Tricyclic graph with maximal Estrada index

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Abstract

Let $G$ be a simple connected graph on $n$ vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the adjacency matrix of $G$. The Estrada index of $G$ is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. Let $T_n$ be the class of tricyclic graphs $G$ on $n$ vertices. In this paper, the graphs in $T_n$ with the maximal Estrada index is characterized.

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1. Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. If $m = n - 1 + c$, then $G$ is called a $c$-cyclic graph. If $c = 0$, 1, 2 and 3, then $G$ is a tree, unicyclic graph, bicyclic graph and tricyclic graph, respectively. Denote by $T_n$ the class of tricyclic graph $G$ on $n$ vertices.

Let $A(G)$ be the $(0, 1)$-adjacency matrix of $G$. The characteristic polynomial $\phi(G; x)$ of $G$ is $|xI - A(G)|$, where $I$ is the unit matrix. We call the eigenvalues $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ (for short $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$) of $A(G)$ the spectrum of $G$. A graph-spectrum-based molecular structure descriptor, named Estrada index, put forward by Estrada [6], is defined as

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

Since then, the Estrada index has found 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 [7–9], and to measure the centrality of complex (reaction, metabolic, communication, social, etc.) networks [10,11]. There is also a connection between the Estrada index and the extended atomic branching of molecules [12]. Besides these applications, the Estrada index has also been extensively studied in mathematics (see [13,14,17–19]). Among these, Ilić and Stevanović [13] obtained the unique tree with minimum Estrada index among the set of trees with given maximum degree. Zhang et al. [17] determined the unique tree with maximum Estrada indices among the set of trees with given matching number. In [4], Z. Du and B. Zhou characterized the unique unicyclic graph with maximum Estrada index, and L. Wang et al. [16] determine the unique graph with maximum Estrada index among bicyclic graphs with fixed order. In this paper, we further consider the Estrada index of tricyclic graphs in $T_n$.

In order to state our results, we introduce some notation and terminology. For other undefined notation we refer to Bollobás [1]. Let $P_n$, $C_n$ and $S_n$ be the path, the cycle and the star on $n$ vertices, respectively. Let $N_C(u) = \{v | uv \in E(G)\}$,

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$N_C(v) = N_G(v) \cup \{v\}$. Denote by $d_C(v) = |N_C(v)|$ the degree of the vertex $v$ of $G$. If $E_G \subseteq E(G)$, we denote by $G - E_0$ the subgraph of $G$ obtained by deleting the edges in $E_0$. If $E_1$ is the subset of the edge set of the complement of $G$, $G + E_1$ denotes the graph obtained from $G$ by adding the edges in $E_1$. Similarly, if $W \subseteq V(G)$, we denote by $G - W$ the subgraph of $G$ obtained by deleting the vertices of $W$ and the edges incident with them. If $E = \{xy\}$ and $W = \{v\}$, we write $G - xy$ and $G - v$ instead of $G - \{xy\}$ and $G - \{v\}$, respectively.

2. Preliminaries

Let $M_k(G)$ be the $k$th spectral moment of the graph $G$, i.e., $M_k(G) = \sum_{i=1}^{n}\lambda_i^k$. We know from [2] that $M_k(G)$ is equal to the number of closed walks of length $k$ in $G$. It is well known that the first few spectral moments satisfy the following relations:

$$M_0(G) = n, \quad M_1(G) = 0, \quad M_2(G) = 2m, \quad M_3(G) = 6t, \quad M_4(G) = 2\sum_{i=1}^{n}d_i^2 - 2m + 8q,$$

where $t$ is the number of triangles, $q$ the number of quadrangles and $d_i = d_C(v)$ the degree of $v_i$ in $G$, respectively. From the Taylor expansion of $e^x$, it is easy to see that the Estrada index and the spectral moments of $G$ are related by

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

Thus, if for two graphs $G_1$ and $G_2$ we have $M_k(G_1) \geq M_k(G_2)$ for all $k \geq 0$, then $EE(G_1) \geq EE(G_2)$. Moreover, if there is at least one positive integer $k_0$ such that $M_{k_0}(G_1) > M_{k_0}(G_2)$, then $EE(G_1) > EE(G_2)$.

