v_t v_i$ . Then  $x^T \bar{L}(G')x \geq x^T \bar{L}(G)x$ , and hence  $\lambda_1(G') \geq \lambda_1(G)$ .*

(ii) *If  $[x(v_i) - x(v_t)][x(v_s) - x(v_j)] \geq 0$ , and  $\{v_i v_j, v_s v_t\} \subseteq E(G)$ ,  $v_i v_s \notin E(G)$ ,  $v_j v_t \notin E(G)$ , let  $G' = G - v_i v_j - v_s v_t + v_i v_s + v_j v_t$ . Then  $x^T \bar{L}(G')x \geq x^T \bar{L}(G)x$ , and hence  $\lambda_1(G') \geq \lambda_1(G)$  with equality if and only if  $x(v_i) = x(v_t)$  and  $x(v_j) = x(v_s)$ .*

**Proof** For the result (i), one can find that

$$\begin{aligned} \lambda_1(G) &= x^T \bar{L}(G)x = \sum_{v_i v_j \in E(G)} [x(v_i) + x(v_j)]^2 \quad (\text{using (2.2)}) \\ &= \left( \sum_{v_k v_l \in E(G) - \{v_t v_j\}} [x(v_k) + x(v_l)]^2 \right) + [x(v_t) + x(v_j)]^2 \\ &\leq \left( \sum_{v_k v_l \in E(G) - \{v_t v_j\}} [x(v_k) + x(v_l)]^2 \right) + [x(v_t) + x(v_i)]^2 \\ &= \sum_{v_k v_l \in E(G')} [x(v_k) + x(v_l)]^2 \\ &\leq \max_{x, \|x\|=1} \sum_{v_k v_l \in E(G')} [x(v_k) + x(v_l)]^2 \\ &= \lambda_1(G'). \quad (\text{using (2.4)}) \end{aligned}$$

If  $\lambda_1(G') = \lambda_1(G)$ , then  $x$  is also a Perron vector of  $\bar{L}(G')$ . Applying (2.6) to the vertex  $v_i$  in the graph  $G$  and in the graph  $G'$ , respectively, we have

$$\begin{aligned} [\lambda_1(G) - d_G(v_i)]x(v_i) &= \sum_{v_k \in N_G(v_i)} x(v_k), \\ [\lambda_1(G') - d_{G'}(v_i)]x(v_i) &= \sum_{v_k \in N_{G'}(v_i)} x(v_k). \end{aligned}$$

As  $\lambda_1(G') = \lambda_1(G)$  and  $N_{G'}(v_i) = N_G(v_i) \cup \{v_t\}$ ,

$$x(v_i) = -x(v_t),$$

which is contradictory to that  $x$  is a positive vector. Thus we have proved the result (i).

For the result (ii), by a similar discussion, we have

$$\begin{aligned} \lambda_1(G) &= \sum_{\{v_i, v_j\} \in E} [x(v_i) + x(v_j)]^2 \\ &= \left( \sum_{v_k v_l \in E(G) - \{v_i v_j, v_t v_s\}} [x(v_k) + x(v_l)]^2 \right) + [x(v_i) + x(v_j)]^2 + [x(v_t) + x(v_s)]^2 \\ &\leq \left( \sum_{v_k v_l \in E(G) - \{v_i v_j, v_t v_s\}} [x(v_k) + x(v_l)]^2 \right) + [x(v_i) + x(v_s)]^2 + [x(v_j) + x(v_t)]^2 \\ &= \sum_{v_k v_l \in E(G')} [x(v_k) + x(v_l)]^2 \\ &\leq \lambda_1(G'), \end{aligned}$$

where the first inequality holds as  $[x(v_i) - x(v_t)][x(v_s) - x(v_j)] \geq 0$ .

