On Maximum Laplacian Estrada Indices of Trees with Some Given Parameters*

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(Received December 1, 2014)

Abstract

The Laplacian Estrada index of a graph G is defined as $LEE(G) = \sum_{i=1}^{n} e^{\mu_i}$, where μ_1, $\mu_2, \ldots, \mu_n$ are the eigenvalues of the Laplacian matrix of G. In this paper, we characterize the trees with maximum Laplacian Estrada indices among trees with given matching number, dominating number, number of pendant vertices, and diameter, respectively.

1 Introduction

In this paper we are concerned with simple finite graphs. Undefined notation and terminology can be found in [3]. Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. We use $d_G(v)$ (or $d(v)$ for short) to denote the degree of a vertex v of G. For two vertices $u, v \in V(G)$, the length of a shortest uv-path is called the distance between u and v and denoted by $d_G(u, v)$. The eccentricity $\varepsilon(v)$ of a vertex v is the maximum distance among the distances from v to the other vertices. Vertices of a graph G with minimum eccentricity form the center of G. A tree T has exactly one or two adjacent center vertices. We use $PV(T)$ to denote the set of pendant vertices of T.

*Supported by NSFC No.11371205 and PCSIRT.

Let $A(G)$ and $D(G)$ denote the adjacency matrix and the diagonal matrix of vertex degrees of G, respectively. The (resp. signless) Laplacian matrix of G is denoted by $L(G) = D(G) - A(G)$ (resp. $Q(G) = D(G) + A(G)$). We denote the eigenvalues of $A(G)$, $L(G)$ and $Q(G)$ by $\lambda_1, \lambda_2, \cdots, \lambda_n$; $\mu_1, \mu_2, \cdots, \mu_n$; and $q_1, q_2, \cdots, q_n$, respectively.

The Estrada index of G, first put forward by Estrada [7], is defined as

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i}.$$

The Estrada index has multiple applications in a large variety of problems, for example, it has been successfully employed to quantify the degree of folding of long-chain molecules, especially proteins [8–10], and it is a useful tool to measure the centrality of complex (reaction, metabolic, communication, social, etc.) networks [11, 12]. There is also a connection between the Estrada index and the extended atomic branching of molecules [13].

Fath-Tabar et al. [14] proposed the Laplacian Estrada index, in full analogy with estrada index as

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i}.$$

They established lower and uper bounds for LEE in terms of different parameters of graphs, and they also pointed out that finding graphs with extremum values of LEE in subcategories of graphs is a part of reaserches about Laplacian Estrada index.

Ayyaswamy et al. [1] defined the signless Laplacian Estrada index as

$$SLEE(G) = \sum_{i=1}^{n} e^{q_i}.$$

They also established lower and upper bounds for $SLEE$ in terms of the numbers of vertices and edges.

Ilić and Stevanović [16] obtained the unique tree with minimum Estrada index among the set of trees with a given maximum degree. Zhang, Zhou and Li [19] determined the unique tree with maximum Estrada indices among the trees with a given matching number. Ilić and Zhou [17] proved that the path and the star are, respectively, the unique trees with minimum and maximum Laplacian Estrada indices, where they also showed that the use of Laplacian Estrada index as a measure of branching in alkanes. In [17], the tree with the second maximum Laplacian Estrada index was also determined. Zhu [21] gave upper bounds for the Laplacian Estrada index in terms of connectivity or matching number and characterized the corresponding extremal graphs. Li and Zhang [18] determined the unicycilc graph with the maximum Laplacian Estrada index. More mathematical properties of the Estrada index and Laplacian Estrada index can be found in [2, 5, 15, 20, 22].

In this paper we characterize the trees with maximum LEE among trees with given matching number, dominating number, number of pendant vertices, and diameter, respectively.