For any vertices $u$, $v$ and $w$ (not necessarily distinct) in $G$, we denote by $M_k(G; u, v)$ the number of walks in $G$ with length $k$ from $u$ to $v$, and by $W_k(G; u, v)$ the number of walks in $G$ with length $k$ from $u$ to $v$ which go through $w$. Denote by $W_k(G; u, v)$ a walk of length $k$ from $u$ to $v$ in $G$, and by $W_k(G; u, v)$ the set of all such walks. Clearly $M_k(G; u, v) = |W_k(G; u, v)|$. Note that

$$M_k(G; u, v) = M_k(G; v, u)$$

for any positive integer $k$ [2].

Let $G$ and $H$ be two graphs with $u_1, v_1 \in V(G)$ and $u_2, v_2 \in V(H)$. If $M_k(G; u_1, v_1) \leq M_k(H; u_2, v_2)$ for all positive integers $k$, then we write $(G; u_1, v_1) \preceq (H; u_2, v_2)$. If $(G; u_1, v_1) \preceq (H; u_2, v_2)$ and there is at least one positive integer $k_0$ such that $M_{k_0}(G; u_1, v_1) < M_{k_0}(H; u_2, v_2)$, then we write $(G; u_1, v_1) \prec (H; u_2, v_2)$.

The following lemmas will be used in this paper.

**Lemma 2.1** ([2]). Let $v$ be a vertex of a graph $G$, and $C(v)$ be the set of all cycles containing $v$. Then the characteristic polynomial of $G$ satisfies

$$\phi(G; x) = x\phi(G - v; x) - \sum_{u \in E(G)} \phi(G - u - v; x) - 2 \sum_{Z \in C(v)} \phi(G \setminus V(Z); x),$$

where $\phi(G - u - v; x) = 1$ if $G$ is a single edge, and $\phi(G \setminus V(Z); x) = 1$ if $G$ is a cycle.

**Lemma 2.2** ([3]). Let $H$ be a graph (not necessarily connected) with $u, v \in V(H)$. Suppose that $w_i \in V(H)$, and $uw_i, vw_i \notin E(H)$ for $i = 1, 2, \ldots, r$, where $r$ is a positive integer. Let $E_u = \{uw_1, uw_2, \ldots, uw_r\}$ and $E_v = \{vw_1, vw_2, \ldots, vw_r\}$. Let $H_u = H + E_u$ and $H_v = H + E_v$. If $(H; u) \prec (H; v)$ and $(H; w_i, u) \preceq (H; w_i, v)$ for $1 \leq i \leq r$, then $EE(H_u) < EE(H_v)$.

**Lemma 2.3** ([5]). Let $G_1$ and $G_2$ be connected graphs with $u \in V(G_1)$ and $v \in V(G_2)$. Let $G$ be the graph obtained by joining $u$ with $v$ by an edge, and let $G'$ be the graph obtained by identifying $u$ with $v$, and attaching a pendant vertex to the common vertex. If $d_G(u), d_G(v) \geq 2$, then $EE(G) < EE(G')$.

The coalescence of two vertex-disjoint connected graphs $G, H$, denoted by $G(u) \circ H(w)$, where $u \in V(G)$ and $w \in V(H)$, is obtained by identifying the vertex $u$ of $G$ with the vertex $w$ of $H$. A graph is called nontrivial if it contains at least two vertices.

**Lemma 2.4** ([16]). Let $H_1$ be a connected graph containing two vertices $u, v$, and let $H_2$ be a connected graph disjoint to $H_1$, which contains a vertex $w$. Let $H'_2$ be a copy of $H_2$, containing the vertex $w'$ corresponding to $w$ of $H_2$. Let $G = (H_1(u) \circ H_2(w))(v) \circ H'_2(w')$.

(i) If there exists an automorphism $\sigma$ of $H_1$ such that it interchanges $u$ and $v$, then $(G; u, t) = (G; v, \sigma(t))$ for any vertex $t$.

(ii) If letting $H_1$ be obtained from $H_1$ by adding some edges incident with $v$ but not $u$, letting $H_2$ be obtained from $H'_2$ by adding some vertices or edges such that the resulting graph is connected, and letting $G$ be obtained from $G$ by replacing $H_1$ with $H_1$ or $H'_2$ with $H_2$, then $(G; u, t) < (G; v, \sigma(t))$.

