

The signless Laplacian Estrada index of tricyclic graphs

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Abstract

The signless Laplacian Estrada index of a simple graph G is defined as $\text{SLEE}(G) = \sum_{i=1}^n e^{q_i}$ where q_1, q_2, \dots, q_n are the eigenvalues of the signless Laplacian matrix of G . In this paper we show that there are exactly two tricyclic graphs with the maximal signless Laplacian Estrada index.

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1 Introduction

Throughout this work, we are concerned with undirected simple graphs. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively, and we assume $|V(G)| = n$ and $|E(G)| = m$. The *cyclomatic number* of a graph G is defined as $r(G) = m - n + c$, where c is the number of connected components of G . For connected graphs it means $r(G) = m - n + 1$. If $r(G) = 3$, i.e, $m = n + 2$, then G is called a *tricyclic graph*. The class of all tricyclic graphs on n vertices is denoted by \mathcal{J}_n .

The adjacency matrix $\mathbf{A} = \mathbf{A}(G) = [a_{ij}]$ of G is a matrix whose (i, j) -th entry is equal to 1 if vertices i and j are adjacent, and 0 otherwise. The set of all eigenvalues of $A(G)$ is the *spectrum* of G , and the largest eigenvalue of G is called the *spectral radius* of G . It is well-known that different graphs can have the same spectrum; the smallest example is the so-called Saltire pair [13]. Hence, the question arises whether it is possible to uniquely reconstruct a graph from its spectrum. If this is possible, i.e., if a graph G is the only graph with a given spectrum, we say that G is *determined by its spectrum* and abbreviate it as G is DS. It is an open problem to determine the asymptotic fraction of DS graphs; we refer the reader to [13] for an in-deep treatment of this problem.

Denote by $\mathbf{Q} = \mathbf{D} + \mathbf{A}$ the signless Laplacian matrix of G , where $\mathbf{D} = \text{diag}(d_1, d_2, \dots, d_n)$ is the diagonal matrix of vertex degrees. The matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is the usual Laplacian matrix of G . The matrix \mathbf{Q} is positive semi-definite, so the eigenvalues of \mathbf{Q} can be ordered as $q_1 \geq q_2 \geq \dots \geq q_n \geq 0$. The largest eigenvalue of \mathbf{Q} is called the *signless Laplacian spectral radius* of graph and it is well known that this eigenvalue is simple and has a unique positive unit eigenvector. In spectral graph theory, the problem of determining graphs with maximum spectral radius of \mathbf{Q} is a prominent one on which many scholars have worked (e.g. [9, 12]). Additional results about spectral properties of the signless Laplacian matrix have been reported in [1, 4, 6, 11, 14]. In [13], the authors present some evidence that the matrix \mathbf{Q} might be better suited than the other graph matrices for studying various graph properties.

The *Estrada index* $\text{EE}(G)$ of a graph G is defined as

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

where λ_j are the eigenvalues of G . It was introduced by Estrada in 2000 [8] and has since found wide applications in chemistry, protein folding and study of complex networks. It was soon generalized also to the Laplacian case [15], and recently Ayyaswamy et al. [2] defined it also for the signless Laplacian matrix. The *signless Laplacian Estrada index* (hereafter denoted by SLEE) is defined as

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

Also, they specified bounds for SLEE in terms of the number of vertices and edges.

graphs on $n \leq 3$ vertices. Moreover, in the case where $n = 4$, H_7^4 (which is the complete graph on 4 vertices) is the unique (extremal) tricyclic graph.

There is an important point in the content of Theorem 2.2. In fact, it consists of two propositions: First, of course, it proposes two graphs H_6^n and H_7^n to be the only possible extremal n -vertex tricyclic graphs with maximum SLEE; second, it expresses that $\text{SLEE}(H_6^n) = \text{SLEE}(H_7^n)$. Actually, to prove the latter, we show (in Section 5) that the graphs H_6^n and H_7^n have the equal signless Laplacian eigenvalues sequences.

3 Preliminaries and lemmas

In this section, we first state some definitions and notations used in our research and restate some results proved in references [5, 7]. Then, we prove an auxiliary lemma which is important for achieving the goals of this article.