2 Preliminary

Denote by $T_k(G)$ the k-th signless Laplacian spectral moment of a graph G, i.e.,

$$T_k(G) = \sum_{i=1}^{n} q_i^k.$$

By using the Taylor expansions of the function e^x, we have that

$$SLEE(G) = \sum_{k\geq 0} \frac{T_k(G)}{k!}.$$

Note that the Laplacian and signlees Laplacian spectra of bipartite graphs coincide. Thus, for a bipartite graph G, we have $SLEE(G) = LEE(G)$. Consequently, if G is bipartite, then

$$LEE(G) = \sum_{k\geq 0} \frac{T_k(G)}{k!}. \tag{1}$$

Trees are obvious bipartite, and so we can use the provided statements in $SLEE$ for LEE in our following analysis.

Definition 2.1. *A semi-edge walk of length k in a graph G is an alternating sequence $W = v_1e_1v_2e_2\cdots v_ke_kv_{k+1}$ of vertices $v_1, v_2, \cdots, v_k, v_{k+1}$ and edges $e_1, e_2, \cdots, e_k$ such that the vertices v_i and v_{i+1} are end-vertices (not necessarily distinct) of the edge e_i, for any $i = 1, 2, \cdots, k$. If $v_1 = v_{k+1}$, then we say that W is a closed semi-edge walk.*

Theorem 2.1. *[4] The signless Laplacian spectral moment T_k is equal to the number of closed semi-edge walks of length k.*

Let G and G' be two graphs with $x, y \in V(G)$ and $x', y' \in V(G)$. We use $SW_k(G; x, y)$ to denote the set of all semi-edge walks of length k in G, starting at vertex x, and ending at vertex y. For convenience, we denote $SW_k(G; x, x)$ by $SW_k(G; x)$, and set $SW_k(G) = \bigcup_{x\in V(G)} SW_k(G; x)$. We use the notation $(G; x, y) \preceq_s (G'; x', y')$ if $|SW_k(G; x, y)| \leq |SW_k(G'; x', y')|$ for any $k \geq 0$. Moreover, if $(G; x, y) \preceq_s (G'; x', y')$, and there exists a k_0 such that $|SW_{k_0}(G; x, y)| < |SW_{k_0}(G'; x', y')|$, then we write $(G; x, y) \prec_s (G'; x', y')$. If $x = y$, we use $(G; x)$ as the short form of $(G; x, x)$. From these notations, we know that

$$T_k(G) = |SW_k(G)| = \sum_{x\in V(G)} |SW_k(G; x)|. \tag{2}$$

3 Lemmas

We will give a few lemmas in this section, which will be used in the sequel.

Lemma 3.1. *Let G_1 and G_2 be two graphs with $u \in V(G_1)$ and $v \in V(G_2)$. Let G be the graph obtained from G_1 and G_2, by joining an edge $e = uv$. If $(G_1; u) \prec_s (G_2; v)$, one has $(G; u) \prec_s (G; v)$.*

Proof. Since $(G_1; u) \prec_s (G_2; v)$, there exists an injection ϕ_k from $SW_k(G_1; u)$ to $SW_k(G_2; v)$ for any $k \geq 1$, and there exists a k_0 such that $|SW_{k_0}(G_1; u)| < |SW_{k_0}(G_2; v)|$. Then ϕ_{k_0} is not a bijection. Let $W \in SW_k(G; u)$ be an arbitrary semi-edge closed walk of G at u. In order to prove the result, it is sufficient to build an injection Φ_k (but not a bijection for all k) from $SW_k(G; u)$ to $SW_k(G; v)$. We distinguish the following cases.

Case 1: $e \notin W$. Then $W \in SW_k(G_1; u)$. Let $\Phi_k(W) = \phi_k(W)$;

Case 2: $e \in W, v \notin W$. Then $W = W_1 e W_2 e \cdots e W_t$, where $e \notin W_i \in SW_{l_i}(G_1; u)$ for $i = 1, 2, \cdots, t$. Let $\Phi_k(W) = \phi_{l_1}(W_1) e \phi_{l_2}(W_2) e \cdots e \phi_{l_t}(W_t)$;

Case 3: $e \in W, v \in W$. Then $W = W_1 e W_2 e W_3$, where $e \notin W_1 \in SW_{l_1}(G_1; u)$ and $e \notin W_3 \in SW_{l_3}(G_1; u)$. Let $\Phi_k(W) = \phi_{l_1}(W_1) e W_2 e \phi_{l_3}(W_3)$.

