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ORIGINAL PAPER

The Estrada index of chemical trees

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Abstract Let G be a simple graph with n vertices and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of its adjacency matrix. The Estrada index of G is a recently introduced molecular structure descriptor, defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, proposed as a measure of branching in alkanes. In order to support this proposal, we prove that among the trees with fixed maximum degree Δ, the broom $B_{n,\Delta}$, consisting of a star $S_{\Delta+1}$ and a path of length $n-\Delta-1$ attached to an arbitrary pendent vertex of the star, is the unique tree which minimizes even spectral moments and the Estrada index, and then show the relation $EE(S_n) = EE(B_{n,n-1}) > EE(B_{n,n-2}) > \cdots > EE(B_{n,3}) > EE(B_{n,2}) = EE(P_n)$. We also determine the trees with minimum Estrada index among the trees with perfect matching and maximum degree Δ. On the other hand, we strengthen a conjecture of Gutman et al. [Z. Naturforsch. 62a (2007), 495] that the Volkmann trees have maximal Estrada index among the trees with fixed maximum degree Δ, by conjecturing that the Volkmann trees also have maximal even spectral moments of any order. As a first step in this direction, we characterize the starlike trees which maximize even spectral moments and the Estrada index.

Keywords Estrada index · Branching · Broom graph · Chemical trees · Volkmann trees · Spectral moments

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1 Introduction

Let $G = (V, E)$ be a simple graph with $|V| = n$ vertices and $|E| = m$ edges. The spectrum of G consists of the eigenvalues

$$\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$$

of its adjacency matrix A. The Estrada index is defined as

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

In the last ten years, the Estrada index found applications in measuring the degree of protein folding [1–3], the centrality of complex networks (such as neural, social, metabolic, protein–protein interaction networks, and the World Wide Web) [4], and it was also proposed as a measure of molecular branching, accounting for the effects of all atoms in the molecule, giving higher weight to the nearest neighbors [5]. Within groups of isomers, EE was found to increase with the increasing extent of branching of the carbon-atom skeleton [6]. Also, EE characterizes the structure of alkanes via electronic partition function [7].

Some mathematical properties of the Estrada index were reported in [8–14]. It is natural problem to study chemical trees (trees with maximum degree four) and generally trees with bounded maximum degree [15,16].

Our goal here is to add some further evidence to support the use of EE as a measure of branching in alkanes. While the measure of branching cannot be formally defined, there are several properties that any proposed measure has to satisfy [17], [18]. Basically, a topological index (TI) acceptable as a measure of branching must satisfy the inequalities

$$TI(P_n) < TI(X_n) < TI(S_n) \qquad \text{or} \qquad TI(P_n) > TI(X_n) > TI(S_n),$$

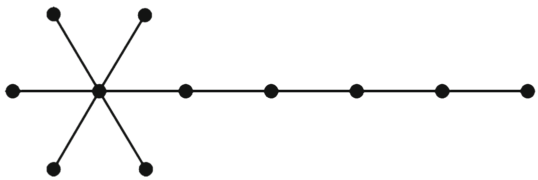
for $n = 5, 6, \ldots$, where P_n is the path, and S_n is the star on n vertices. For example, the first relation is obeyed by the largest graph eigenvalue [19] and EE [20], while the second relation is obeyed by the Wiener index [21], Hosoya index and graph energy [22].

We refine the above relation by showing that

$$\begin{aligned} EE(S_n) &= EE(B_{n,n-1}) > EE(B_{n,n-2}) > \cdots > EE(B_{n,3}) > EE(B_{n,2}) \\ &= EE(P_n), \end{aligned} \tag{1}$$

where the broom $B_{n,\Delta}$ is a tree consisting of a star $S_{\Delta+1}$ and a path of length $n-\Delta-1$ attached to an arbitrary pendent vertex of the star (see Fig. 1). It is proven in [23] that among trees with perfect matching and maximum degree equal to Δ, the broom $B_{n,\Delta}$ uniquely minimizes the largest eigenvalue of adjacency matrix. Also it is shown that among trees with bounded degree Δ, the broom has minimal Wiener index and

Fig. 1 The broom $B_{11,6}$



Laplacian-like energy [24]. In [25] and [26] the broom has minimal energy among trees with fixed diameter or fixed number of pendant vertices.