Recall that the k -th signless Laplacian spectral moment of a graph G is denoted by $T_k(G)$, and defined by $T_k(G) = \sum_{i=1}^n q_i^k$. Let \mathbf{Q}^k be the k -th power of signless Laplacian matrix of the graph G . Then, by definition of $T_k(G)$, one can easily see that $T_k(G)$ is equal to the trace of matrix \mathbf{Q}^k , i.e. $T_k(G) = \text{Tr}(\mathbf{Q}^k)$. Therefore, by Taylor expansion of exponential function e^{q_i} and the definition of $\text{SLEE}(G)$, we conclude

$$\text{SLEE}(G) = \sum_{k \geq 0} \frac{T_k(G)}{k!}. \quad (2)$$

This equation leads us to the idea of using the notion of signless Laplacian spectral moments of graphs to compare their SLEE's. To exploit this idea, we need a notion which is very closely related to the signless Laplacian spectral moments of a graph. The following definition and the proposition after that provide this suitable notion for us and state this close relation.

Definition 3.1. [5] A *semi-edge walk* of length k in graph G , is an alternating sequence $W = v_1 e_1 v_2 e_2 \cdots v_k e_k v_{k+1}$ of vertices $v_1, v_2, \dots, v_k, v_{k+1}$ and edges e_1, e_2, \dots, e_k such that the vertices v_i and v_{i+1} are end-vertices (not necessarily distinct) of edge e_i , for any $i = 1, 2, \dots, k$. If $v_1 = v_{k+1}$, then we say W is a *closed semi-edge walk*.

Proposition 3.2. [5] Let G be a graph and \mathbf{Q} be its signless Laplacian matrix. The number of semi-edge walks of length k starting at vertex v and ending at vertex u is equal to the (v, u) -th entry of the matrix \mathbf{Q}^k .

As a consequence of the above propositions, it follows that the number of closed semi-edge walks of length k in a graph G is equal to $T_k(G)$. Therefore, to calculate $T_k(G)$ we may use the set of all (closed) semi-edge walks of length k and its cardinality.

Let G and H be two graphs, $x, y \in V(G)$, and $u, v \in V(H)$. We denote by $SW_k(G; x, y)$, the set of all semi-edge walks, each of which is of length k in G , starting at vertex x , and ending at vertex y . For convenience, we may denote $SW_k(G; x, x)$

by $SW_k(G; x)$, and set $SW_k(G) = \bigcup_{x \in V(G)} SW_k(G; x)$. Given the above argument, we know that $T_k(G) = |SW_k(G)|$. We use the notation $(G; x, y) \preceq_s (H; u, v)$ for, if $|SW_k(G; x, y)| \leq |SW_k(H; u, v)|$, for all $k \geq 0$. Moreover, if $(G; x, y) \preceq_s (H; u, v)$, and there exists some k_0 such that $|SW_{k_0}(G; x, y)| < |SW_{k_0}(H; u, v)|$, then we write $(G; x, y) \prec_s (H; u, v)$.

Now, we restate the following lemma, which is an excellent tool to compare the SLEE's of two graphs, each of which has a particular subgraph that are isomorphic.

Lemma 3.3. [7] *Let G be a graph and $v, u, w_1, w_2, \dots, w_r \in V(G)$. Suppose that $E_v = \{e_1 = vw_1, \dots, e_r = vw_r\}$ and $E_u = \{e'_1 = uw_1, \dots, e'_r = uw_r\}$ where $e_i, e'_i \notin E(G)$, for $i = 1, 2, \dots, r$. Let $G_u = G + E_u$ and $G_v = G + E_v$. If $(G; v) \prec_s (G; u)$, and $(G; w_i, v) \preceq_s (G; w_i, u)$ for each $i = 1, 2, \dots, r$, then $SLEE(G_v) < SLEE(G_u)$.*

To use the above lemma, we say that the graph G_u is obtained from G_v by transferring vertices w_1, \dots, w_r from $N(v)$, the set of neighbors of v , to $N(u)$. In this situation, we call the vertices w_1, \dots, w_r the *transferred neighbors*, and the graph G is named the *transfer route*. Note that G is a subgraph of both G_u and G_v .

Although Lemma 3.3 is an excellent tool, it has many conditions which have to be provided when we want to use it. The following lemma enables us to discover a special case that provides such conditions.