It is obvious that Φ_k is an injection. Furthermore, as ϕ_{k_0} is not a bijection, we have that Φ_{k_0} is not a bijection, i,e., $(G; u) \prec_s (G; v)$. □

Corollary 3.2. *Let $P_n = v_1 v_2 \cdots v_n$ be an n-vertex path. Then one has*

$$(P_n; v_1) \prec_s (P_n; v_2) \prec_s \cdots \prec_s (P_n; v_{\lfloor \frac{n}{2} \rfloor}).$$

Lemma 3.3. *[6] Let H_1 and H_2 be two bipartite graphs with $u, v \in V(H_1)$ and $w \in V(H_2)$. Let G_u (G_v, respectively) be the graph obtained from H_1 and H_2 by identifying u (v, respectively) with w. If $(H_1; v) \prec_s (H_1; u)$, then $LEE(G_v) < LEE(G_u)$ (see Figure 1).*

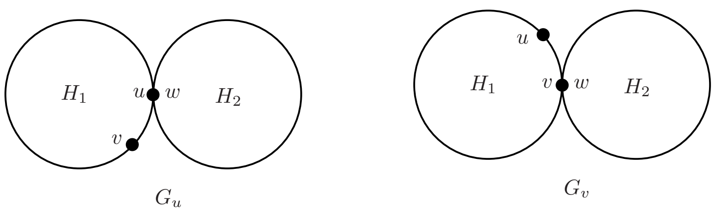

Figure 1. G_u and G_v

Definition 3.1. *Let G_1 and G_2 be two graphs with $u \in V(G_1)$ and $v \in V(G_2)$. Let G be the graph obtained from G_1 and G_2 by joining an edge uv, and G' be the graph obtained from G_1 and G_2 by identifying u with v and attaching a pendant vertex to u. We call the procedure of constructing G' from G the A-transformation of G at edge uv; see Figure 2.*

Lemma 3.4. *[6] Let G and G' be two bipartite graphs, where G' is an A-transformation of G at edge uv. If $d_G(u), d_G(v) \geq 2$, then $LEE(G) < LEE(G')$.*

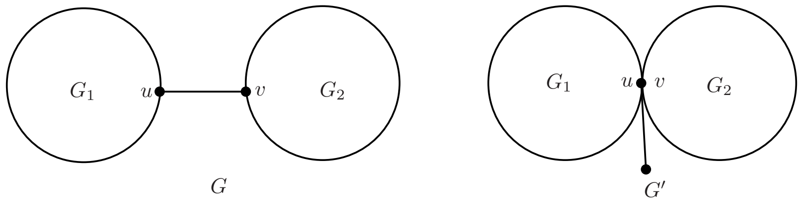

Figure 2. G and G'

Let T be an arbitrary tree rooted at a center vertex u, and let v be a vertex which is distinct from u such that $N_T(v) = \{v_1, v_2, \cdots, v_s\}$. It is obvious that $T - v$ has s components, denoted by $T_1, T_2, \cdots, T_s$ with $v_i \in V(T_i)$ for $1 \leq i \leq s$. Without loss of generality, we may assume $u \in V(T_1)$. If there exists an i $(2 \leq i \leq s)$ such that T_i is a path, say $T_s = P_r$, we define a graph transformation as follows:

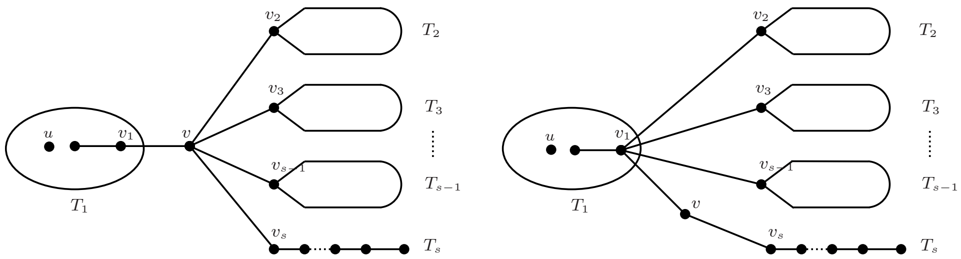

Figure 3. T and T'

Definition 3.2. *Let T' be the tree obtained from T by removing the edges $vv_2, vv_3, \ldots, vv_{s-1}$ and adding new edges $v_1v_2, v_1v_3, \ldots, v_1v_{s-1}$; see Figure 3. We call T' a B-transformation of T at v with vv_s remained.*

Lemma 3.5. *Let T and T' be the trees defined as above. If v is not a center of T or $d_T(v_1) > 2$, then $LEE(T) < LEE(T')$.*

Proof. Let H_1 be the component that contains v_1 in $T - \{vv_2, vv_3, \cdots, vv_{s-1}\}$, and H_2 be the component that contains v in $T - \{v_1, v_s\}$. Let $\hat{T}_s = T[V(T_s) \cup \{v\}] \cong P_{r+1}$. If v is not a center of T, since $u \in V(T_1)$ and u is the center of T, we know that there exists a path P in T_1 of length at least $r + 1$ with an end vertex v_1, and so $(\hat{T}_s; v) \prec_s (T_1; v_1)$;

If v is a center and $d_T(v_1) > 2$, then there exists a path P in T_1 having a length at least r with an end vertex v_1, together with the fact that $|SW_1(\hat{T}_s; v)| = 1 < |SW_1(T_1; v_1)|$, we have that $(\hat{T}_s; v) \prec_s (T_1; v_1)$.

By Lemma 3.1, we have $(H_1; v) \prec_s (H_1; v_1)$. Consequently, we can obtain $LEE(T) < LEE(T')$ by Lemma 3.3. $\square$

4 The maximum LEE trees with given parameters

The matching number of a graph G is the maximum size of an independent (pairwise nonadjacent) set of edges of G and will be denoted by $\alpha'(G)$. Let $\mathcal{M}(n, q)$ be the set of all n-vertex trees with matching number q. Let $A(n, q)$ be the tree that is obtained by attaching $q-1$ pendant edges to $q-1$ pendant vertices of the star $K_{1,n-q}$; see Figure 4. It is routine to check that $A(n, q) \in \mathcal{M}(n, q)$. Given a vertex w in G, call w a perfectly matched vertex if it is matched in any maximum matching of G.

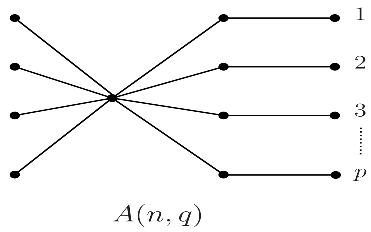

Figure 4. $A(n, q)$

Theorem 4.1. *Among $\mathcal{M}(n, q)$, the tree $A(n, q)$ is the unique graph with the maximum Laplacian Estrada index.*

Proof. Choose $T \in \mathcal{M}(n, q)$ such that its Laplacian Estrada index is as large as possible. If T contains a pendant path of length $p > 2$, say $v_1v_2v_3...v_pv_{p+1}$ with $v_1 \in PV(T)$, then $(T - v_2 - v_1; v_3) \prec_s (T - v_2 - v_1; v_4)$ by Lemma 3.1. Let $T_0 = T - v_2v_3 + v_2v_4$. It is routine to check that T_0 is in $\mathcal{M}(n, q)$. By Lemma 3.3, we can get $LEE(T) < LEE(T_0)$, a contradiction. Hence, any pendant path contained in T must have a length at most 2.