In particular, we show in Sect. 3 that the broom $B_{n,\Delta}$ has minimal EE among the trees on n vertices and maximum degree Δ, and we also determine the tree with the second minimal EE. Next, in Sect. 4 we determine the tree with minimal EE among n-vertex trees with perfect matching and maximum degree Δ, and prove a relation analogous to (1).

The question may also be asked which are the most branched alkanes [27]. This problem was examined in due detail [18] and several molecular structure-descriptors imply that the most branched alkanes are those represented by the Volkmann trees. In Sect. 5 we strengthen a conjecture from [6] that the Volkmann trees have maximal EE among the trees with fixed maximum degree Δ, by conjecturing that the Volkmann trees also have maximal even spectral moments of any order. As a first step in this direction, we characterize the starlike trees which maximize even spectral moments and EE.

2 Preliminaries

In our proofs, we will use a connection between EE and the spectral moments of a graph. For $k \geqslant 0$, we denote by M_k the kth spectral moment of G,

$$M_k(G) = \sum_{i=1}^{n} \lambda_i^k.$$

A walk of length k in G is any sequence of vertices and edges of G,

$$w = w_0, e_1, w_1, e_2, \ldots, w_{k-1}, e_k, w_k,$$

such that e_i is the edge joining w_{i-1} and w_i for every $i = 1, 2, \ldots, k$. The walk is closed if $w_0 = w_k$. It is well-known (see [28]) that $M_k(G)$ represents the number of closed walks of length k in G. Obviously, for every graph $M_0 = n$, $M_1 = 0$ and $M_2 = 2m$. For the third moment we have $M_3 = 6t$, where t is the number of triangles in graph G. The fourth moment is equal to

$$M_4 = 2\sum_{i=1}^{n} d_i^2 - 2m + 8q, \tag{2}$$

where d_i is the degree of the ith vertex, and q the number of quadrangles in G.

From the Taylor expansion of e^x, we have that the Estrada index and the spectral moments of G are related by

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k}{k!}. \tag{3}$$

Thus, if for two graphs G and H we have $M_k(G) \geqslant M_k(H)$ for all $k \geqslant 0$, then $EE(G) \geqslant EE(H)$. Moreover, if the strict inequality $M_k(G) > M_k(H)$ holds for at least one value of k, then $EE(G) > EE(H)$.

The Δ-starlike tree $T(n_1, n_2, \ldots, n_\Delta)$ is a tree composed of the root v, and the paths $P_1, P_2, \ldots, P_\Delta$ of lengths $n_1, n_2, \ldots, n_\Delta$ attached at v. The number of vertices of a tree $T(n_1, n_2, \ldots, n_\Delta)$ equals $n = n_1 + n_2 + \cdots + n_\Delta + 1$. The Δ-starlike tree is *balanced* if all paths have almost equal lengths, i.e., $|n_i - n_j| \leqslant 1$ for every $1 \leqslant i \leqslant j \leqslant \Delta$. Notice that the broom $B_{n,\Delta} = T(n - \Delta, 1, 1, \ldots, 1)$ is a Δ-starlike tree.

3 The minimum spectral moments and Estrada index

Let $M_k(n, i)$ be the number of closed walks of length k starting from the vertex v_i in the path $P_n = v_0 v_1 v_2 \ldots v_n$. Since every tree is a bipartite graph, we have identity $M_{2k+1}(n, i) = 0$ for $0 \leqslant i \leqslant n$. By symmetry, we have $M_k(n, i) = M_k(n, n - i)$.

Recall that the sequence of numbers $c_1, c_2, \ldots, c_k$ is *unimodal* if there exists no indices $1 \leqslant p < q < r \leqslant k$ such that $c_p > c_q < c_r$.

Lemma 3.1 *For every even $k > 2$ holds*

$$M_k(n, 0) \leqslant M_k(n, 1) \leqslant \cdots \leqslant M_k\left(n, \left\lceil \frac{n}{2} \right\rceil - 1\right) \leqslant M_k\left(n, \left\lceil \frac{n}{2} \right\rceil\right).$$

For sufficiently large k, strict inequalities hold.