If  $\lambda_1(G) = \lambda_1(G')$ , then  $x$  is also a Perron vector of  $\bar{L}(G')$ . Applying (2.6) to the vertex  $v_i$  (and the vertex  $v_j$ ) in the graph  $G$  and in the graph  $G'$ , respectively, we get  $x(v_j) = x(v_s)$  (and  $x(v_i) = x(v_t)$ ). Conversely, if  $x$  satisfies that  $x(v_j) = x(v_s)$  and  $x(v_i) = x(v_t)$ , then by (2.6)  $x$  is an eigenvector of  $\bar{L}(G')$  corresponding to the eigenvalue  $\lambda_1(G)$ . As  $x$  is positive, by Perron-Frobenius theory,  $\lambda_1(G)$  is necessarily the spectral radius of  $\bar{L}(G')$ .  $\square$

By (2.1), (2.3), (2.5) and a similar discussion of Lemma 2.2, we have

**Lemma 2.3** *Let  $G$  be a graph on vertices  $v_1, v_2, \dots, v_n$ , with  $x$  as a unit Perron vector of  $A(G)$ .*

(i) *If  $x(v_i) \geq x(v_j)$ ,  $v_t v_j \in E(G)$  and  $v_t v_i \notin E(G)$ , let  $G' = G - v_t v_j + v_t v_i$ . Then  $x^T A(G')x \geq x^T A(G)x$ , and hence  $\mu_1(G') > \mu_1(G)$ .*

(ii) *If  $[x(v_i) - x(v_t)][x(v_s) - x(v_j)] \geq 0$ , and  $\{v_i v_j, v_s v_t\} \subseteq E(G)$ ,  $v_i v_s \notin E(G)$ ,  $v_j v_t \notin E(G)$ , let  $G' = G - v_i v_j - v_s v_t + v_i v_s + v_j v_t$ . Then  $x^T A(G')x \geq x^T A(G)x$ , and hence  $\mu_1(G') \geq \mu_1(G)$  with equality if and only if  $x(v_i) = x(v_t)$  and  $x(v_j) = x(v_s)$ .*

Now we specify a tree  $T^\#(n, \Delta) \in \mathcal{T}(n, \Delta)$  on vertex set  $V = \{v_1, v_2, \dots, v_n\}$ , which can be constructed inductively until the resulting tree has  $n$  vertices. Let  $T_0^\# = \{v_1\}$ . Assume that the tree  $T_k^\#$  ( $k \geq 0$ ) is constructed. The tree  $T_{k+1}^\#$  is obtained from  $T_k$  by joining vertices of  $V - V(T_k^\#)$  with subscripts as small as possible to the pendent vertices of  $T_k^\#$  with subscripts as small as possible such that  $\Delta(T_{k+1}^\#) = \Delta$ , where a vertex of a graph is said pendent if it has degree 1 in that graph. In other words, if  $v_j \in V - V(T_k^\#)$  is adjacent to a pendent vertex  $v_i$  of  $V(T_k^\#)$ , then each vertex  $v_p \in V - V(T_k^\#)$  with  $p < j$  is adjacent to some pendent vertex  $v_q \in V(T_k^\#)$  with  $q \leq i$  such that  $\Delta(T_{k+1}^\#) = \Delta$ . For example, the tree  $T^\#(6, 2), T^\#(15, 3)$  are respectively listed in Figure 1. We adopt the convention that the tree  $T^\#(n, \Delta)$  always has the vertices with subscripts arranged as those in above construction.

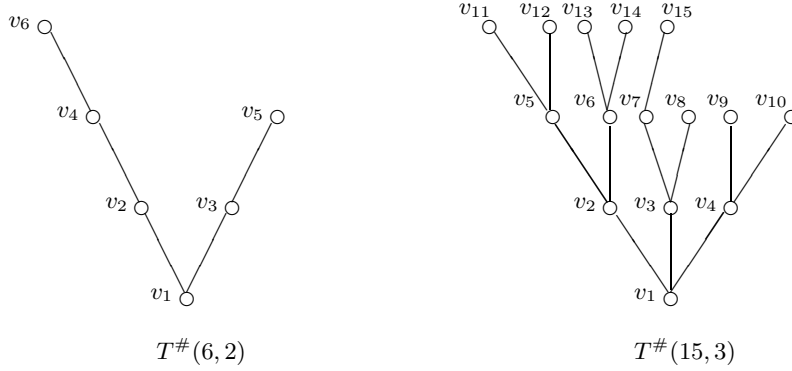


Figure 1 Two trees  $T^\#(6, 2)$  and  $T^\#(15, 3)$

For the class  $T^\#(n, \Delta)$ , if  $\Delta = 1$ , then  $T^\#(n, \Delta)$  contains exactly one tree, i.e., an edge joining two vertices. In the following we assume  $\Delta \geq 2$ .