Suppose that there exists a non-center vertex $v \in V(T)$ with $d_T(v) = r + s + 1$ such that T contains r pendant edges $vv_1, vv_2, \cdots, vv_r$ and s pendant paths of length 2 $vu_1u'_1, vu_2u'_2, \cdots, vu_su'_s$ attached to v. Let u be the center of T and w be the neighbor of v in the path $P_T(v, u)$, where $P_T(v, u)$ is the path from v to u in T. We consider the following possible cases.

Case 1: $s = 0$ and w is perfectly matched. Let M be a maximum matching of T. Since w is perfectly matched, there exists a vertex $s \neq v$ such that $sw \in M$, and $vv_i \in M$ for some $1 \leq i \leq r$. Without loss of generality, suppose $vv_1 \in M$. Apply $B-$transformation at v with vv_1 remained. Then M is also a matching of the resulting tree T'. If M is not a maximum matching of T', then T' has a matching M' such that $|M'| \geq q + 1$. There exists an i $(2 \leq i \leq r)$ such that $wv_i \in M'$. Obviously, $M' \setminus \{wv_i\}$ is a matching of T. Note that $|M' \setminus \{wv_i\}| \geq q$ and w is not matched in $M' \setminus \{wv_i\}$, we can obtained a contradiction. Hence $T' \in \mathcal{M}(n, q)$. By Lemma 3.5 we get $LEE(T) < LEE(T')$, a contradiction.

Case 2: $s = 0$ and w is not perfectly matched. Applying A-transformation at edge wv. Let T' be the resulting tree. Note that a matching of T' is also a matching of T, and so $\alpha'(T') \leq \alpha'(T) = q$. Since w is not perfectly matched, there exists a maximum matching M of T such that w is not matched in M. We can easily check that M is also a matching of T'. Hence, we have $\alpha'(T') = q$. By Lemma 3.4 we get $LEE(T) < LEE(T')$, a contradiction.

Case 3: $r = 0$. Applying B-transformation at v with vu_1 remained. It is routine to check that the resulting tree T' is in $\mathcal{M}(n, q)$. By Lemma 3.5 we get $LEE(T) < LEE(T')$, a contradiction.

Case 4: $r > 0, s > 0$ and w is perfectly matched. For a maximum matching M of T, we know that there exists an i $(1 \leq i \leq r)$ such that $vv_i \in M$. Without loss of generality, suppose $vv_1 \in M$. Apply $B-$transformation at v with vv_1 remained. It is routine to check that T' is in $\mathcal{M}(n, q)$. By Lemma 3.5 we get $LEE(T) < LEE(T')$, a contradiction.

Case 5: $r > 0, s > 0$ and w is not perfectly matched. Applying A-transformation at edge wv. By a similar analysis in case 2, we can easily check that T' is in $\mathcal{M}(n, q)$. By Lemma 3.4 we get $LEE(T) < LEE(T')$, a contradiction.

Hence, all the pendant paths of length at most 2 are attached only to the centers of T. In order to characterize the structure of T, it suffices to show that T contains just one center whose degree is larger than 2. Otherwise, assume that T contains two centers, say c_1 and c_2, with $d_T(c_1) > 2$ and $d_T(c_2) > 2$. Applying B-transformation at c_1 with c_1u remained in T, where $N_T(u) = \{c_1\}$, we get a new tree, say T'. It is routine to check that T' is in $\mathcal{M}(n, q)$. By Lemma 3.5 we get $LEE(T) < LEE(T')$, a contradiction.

The proof is now complete. □

A dominating set in a graph G is a subset S of $V(G)$ such that each vertex of G either belongs to S or is adjacent to some elements of S. The dominating number of a graph G, denoted by $\gamma(G)$, is defined as the cardinality of a minimum dominating set of G. Let $\mathcal{D}(n, q)$ be the set of all n-vertex trees with dominating number q.