Proof Let A be the adjacency matrix of the path P_n. It is well-known that the element $(A^k)_{i,j}$ represents the number of walks of length k from vertex i to vertex j. We will prove that the matrix A^k has the following property: every diagonal parallel to the main diagonal is unimodal. First, the matrix A^k is symmetric. Next, by automorphism $f : \{v_0, v_1, \ldots, v_n\} \to \{v_0, v_1, \ldots, v_n\}$ of P_n, given by $f(v_i) = v_{n-i}$, we can see that $(A^k)_{i,j} = (A^k)_{n-i,n-j}$. Therefore, we only have to prove that the diagonals that are parallel to the main diagonal, increase for $i + j \leqslant n$.

We will proceed by mathematical induction on k and prove that for all $1 \leqslant i, j \leqslant n$ such that $i + j \leqslant n$, holds:

$$(A^k)_{i,j} \geqslant (A^k)_{i-1,j-1}. \tag{4}$$

For $k = 0$ and $k = 1$, this is obvious. Using the recurrent formulas derived from matrix multiplication, we have:

$$(A^{k+1})_{i-1,j-1} = (A^k)_{i-1,j-2} + (A^k)_{i-1,j}$$
$$(A^{k+1})_{i,j} = (A^k)_{i,j-1} + (A^k)_{i,j+1}$$

From the induction hypothesis we have $(A^k)_{i,j-1} \geqslant (A^k)_{i-1,j-2}$. If $i + j + 1 \leqslant n$, we also have $(A^k)_{i,j+1} \geqslant (A^k)_{i-1,j}$. For $i + j + 1 = n + 1$, i.e., $j = n - i$, we have that $(A^k)_{i-1,j} = (A^k)_{i,j+1}$. This proves inequality (4).

For the strict inequality, consider two neighboring rows $i - 1$ and i. Eventually, the element $(A^k)_{i,0}$ becomes nonzero and it forces the strict inequality $(A^{k+1})_{i,1} > (A^{k+1})_{i-1,0}$. This causes the chain of strict inequalities $(A^{k+2})_{i,2} > (A^{k+2})_{i-1,1}$, $(A^{k+3})_{i,3} > (A^{k+3})_{i-1,2}$, and finally

$$(A^{k+n-i})_{i,n-i} > (A^{k+n-i})_{i-1,n-i-1}.$$

The number of closed walks of length k starting from the vertex i equals to the element (i, i) in matrix A^k. Therefore,

$$M_k(n, i) = (A^k)_{i,i}$$

and using inequalities (4) we conclude that $M_k(n, i) \leqslant M_k(n, i+1)$ for every $0 \leqslant i \leqslant \lceil \frac{n}{2} \rceil - 1$. If k is large enough, we have strict inequality $M_k(n, i) < M_k(n, i + 1)$. □

Theorem 3.2 *Let w be a vertex of the nontrivial connected graph G and for nonnegative integers p and q, let $G(p, q)$ denote the graph obtained from G by attaching pendent paths $P = wv_1v_2 \ldots v_p$ and $Q = wu_1u_2 \ldots u_q$ of lengths p and q, respectively, at w. If $p \geqslant q \geqslant 1$, then*

$$M_k(G(p, q)) \geqslant M_k(G(p + 1, q - 1)). \tag{5}$$

For sufficiently large k, the strict inequalities hold.

Proof Since this transformation does not affect the number of vertices or the edges, we have that $M_k(G(p, q)) = M_k(G(p + 1, q - 1))$ for $k = 0, 1, 2$.

Thus, assume that $k \geqslant 3$ is fixed. Inequality (5) will be proved if we show that $G(p, q)$ has more closed walks of length k than $G(p+1, q-1)$. For that purpose, we will construct an injection i^* from the set $\mathcal{W}'_k = \mathcal{W}_k(G(p+1, q-1))$ of closed walks of length k in $G(p+1, q-1)$ to the set $\mathcal{W}_k = \mathcal{W}_k(G(p, q))$ of closed walks of length k in $G(p, q)$. Denote with P' and Q', the paths $wv_1v_2 \ldots v_pv_{p+1}$ and $wu_1u_2 \ldots u_{q-1}$.