**Theorem 2.4**  $T^\#(n, \Delta)$  is the unique tree in  $\mathcal{T}(n, \Delta)$  which has the maximal Laplacian spectral radius.

**Proof** Suppose that  $T^* \in \mathcal{T}(n, \Delta)$  has maximal Laplacian spectral radius, which has vertices  $v_1, v_2, \dots, v_n$ . Let  $x$  be the unit Perron vector of  $\bar{L}(T^*)$  such that

$$x(v_1) \geq x(v_2) \geq \dots \geq x(v_n) > 0.$$

We first consider the vertex  $v_1$ , and assert that  $v_1$  has following property.

- (1)  $d(v_1) = \Delta$ .

If  $d(v_1) < \Delta$ , then there exists a vertex  $u$  not adjacent to  $v_1$ , and a path  $P$  joining  $u$  and  $v_1$ . Let  $w$  be the vertex on  $P$  that is adjacent to  $u$ . Deleting the edge  $uw$  and adding the edge  $v_1u$ , we obtain a tree  $T$ . By Lemma 2.2(i),  $\lambda_1(T) > \lambda_1(T^*)$ , a contradiction.

- (2)  $v_1$  is adjacent to  $\Delta$  vertices respectively with values  $x(v_2), \dots, x(v_{\Delta+1})$ , that is,  $v_1$  is adjacent to vertices respectively with the 2nd to the  $(\Delta + 1)$ th largest values of the entries of  $x$ .

If not, then  $v_1$  is adjacent to some vertex  $v_k$  ( $k > \Delta + 1$ ) and is not adjacent to some vertex  $v_t$  ( $t \leq \Delta + 1$ ), and  $x(v_k) < x(v_t)$ . Let  $P$  be a path joining  $v_1$  to  $v_t$ . We divide the discussion into two cases.

**Case 1**  $P$  does not contain  $v_k$ . Let  $w$  be the vertex on  $P$  adjacent to  $v_t$ . Deleting the edges  $v_t w$  and  $v_1 v_k$ , and adding new edges  $v_t v_1$  and  $w v_k$ , we obtain a tree  $T'$ , and by Lemma 2.2(ii),  $\lambda_1(T') > \lambda_1(T^*)$  as  $x(v_k) < x(v_t)$ , a contradiction.

**Case 2**  $P$  contains  $v_k$ . If  $d(v_t) < \Delta$ , deleting the edge  $v_1 v_k$ , and adding a new edge  $v_t v_1$ , we obtain a tree  $T' \in \mathcal{T}(n, \Delta)$ . By Lemma 2.2(i),  $\lambda_1(T') > \lambda_1(T^*)$ , a contradiction. If  $d(v_t) = \Delta (\geq 2)$ , there exists a vertex  $w$  not on  $P$ , which is adjacent to  $v_t$ . Deleting the edges  $v_1 v_k$  and

$v_t w$ , and adding new edges  $v_1 v_t$  and  $w v_k$  to  $T^*$ , then we get a new tree  $T'$ . By Lemma 2.2(ii),  $\lambda_1(T') > \lambda_1(T^*)$  as  $x(v_k) < x(v_t)$ , a contradiction.

Next we consider the vertex  $v_2$ . If  $|V(T^*) - N(v_1) \cup \{v_1\}| \geq \Delta - 1$ , then by a similar discussion to (1) we can prove that  $d(v_2) = \Delta$ , where  $|S|$  denotes the cardinality of a finite set  $S$ . Next we assert that  $v_2$  is adjacent to the vertices (except  $v_1$ ) with the  $(\Delta + 2)$ nd to the  $(2\Delta)$ th largest values of the entries of  $x$ ; otherwise, by a similar discussion to Case 1 or Case 2, there exists a tree with Laplacian spectral radius greater than  $\lambda_1(T^*)$ . If  $|V(T^*) - N(v_1) \cup \{v_1\}| < \Delta - 1$ , then  $v_2$  is adjacent to all vertices of  $V(T) - N(v_1) \cup \{v_1\}$  also by a similar discussion to Case 1 or Case 2.