Lemma 3.4. *Let G be a graph and $u, v \in V(G)$. If $N(v) \subseteq N(u) \cup \{u\}$, then $(G; v) \preceq_s (G; u)$, and $(G; w, v) \preceq_s (G; w, u)$ for each $w \in V(G)$. Moreover, if $deg_G(v) < deg_G(u)$, then $(G; v) \prec_s (G; u)$, where $deg_G(v)$ is the degree of vertex v in the graph G .*

Proof. Let $k \geq 0$, and $W \in SW_k(G; v)$. We can decompose W uniquely to $W_1W_2W_3$, such that W_1 and W_3 are as long as possible and consist of just the vertex v and edges vw where $w \in N(v) \setminus \{u\}$. Note that W_2 and W_3 are empty if W does not contain any other vertex than v . Let W'_j be obtained from W_j , for $j = 1, 3$, by replacing the vertex v by u , and edges vw by uw , where $w \in N(v) \setminus \{u\}$. The map $f : SW_k(G; v) \rightarrow SW_k(G; u)$, defined by the rule $f(W_1W_2W_3) = W'_1W_2W'_3$, is injective. Thus $(G; v) \preceq_s (G; u)$.

Similarly, by decomposing each semi-edge walk in $SW_k(G; w, v)$ and changing the end part of them, we conclude that $(G; w, v) \preceq_s (G; w, u)$.

Finally, since $deg_G(v) = SW_1(G; v)$, the last part of the lemma is obvious. □

4 The proof of Theorem 2.1

In this section, we determine the unique n -vertex extremal tricyclic graph with maximum SLEE which exactly has j simple cycles, for $j = 3, 4, 6, 7$.

The *base* of a tricyclic graph G , denoted by $B(G)$, and defined to be the unique maximal subgraph of G , containing no pendent vertices. Indeed, $B(G)$ is the unique minimal tricyclic subgraph of G , and G can be obtained from $B(G)$ by planting some trees on it.

The following lemma is expressing the importance of the rule of the base of an extremal graph with maximum SLEE.

Lemma 4.1. *Let G be an extremal graph with maximum SLEE over \mathcal{J}_n . Then each vertex in G is either in $B(G)$ or a pendent vertex.*

Proof. Let T be a subgraph of G with exactly one vertex in common with $B(G)$, say u . If T is not a star with center vertex u , then there is a neighbor of u in T , say v , such that $deg_G(v) > 1$. Let G' be the graph obtained from G by transferring all of the vertices in $N(v) \setminus \{u\}$ from $N(v)$ to $N(u)$, and H be the transfer route graph. Then, Lemma 3.4 implies that $(H; v) \prec_s (H; u)$, and therefore $SLEE(G) < SLEE(G')$, by Lemma 3.3, which is a contradiction. Hence, each subgraph of G with just one common vertex u with $B(G)$, is a star with center vertex u , and this is the desired result. \square

By [10], we know that there are 15 different bases of tricyclic graphs, and they can be classified to four classes according to their number of simple cycles (as shown in Figure 2):