Consider an arbitrary closed walk C' from $\mathcal{W}'$. If C' is entirely contained in G or does not contain the edge (v_p, v_{p+1}), then $i^*(C') = C'$ is also a closed walk in $G(p, q)$. If C' is entirely contained in the union of paths $P' \cup Q'$, we can construct the corresponding walk $i^*(C')$ in $P \cup Q$ by shifting it for one place, since both unions are isomorphic to P_{p+q+1}. Therefore, we can assume that C' contains the edge (v_p, v_{p+1})

and some vertices from G. Without loss of generality, assume that the closed walk C' starts at vertex w and that it is decomposed as follows:

$$C' = C_1' \, C_2' \, C_3' \, C_4' \ldots, \tag{6}$$

where C_i' is a closed walk that starts at w that is either contained completely in $P' \cup Q'$ or in G. Let $l_1, l_2, l_3, \ldots$ be the lengths of closed walks $C_1', C_2', C_3', \ldots$, respectively. Since $q \leqslant p$, from Lemma 3.1 we have that

$$M_{l_j}(p+q+1, q-1) \leqslant M_{l_j}(p+q+1, q).$$

Thus, one can construct an injection i_j^* mapping the closed walks of length l_j starting at w in $P' \cup Q'$ into the closed walks of length l_j starting at w in $P \cup Q$.

Now, if we assume that the walks C_{2i+1}', $i \geqslant 0$ are contained in G, while the walks C_{2i}', $i \geqslant 1$ are contained in $P' \cup Q'$, then

$$i^*(C') = C_1' \, i_{l_2}^*(C_2') \, C_3' \, i_{l_4}^*(C_4') \, \ldots$$

is a corresponding closed walk in $G(p, q)$. The mapping i^* is an injection by its construction, and that fact proves (5).

For k large enough and the closed walks which are decomposable by (6) into a fixed number of parts, at least one of the numbers $l_2, l_4, \ldots$ is large enough such that the strict inequality $M_{l_{2j}}(p+q+1, q-1) < M_{l_{2j}}(p+q+1, q)$ holds. Then $M_k(G(p+1, q-1)) < M_k(G(p, q))$ holds as well. □

Corollary 3.3 *Let w be a vertex of the nontrivial connected graph G and for nonnegative integers p and q, let $G(p, q)$ denote the graph obtained from G by attaching pendent paths $P = wv_1v_2 \ldots v_p$ and $Q = wu_1u_2 \ldots u_q$ of lengths p and q, respectively, at w. If $p \geqslant q \geqslant 1$, then*

$$EE(G(p, q)) > EE(G(p+1, q-1)).$$

Proof The result follows directly from (3) and previous theorem. □

Theorem 3.4 *Let $T \ncong B_{n,\Delta}$ be an arbitrary tree on n vertices with the maximum vertex degree Δ. Then*

$$EE(B_{n,\Delta}) < EE(T). \tag{7}$$

Proof Fix a vertex v of degree Δ as a root and let $k > 2$ be an even number. Let $T_1, T_2, \ldots, T_\Delta$ be the trees attached at v. We can repeatedly apply the transformation from Corollary 3.3 at any vertex of degree at least three with largest eccentricity from the root in every tree T_i, as long as T_i does not become a path. From Corollary 3.3 it follows that each application of this transformation strictly decreases its Estrada index.

When all trees $T_1, T_2, \ldots, T_\Delta$ turn into paths, we can again apply Corollary 3.3 at the vertex v as long as there exists at least two paths of length at least two, further decreasing the Estrada index. In the end of this process, we arrive at the broom $B_{n,\Delta}$. $\square$

Let $B'_{n,\Delta} = T(n-\Delta-1, 2, 1, \ldots, 1)$ be a starlike tree obtained from $B_{n,\Delta}$ by removing the last edge from the longest path and attaching it to another pendent vertex. From the above proof, we also get that $B'_{n,\Delta}$ has the second minimal EE among trees with maximum vertex degree Δ.