Theorem 4.2. *Among $\mathcal{D}(n, q)$, the tree $A(n, q)$ is the unique graph with the maximum Laplacian Estrada index.*

Proof. Let T be a tree which maximizes the Laplacian Estrada index among $\mathcal{D}(n, q)$. In order to complete the proof, it suffices to show that $\gamma(T) = \alpha'(T)$. It is known from [3] that $\gamma(T) \leq \alpha'(T)$. So we only need to show $\gamma(T) \geq \alpha'(T)$. Assume that $S = \{v_1, v_2, \cdots, v_q\}$ is a dominating set of T with cardinality q. We claim that $T - S$ is an empty graph. In fact, if there exists an edge $w_1w_2 \in E(T - S)$, then w_1 and w_2 are dominated by two different vertices of S. Without loss of generality, assume that w_i is dominated by the vertex v_i for $i = 1, 2$. Now we construct a new tree $T' \in \mathcal{D}(n, q)$ by using A-transformation in T at edges v_1w_1 and v_2w_2. By Lemma 3.4 we get $LEE(T) < LEE(T')$, a contradiction. The claim follows and hence, we can easily get that $\alpha'(T) \leq q$. This completes the proof. $\square$

Let $\mathcal{P}(n, k)$ be the set of all n-vertex trees with k leaves ($2 \leq k \leq n-1$). A spider is a tree with at most one vertex of degree more than 2, and this vertex is called the hub of the spider (if no vertex of degree more than two, then any vertex can be the hub). A leg of a spider is a path from the hub to a leaf. Let T_n^k be an n-vertex tree with k legs satisfying all the lengths of the k legs, say $l_1, l_2, \cdots, l_k$, are almost equal, i.e., $|l_i - l_j| \leq 1$ for $1 \leq i, j \leq k$. It is easy to see that $T_n^k \in \mathcal{P}(n, k)$ and $l_i = \lfloor \frac{n-1}{k} \rfloor$ or $\lceil \frac{n-1}{k} \rceil$, for any $1 \leq i \leq k$.

Theorem 4.3. *Among $\mathcal{P}(n, k)$, the tree T_n^k is the unique graph with the maximum Laplacian Estrada index.*

Proof. Choose $T \in \mathcal{P}(n, k)$ such that its Laplacian Estrada index is as large as possible. If $k = 2$ or $n - 1$, our result follows immediately. Hence, we consider $2 < k < n - 1$. For convenience, let W be the set of vertices of degree larger than 2 in T.

First, we show that for any $v \in W$, v is a center of T. Otherwise, there exists a vertex $v \in W$ that is not a center of T, and v satisfies that $T - v$ has a path component T_1 with $vv_1 \in E(T)$ and v_1 is not a center of T. Apply B-transformation of T at v with vv_1 remained to get a new tree T'. It is straightforward to check that $T' \in \mathcal{P}(n, k)$. By Lemma 3.5, we have that $LEE(T) < LEE(T')$, a contradiction to the choice of T. Hence, for any vertex $w \in V(T)$ that is not a center of T, we have $d_T(w) \leq 2$. If there are two center vertices c_1 and c_2 in W, we can similarly apply a B-transformation of T at c_1 with c_1u remained to get a new tree T', where $u \in N_T(c_1) \setminus \{c_2\}$. Then T' is a spider, and by Lemma 3.5 we have $LEE(T) < LEE(T')$, a contradiction.

Now suppose that c is the only vertex in W. We show that$|d_T(c, u_i) - d_T(c, u_j)| \leq 1$ for any $u_i, u_j \in PV(T)$. Assume, to the contrary, that there exist two pendant vertices, say u_t, u_l, such that

$$|d_T(c, u_t) - d_T(c, u_l)| > 2. \tag{1}$$

Denote the unique path connecting u_t and u_l by $P_s = w_1 w_2 \cdots w_{i-1} w_i w_{i+1} \cdots w_s$, where $w_1 = u_t, w_s = u_l$ and $w_i = c, 1 < i < s$. In view of (1), we have

$$c = w_i \neq w_{\lfloor \frac{s+1}{2} \rfloor} \, and \; c = w_i \neq w_{\lceil \frac{s+1}{2} \rceil}.$$