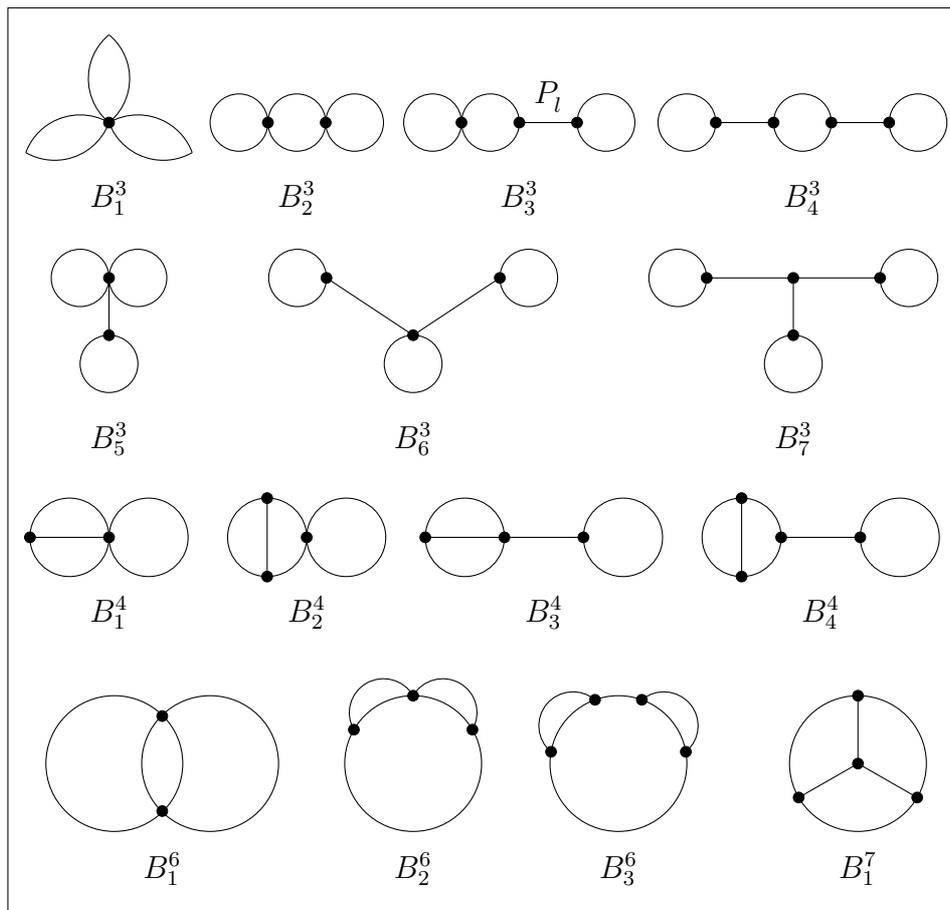


Figure 2: A demonstration of all possible bases in \mathcal{J}_n .

$$\begin{aligned} \mathcal{J}_n^3 &= \{G \in \mathcal{J}_n : B(G) \cong B_i^3 : i \in \{1, 2, \dots, 7\}\}, \\ \mathcal{J}_n^4 &= \{G \in \mathcal{J}_n : B(G) \cong B_i^4 : i \in \{1, 2, \dots, 4\}\}, \\ \mathcal{J}_n^6 &= \{G \in \mathcal{J}_n : B(G) \cong B_i^6 : i \in \{1, 2, 3\}\}, \\ \mathcal{J}_n^7 &= \{G \in \mathcal{J}_n : B(G) \cong B_i^7 : i \in \{1\}\}. \end{aligned}$$

With this classification, we surely have $\mathcal{J}_n = \mathcal{J}_n^3 \cup \mathcal{J}_n^4 \cup \mathcal{J}_n^6 \cup \mathcal{J}_n^7$. Through all infinite number of bases of tricyclic graphs, there are just 7 bases with the property that each of their edges belongs to at least one triangle. We denote these bases by $A_1^3, A_1^4, A_1^6, A_1^7, A_2^3, A_2^4$ and A_2^6 (as shown in Figure 3).

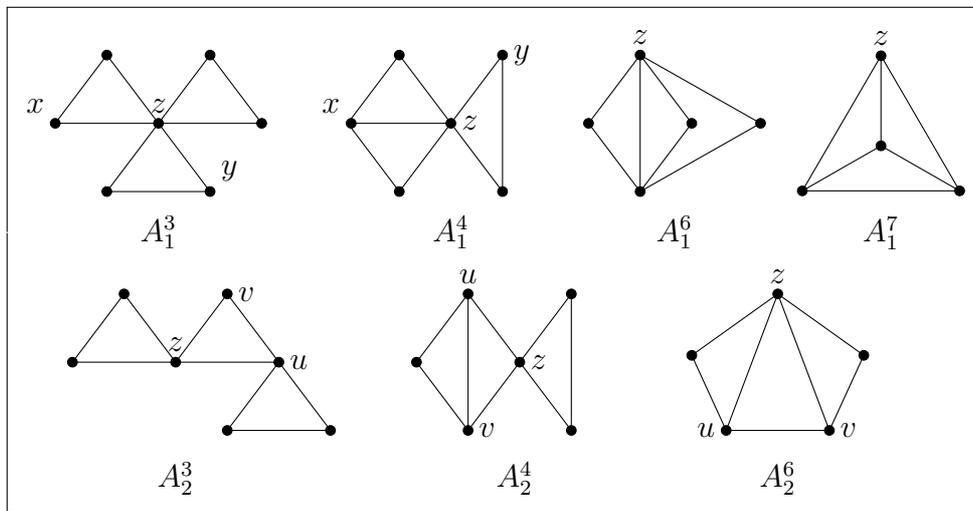


Figure 3: Bases A_i^j and A_1^7 , for $i \in \{1, 2\}$ and $j \in \{3, 4, 6\}$.