Corollary 3.5 *Let $T \ncong B_{n,\Delta}, B'_{n,\Delta}$ be an arbitrary tree on n vertices with the maximum vertex degree Δ. Then*

$$EE(B'_{n,\Delta}) < EE(T).$$

It was conjectured in [29] that the path P_n has minimum Estrada index among connected graphs on n vertices. While the conjecture has been proved recently in [20], Corollary 3.3 enables us to give a new proof of this conjecture. Namely, deleting an edge from a graph decreases the number of closed walks, and by (3) also decreases the Estrada index. Thus, any graph will have larger Estrada index than its spanning tree, showing that the graph with minimum Estrada index has to be a tree itself. Next, from Theorem 3.4 we know that the minimum Estrada index among trees on n vertices is achieved for one of the brooms $B_{n,\Delta}$. If $\Delta > 2$, we can apply the transformation from Corollary 3.3 at the vertex of degree Δ in $B_{n,\Delta}$ and obtain $B_{n,\Delta-1}$. Thus, $EE(B_{n,\Delta}) > EE(B_{n,\Delta-1})$ for $\Delta > 2$, which shows that

$$EE(S_n)=EE(B_{n,n-1}) > EE(B_{n,n-2}) > \cdots > EE(B_{n,3}) > EE(B_{n,2})=EE(P_n).$$

In [30] the authors estimate the Estrada index of a path P_n and proved that

$$EE(P_n) \approx (n+1)I_0 - \cosh 2,$$

where $I_0 = \sum_{k=0}^{\infty} \frac{1}{(k!)^2} = 2.27958530$. Since, the spectra of graph $B_{n,3} \cong Z_n$ consists of

$$\{0\} \bigcup \left\{ 2\cos\frac{(2k+1)\pi}{2(n-1)} \mid k = 0, 1, 2, \ldots, n-2 \right\},$$

we have the following approximation $EE(Z_n) \approx nI_0$ from [31]. The path P_n is the unique graph with maximal degree 2, and therefore Z_n has the second minimal Estrada index among trees on n vertices.

4 The minimum Estrada index of trees with perfect matchings

It is well known that if a tree T has a perfect matching, then the perfect matching M is unique: namely, a pendent vertex v has to be matched with its unique neighbor w, and then $M - \{vw\}$ forms the perfect matching of $T - v - w$.

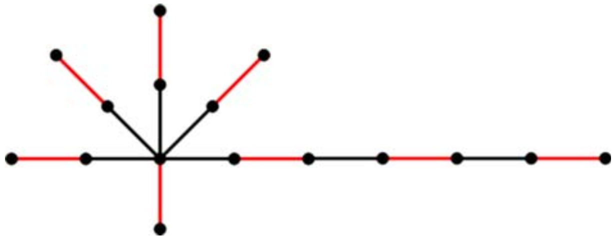


Fig. 2 The tree $A_{16,6}$

Let $A_{n,\Delta}$ be a Δ-starlike tree $T(n-2\Delta, 2, 2, \ldots, 2, 1)$ consisting of a central vertex v, a pendant edge, a pendant path of length $n-2\Delta$ and $\Delta-2$ pendant paths of length 2, all attached at v (see Fig. 2).

Theorem 4.1 *The tree $A_{n,\Delta}$ has minimum EE among trees with perfect matching and maximum degree Δ.*

Proof Let T be an arbitrary tree with perfect matching and let v be a vertex of degree Δ, with neighbors $v_1, v_2, \ldots, v_\Delta$. Let $T_1, T_2, \ldots, T_\Delta$ be the maximal subtrees rooted at $v_1, v_2, \ldots, v_\Delta$, respectively, such that neither of these trees contains v. Then at most one of the numbers $|T_1|, |T_2|, \ldots, |T_\Delta|$ can be odd (if T_i and T_j have odd number of vertices, then their roots v_i and v_j will be unmatched). Actually, since the number of vertices in T is even, there exists exactly one among $T_1, T_2, \ldots, T_\Delta$ with odd number of vertices.

Using Corollary 3.3, we may transform each T_i into a pendant path attached at v—while simultaneously decreasing EE and keeping the existence of a perfect matching. Assume that T_Δ has odd number of vertices, while the remaining trees have even number of vertices. We apply similar transformation to the one in Theorem 3.2, but instead of moving one edge, we move two edges in order to keep the existence of a perfect matching. Thus, if $p \geqslant q \geqslant 2$ then from Corollary 3.3

$$EE(G(p,q)) > EE(G(p+2, q-2)).$$

Using this transformation we may reduce T_Δ to one vertex, the trees $T_2, \ldots, T_{\Delta-1}$ to two vertices, leaving T_1 with $n-2\Delta$ vertices, and thus obtaining $A_{n,\Delta}$. Since we have been strictly decreasing EE at all times, we conclude that $A_{n,\Delta}$ indeed has minimum EE among the trees with perfect matching. □