Continue above procedure inductively. Assume we know  $N(v_k)$  for  $k \geq 2$ . If  $|V(T^*) - \cup_{i=1}^k N(v_i) \cup \{v_1\}| \geq 1$ , then we consider the vertex  $v_{k+1}$  by a similar discussion to  $v_2$ ; otherwise the procedure is finished. We finally find that  $T^*$  is exactly the tree  $T^\#(n, \Delta)$ .  $\square$

By a similar discussion, we have

**Theorem 2.5**  $T^\#(n, \Delta)$  is the unique tree in  $\mathcal{T}(n, \Delta)$  which has the maximal adjacency spectral radius.

From the proof of Theorem 2.4, we also find

**Corollary 2.6** Let  $x, y$  be respectively the Perron vectors of  $\bar{L}(T^\#(n, \Delta))$  and  $A(T^\#(n, \Delta))$ . Then

$$\begin{aligned} x(v_1) &\geq x(v_2) \geq \dots \geq x(v_n) > 0, \\ y(v_1) &\geq y(v_2) \geq \dots \geq y(v_n) > 0. \end{aligned}$$

**Theorem 2.7** For each integer  $n$  ( $n \geq 4$ ) and each integer  $\Delta$  ( $2 \leq \Delta \leq n - 2$ ), we have

$$\lambda_1(T^\#(n, \Delta)) < \lambda_1(T^\#(n, \Delta + 1)),$$

or equivalently,

$$\lambda_1(T^\#(n, n - 1)) > \lambda_1(T^\#(n, n - 2)) > \dots > \lambda_1(T^\#(n, 3)) > \lambda_1(T^\#(n, 2)).$$

**Proof** Let  $x$  be a unit Perron vector of  $\bar{L}(T^\#(n, \Delta))$ . By Corollary 2.6, we have  $x(v_1) \geq x(v_2) \geq \dots \geq x(v_n) > 0$ . Note that there exists a pendant vertex  $u$  of  $T^\#(n, \Delta)$  adjacent to the vertex  $w \neq v_1$ . Deleting the edge  $uw$  and adding an edge  $uv_1$ , we get a tree  $T \in \mathcal{T}(n, \Delta + 1)$ . By Lemma 2.2(i) and Theorem 2.4, we obtain

$$\lambda_1(T^\#(n, \Delta)) < \lambda_1(T) \leq \lambda_1(T^\#(n, \Delta + 1)).$$

$\square$

Similarly, we have the following result.

**Theorem 2.8** For each integer  $n$  ( $n \geq 4$ ) and each integer  $\Delta$  ( $2 \leq \Delta \leq n - 2$ ), we get

$$\mu_1(T^\#(n, \Delta)) < \mu_1(T^\#(n, \Delta + 1)),$$

or equivalently,

$$\mu_1(T^\#(n, n - 1)) > \mu_1(T^\#(n, n - 2)) > \dots > \mu_1(T^\#(n, 3)) > \mu_1(T^\#(n, 2)).$$

Note that  $T^\#(n-1, n)$  is a star and  $T^\#(n, 2)$  is a path, both on  $n$  vertices.

**Corollary 2.9**<sup>[3,12]</sup> *Let  $T$  be an arbitrary tree on  $n$  ( $n \geq 4$ ) vertices. Then*

$$2\left(1 + \cos \frac{\pi}{n}\right) = \lambda_1(T^\#(n, 2)) \leq \lambda_1(T) \leq \lambda_1(T^\#(n, n-1)) = n$$

with left equality if and only if  $T = T^\#(n, 2)$ , and with right equality if and only if  $T = T^\#(n, n-1)$ .

**Corollary 2.10**<sup>[1]</sup> *Let  $T$  be an arbitrary tree on  $n$  ( $n \geq 4$ ) vertices. Then*

$$2 \cos \frac{\pi}{n+1} = \mu_1(T^\#(n, 2)) \leq \mu_1(T) \leq \mu_1(T^\#(n, n-1)) = \sqrt{n-1}$$

with left equality if and only if  $T = T^\#(n, 2)$ , and with right equality if and only if  $T = T^\#(n, n-1)$ .

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