Note that according to the above notations, the aim of this section is to show that H_j^n is the unique extremal graph with maximum SLEE among the members of \mathcal{J}_n^j , for any $j \in \{3, 4, 6, 7\}$. To reach this goal, we need a suitable tool to compare the SLEE's of graphs with the same type of bases. Such a tool is provided in the following lemma.

Lemma 4.2. *Let G be a tricyclic graph with $u, v \in V(G)$, where $e = uv \in E(G)$ and $N(u) \cap N(v) = \emptyset$. If $G \in \mathcal{J}_n^j$, for some $j \in \{3, 4, 6, 7\}$, then there exists a graph $G' \in \mathcal{J}_n^j$ such that $\text{SLEE}(G) < \text{SLEE}(G')$.*

Proof. Let G' be the graph obtained from G , by transferring all of vertices in $N(v) \setminus \{u\}$ from $N(v)$ to $N(u)$, and H be the transfer route graph. By Lemma 3.4 we have $(H; v) \prec_s (H; u)$, which, according to the Lemma 3.3, implies that $\text{SLEE}(G) < \text{SLEE}(G')$. On the other hand, since the aforesaid transferring does not change the number of neither simple cycles nor edges, we conclude that $G' \in \mathcal{J}_n^j$. \square

Remark 4.3. By previous lemma, if the base of a tricyclic graph G has a path which is not in a simple cycle (e.g. B_3^3 has the path P_1 , as shown in Figure 2), then G is not

an extremal graph with maximum SLEE through \mathcal{J}_n^j , for $j \in \{3, 4\}$. Moreover, if two successive vertices of a simple cycle of G , say the vertices v_1 and v_2 of the simple cycle $c_q = v_1v_2 \cdots v_qv_1$, have no common neighbors (i.e. $N(v_1) \cap N(v_2) = \emptyset$), then G is not an extremal graph with maximum SLEE in \mathcal{J}_n^j , for $j \in \{3, 4, 6, 7\}$. Therefore, if $B(G)$ is the base of an extremal tricyclic graph in \mathcal{J}_n^j with maximum SLEE, then we have $B(G) \cong A_i^j$, for some $i \in \{1, 2\}$.

Lemma 4.4. *If G is an extremal graph with maximum SLEE in \mathcal{J}_n^j , for $j = 3, 4, 6, 7$, then $B(G) \cong A_1^j$.*

Proof. The case $j = 7$ is obvious. Let $j = 3$, and G be an extremal graph with maximum SLEE in \mathcal{J}_n^3 , such that $B(G) \cong A_2^3$. Suppose that G' is the graph obtained from G by transferring all of vertices in $N(u) \setminus \{z, v\}$ from $N(u)$ to $N(z)$, and H be the transfer route graph. Note that $B(G') \cong A_1^3$. Since $N_H(u) \subseteq N_H(z) \cup \{z\}$, Lemma 3.4 implies that $(H; u) \prec_s (H; z)$. Thus, by Lemma 3.3, $\text{SLEE}(G) < \text{SLEE}(G')$, which is a contradiction. Therefore, if G is an extremal graph with maximum SLEE in \mathcal{J}_n^3 , then $B(G) \cong A_1^3$.

For the case $i = 4$ (respectively, $i = 6$), the result follows by a method similar to the one used above and transferring all of vertices in $N(u) \setminus \{v, z\}$ from $N(u)$ to $N(z)$ (respectively, $N(v)$), where vertices v, u and z are shown in Figure 3. \square

Now, we are ready to prove our first main theorem. More precisely, in the proof of the Theorem 2.1 we show that H_j^n is, up to isomorphism, the unique extremal tricyclic graph with maximum SLEE among all tricyclic graphs with exactly j simple cycles, where $j \in \{3, 4, 6, 7\}$.