If $\Delta > 2$, we can apply the transformation from Corollary 3.3 (by moving two vertices) at the vertex of degree Δ in $A_{n,\Delta}$ to obtain $A_{n,\Delta-1}$. Thus, it follows that

$$EE(A_{n,n/2}) > EE(A_{n,n/2-1}) > \cdots > EE(A_{n,3}) > EE(A_{n,2}) = EE(P_n).$$

5 The maximum spectral moments and Estrada index

The complete Δ-ary tree is defined as follows. Start with the root having Δ children. Every vertex different from the root, which is not in one of the last two levels, has

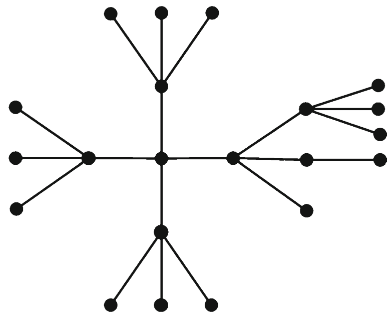


Fig. 3 The complete 4-ary tree of order 21

exactly $\Delta - 1$ children. In the last level, while not all nodes have to exist, the nodes that do exist fill the level consecutively (see Fig. 3). Thus, at most one vertex on the level second to last has its degree different from Δ and 1.

In [6] the authors proposed these trees to be called *Volkmann trees*, as they represent alkanes with minimal Wiener index [32]. Volkmann trees also have maximal greatest eigenvalue among trees with maximum degree Δ, as shown in [33].

The computer search among trees with up to 24 vertices revealed that the complete Δ-ary trees attain the maximum values of EE and even spectral moments of orders up to 16 among the trees with the maximum vertex degree Δ.

It is well-known that an integer sequence $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n \geqslant 1$ represents the degrees sequence of a tree if and only if $d_1 + d_2 + \cdots + d_n = 2n - 2$. Consider an arbitrary tree T with vertex degrees

$$\Delta = d_1 \geqslant d_2 \geqslant \cdots \geqslant d_{n-1} \geqslant d_n = 1.$$

From (2), the fourth spectral moment of trees depends only on the sum of squares of degrees, also known as the first Zagreb index [34]. In order to maximize the sum $Z(T) = \sum_{i=1}^{n} d_i^2$, assume that there exist two vertices i and j such that $1 < d_i \leqslant d_j < \Delta$. Simple transformation $d_i' = d_i - 1$, $d_j' = d_j + 1$ strictly increases M_4, as

$$Z(T') - Z(T) = (d_i - 1)^2 + (d_j + 1)^2 - d_i^2 - d_j^2 = 2(d_j - d_i + 1) \geqslant 2.$$

Therefore, the fourth spectral moment is maximized if at most one vertex of a tree has degree different from 1 and Δ, which is satisfied for the complete Δ-ary tree.

Based on this argument and the above-mentioned empirical observations, we pose the following

Conjecture 5.1 *For any $k \geqslant 2$, the complete Δ-ary tree has maximum spectral moment M_{2k} among trees on n vertices with maximum degree Δ.*

This conjecture implies the conjecture of Gutman et al. [6], thanks to Eq. (3).

While we do not have the proof of the above conjecture at the moment, we make a humble step forward by characterizing the starlike trees which maximize even spectral moments and the Estrada index.

Theorem 5.2 *The balanced Δ-starlike tree has maximum even spectral moments and maximum EE among Δ-starlike trees of order n.*

Proof Let $T = T(n_1, \ldots, n_\Delta)$ be an arbitrary Δ-starlike tree. If there exists i and j, $1 \le i, j \le \Delta$, such that $|n_i - n_j| > 1$, we can strictly increase its even spectral moments by applying Theorem 3.2 repeatedly until we obtain Δ-starlike tree with paths of lengths $\lfloor \frac{n_i+n_j}{2} \rfloor$ and $\lceil \frac{n_i+n_j}{2} \rceil$ instead of n_i and n_j.

The maximality of EE in such trees is shown analogously using Corollary 3.3. $\square$

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