Hence, by Corollary 3.2 and Lemma 3.3 there exists an n-vertex tree $T \in \mathcal{P}(n, k)$ such that $LEE(T) < LEE(T')$, a contradiction to the choice of T. So we have $T \cong T_n^k$. $\square$

Let $\mathcal{D}_n^d$ denote the set of all n-vertex trees of diameter d. Let $\hat{T}_{n,k}^d$ be the n-vertex tree obtained from $P_{d+1} = v_1 v_2 \cdots v_d v_{d+1}$ by attaching $n - d - 1$ pendant edges to v_k; see Figure 5.

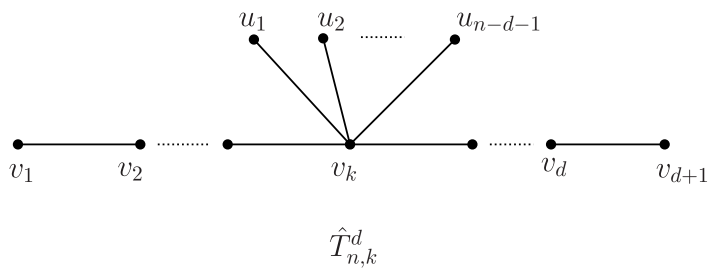

Figure 5. $\hat{T}_{n,k}^d$

Theorem 4.4. *Among $\mathcal{D}_n^d$, the tree $\hat{T}_{n,i}^d$ is the unique graph with the maximum Laplacian Estrada index, where $i = \lfloor \frac{d}{2} \rfloor + 1$ or $\lceil \frac{d}{2} \rceil + 1$.*

Proof. Choose $T \in \mathcal{D}_n^d$ such that its Laplacian Estrada index is as large as possible. Let $P_{d+1} = v_1 v_2 \cdots v_d v_{d+1}$ be a longest path in T. Let $e = uv$ be an edge of T. If $\{u, v\} \cap \{v_1, v_2 \cdots, v_{d+1}\} = \emptyset$, we can apply A-transformation at edge uv to get T'. Note that $T' \in \mathcal{D}_n^d$, and $LEE(T) < LEE(T')$ by Lemma 3.4, we can obtain a contradiction. Hence $\{u, v\} \cap \{v_1, v_2 \cdots, v_{d+1}\} \neq \emptyset$

For any $e = uv_i \in E(G) \setminus E(P_{d+1})(1 < i < d+1)$, we prove that $i = \lfloor \frac{d}{2} \rfloor + 1$ or $\lceil \frac{d}{2} \rceil + 1$. Suppose $i < \lfloor \frac{d}{2} \rfloor + 1$, and let $j = \min\{i : 1 < i < \lfloor \frac{d}{2} \rfloor + 1, d_T(v_i) > 2\}$. We can apply a B-transformation at v_j with $v_j v_{j-1}$ remained. It is routine to check that the resulting tree T' is in $\mathcal{D}_n^d$. By Lemma 3.5, we have $LEE(T) < LEE(T')$, a contradiction. We can similarly get a contradiction if $i > \lceil \frac{d}{2} \rceil + 1$.

If $d_T(v_{\lfloor \frac{d}{2} \rfloor + 1}) > 2$ and $d_T(v_{\lceil \frac{d}{2} \rceil + 1}) > 2$, By applying a B-transformation at $v_{\lceil \frac{d}{2} \rceil + 1}$ with $v_{\lceil \frac{d}{2} \rceil + 1} v_{\lceil \frac{d}{2} \rceil + 2}$ remained, we get a new tree $T' \in \mathcal{D}_n^d$, and $LEE(T) < LEE(T')$, a contradiction. Hence $d_T(v_{\lfloor \frac{d}{2} \rfloor + 1}) = 2$ or $d_T(v_{\lceil \frac{d}{2} \rceil + 1}) = 2$. This completes our proof. $\square$

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