Proof of Theorem 2.1 Let $j \in \{3, 4, 6, 7\}$ and G be an extremal graph with maximum SLEE over \mathcal{J}_n^j . By previous lemmas, G is obtained by attaching some pendent vertices to some vertices of A_1^j . Let x be a vertex of A_1^j , where $x \neq z$ and it has some pendent neighbors (the vertex z is shown in Figure 3). Further, let $N^{np}(x)$ be the set of all non-pendent neighbors of x . Since $N^{np}(x) \subseteq N(z) \cup \{z\}$, by transferring pendent neighbors of x from $N(x)$ to $N(z)$ and applying Lemma 3.4, we get a graph G' such that $\text{SLEE}(G) < \text{SLEE}(G')$, which is a contradiction. Therefore, all of $n - |V(A_1^j)|$ pendent vertices of G are attached to z . It means that G is isomorphic to H_j^n \square

5 The proof of Theorem 2.2

In this section, we prove the first claim of Theorem 2.2 in the next lemma. Afterward, we present the proof of the second claim of the theorem to close the section.

Lemma 5.1. *Let G be an extremal graph with the maximum SLEE among the graphs in \mathcal{J}_n . Then $B(G) \cong A_1^j$, where $j \in \{6, 7\}$.*

Proof. Let G be an extremal graph with maximum SLEE in \mathcal{J}_n . By Lemma 4.4, it is enough to show that $B(G)$ is isomorphic to neither A_1^3 nor A_1^4 .

Let $B(G) \cong A_1^3$ or A_1^4 (as shown in Figure 3). Suppose that G' is the graph obtained from G by transferring all of vertices in $N(y) \setminus \{z\}$ from $N(y)$ to $N(x)$, and let H be the transfer route graph. Since $N_H(y) \subset N_H(x)$, we have $(H; y) \prec_s (H; x)$ and $(H; w, y) \preceq_s (H; w, x)$, by Lemma 3.4, for each $w \in N(y) \setminus \{z\}$. Thus by Lemma 3.3, we get $\text{SLEE}(G) < \text{SLEE}(G')$, which is a contradiction. Therefore $B(G) \cong A_1^6$ or A_1^7 . \square

Proof of Theorem 2.2 For the first claim of the theorem, we turn your attention to the fact that Theorem 2.1 and the previous lemma guarantee that only graphs H_6^n and H_7^n are candidates for being extremal graphs with maximum SLEE over \mathcal{J}_n .

In the following, we show that these two graphs have simultaneous maximum SLEE value over the members of \mathcal{J}_n . To do this, it is enough to show that the characteristic polynomials of $\mathbf{Q}(H_6^n)$ and $\mathbf{Q}(H_7^n)$ are equal. This means that the eigenvalue sequences of these matrices are equal. Therefore, by Equation 1, $\text{SLEE}(H_6^n) = \text{SLEE}(H_7^n)$ as desired.

Let us use labels for vertices of H_6^n and H_7^n as shown in Figure 4.

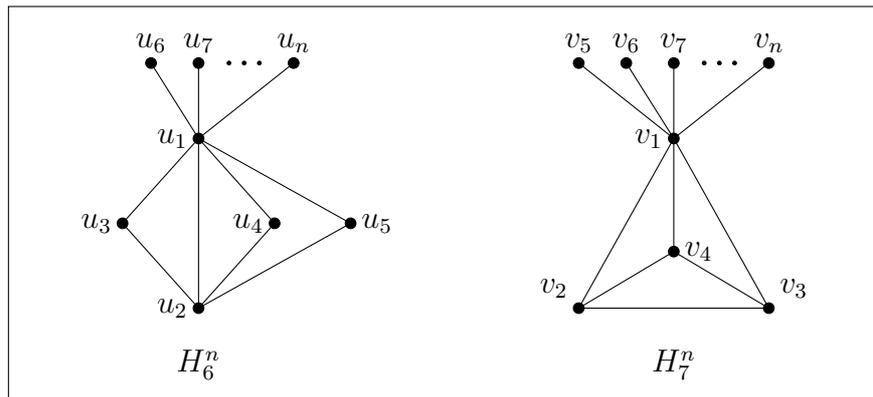


Figure 4: The two n -vertex tricyclic graphs which are simultaneous extremal with maximum SLEE value.

For $j \in \{6, 7\}$, let \mathbf{S}_j be the sub-matrix of $\mathbf{Q}(H_j^n)$, obtained by removing the first row and column. Moreover, suppose that $\mathbf{M}_j^{n,r}$ is the sub-matrix of $\mathbf{Q}(H_j^n)$ obtained by removing last $n - r$ rows and columns, for $5 \leq r \leq n$. Obviously, $\mathbf{Q}(H_j^n) = \mathbf{M}_j^{n,n}$. Indeed, we have:

$$\mathbf{S}_6 = \begin{bmatrix} 4 & 1 & 1 & 1 \\ 1 & 2 & 0 & 0 \\ 1 & 0 & 2 & 0 \\ 1 & 0 & 0 & 2 \end{bmatrix} \quad \mathbf{S}_7 = \begin{bmatrix} 3 & 1 & 1 & 0 \\ 1 & 3 & 1 & 0 \\ 1 & 1 & 3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

and

$$\mathbf{Q}(H_j^n) = \begin{bmatrix}
 \overbrace{\begin{matrix} (n-1) & 1 & 1 & 1 & 1 & 1 & \dots & 1 \\
 1 & \mathbf{S}_j & 0 & \dots & 0 & 0 & \dots & 0 \\
 1 & \mathbf{S}_j & 0 & \dots & 0 & 0 & \dots & 0 \\
 1 & \mathbf{S}_j & 0 & \dots & 0 & 0 & \dots & 0 \\
 1 & \mathbf{S}_j & 0 & \dots & 0 & 0 & \dots & 0 \\
 1 & 0 & 0 & 0 & 0 & 1 & \dots & 0 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
 1 & 0 & 0 & 0 & 0 & 0 & \dots & 1 \\
 1 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\
 \vdots & \vdots \\
 1 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\
 \vdots & \vdots \\
 1 & 0 & 0 & 0 & 0 & 0 & \dots & 1 \end{matrix}}^{\mathbf{M}_j^{n,r}} & 1 & \dots & 1 \\
 \end{bmatrix}$$

Recall that the characteristic polynomial of any $n \times n$ -matrix \mathbf{M} is defined to be $\phi(\mathbf{M}) = \det(\mathbf{M} - x \mathbf{I}_n)$, where \mathbf{I}_n is the $n \times n$ identity matrix.

Now, let $n \geq 6$ and $5 < r \leq n$. We evaluate $\phi(\mathbf{M}_j^{n,r})$ by computing the cofactor expansion along the last row and then computing the subsequent cofactor expansions along the last column. We get the following recursive formula for both $j = 6$ and 7 :

$$\phi(\mathbf{M}_j^{n,r}) = -(1-x)^{n-6} \phi(\mathbf{S}_j) + (1-x) \phi(\mathbf{M}_j^{n,r-1}).$$

Therefore,

$$\phi(\mathbf{Q}(H_j^n)) = \phi(\mathbf{M}_j^{n,n}) = -(n-5)(1-x)^{n-6} \phi(\mathbf{S}_j) + (1-x)^{n-5} \phi(\mathbf{M}_j^{n,5}).$$

Also, for $r = 5$, by a few algebraic calculations, one can easily show that

$$\begin{aligned}
 \phi(\mathbf{M}_6^{n,5}) &= x^5 + (-n-9)x^4 + (10n+19)x^3 + (13-33n)x^2 + (44n-72)x - 20n + 52 \\
 &= \phi(\mathbf{M}_7^{n,5}),
 \end{aligned}$$

$$\phi(\mathbf{S}_6) = x^4 - 10x^3 + 33x^2 - 44x + 20 = \phi(\mathbf{S}_7).$$

Therefore the result holds for $n \geq 5$ by using the last three formulas. □

6 Concluding remarks

In this paper we have studied the signless Laplacian Estrada index and determined its maximum values and corresponding graphs over the class of all tricyclic graphs on a given number of vertices. It would be of interest to study its behavior also on other classes of connected graphs with simple connectivity patterns and cycle structure. Among the most promising candidates are linear polymers and cactus graphs, as well as the graphs that arise from simpler components via binary operations of splice and link.

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