3. Tricyclic graphs with maximal Estrada index

For a graph $G \in \mathcal{G}_n$, the base of $G$, denoted by $B(G)$, is the minimal tricyclic subgraph of $G$. Obviously, $B(G)$ is the unique tricyclic subgraph of $G$ containing no pendant vertex, and $G$ can be obtained from $B(G)$ by planting trees to some vertices of
B(G). By [15], we know that tricyclic graphs have the following four types of bases (as shown in Figs. 1–4): $G^3_j$ $(j = 1, \ldots, 7)$, $G^4_j$ $(j = 1, \ldots, 4)$, $G^6_j$ $(j = 1, \ldots, 3)$ and $G^7_1$. Let

$$\mathcal{T}^3_n = \{G|B(G) \cong G^3_j, j \in \{1, \ldots, 7\}\}; \quad \mathcal{T}^4_n = \{G|B(G) \cong G^4_j, j \in \{1, \ldots, 4\}\};$$

$$\mathcal{T}^6_n = \{G|B(G) \cong G^6_j, j \in \{1, \ldots, 3\}\}; \quad \mathcal{T}^7_n = \{G|B(G) \cong G^7_1\}.$$

Then $\mathcal{T}_n = \mathcal{T}^3_n \cup \mathcal{T}^4_n \cup \mathcal{T}^6_n \cup \mathcal{T}^7_n$.

Repeatedly by Lemma 2.3, we have the following lemmas.

**Lemma 3.1.** If $G^*$ be a extremal graph with maximal Estrada index in $\mathcal{T}_n$, then $G^*$ is obtained from its base by attaching some pendent vertices.

**Lemma 3.2.** (i) If $G^*$ be a extremal graph with maximal Estrada index in $\mathcal{T}^3_n$, then $B(G^*) \cong G^3_j, j \in \{1, 2\}$.

(ii) If $G^*$ be a extremal graph with maximal Estrada index in $\mathcal{T}^4_n$, then $B(G^*) \cong G^4_j, j \in \{1, 2\}$. 
Lemma 3.3. If $G_1$ be a extremal graph with maximal Estrada index in $\mathcal{F}^4_n$, then there exists a graph $G_2$ in $\mathcal{F}^4_n$ such that $EE(G_2) > EE(G_1)$.

Proof. By Lemma 3.2(i), we know that $B(G_1) \cong G^3_1$, $j \in \{1, 2\}$. If $B(G_1) \cong G^1_1$, let $uv, vt, uw, ws \in E(G_1)$ (as shown in Fig. 1). Without loss of generality, let $d_{G_1}(w) \geq d_{G_1}(v).$

Let $H_1$ be the graph obtained from $G_1$ by deleting $ws$, $vt$, $d_{G_1}(w) - 2$ pendent edges attached at $w$ and $d_{G_1}(v) - 2$ pendent edges attached at $v$. Then there exists an automorphism $\sigma$ of $H_1$ which interchange $v$ and $w$, and preserves all other vertices.

Let $H_2 \cong K_1d_{G_1}(v) - 2$ with center $v'$ and $G_0 = (H_1(v) \circ H_2(v'))(w) \circ H_2(v')$. By Lemma 2.4(i), we have $(G_0; v, x) = (G_0; x, v, (x))$ for any vertex $x \in V(G_0).$ Further, let $G_3$ be the graph obtained from $G_0$ by adding edge $uw, wu$, $w_1w_2 \in E(G_1)$ (as shown in Fig. 2). Note that $C_4 \cap C_6 = P$ in $G_4$. Without loss of generality, let $d_{G_1}(w_1) \geq d_{G_1}(v_1).

Case 1. If $r \neq 1$, let $H_1$ be the graph obtained from $G_1$ by deleting $w_1w_2, v_1v_2, d_{G_1}(w_1) - 2$ pendent edges attached at $w_1$ and $d_{G_1}(v_1) - 2$ pendent edges attached at $v_1$. Then there exists an automorphism $\sigma$ of $H_1$ which interchange $v_1$ and $w_1$, and preserves all other vertices.

Let $H_2 \cong K_1d_{G_1}(v_1) - 2$ with center $v'$ and $G_0 = (H_1(v_1) \circ H_2(v'))(w_1) \circ H_2(v').$ By Lemma 2.4(i), we have $(G_0; v_1, x) = (G_0; v_1, x, (x))$ for any vertex $x \in V(G_0).$ Further, let $G_3$ be the graph obtained from $G_0$ by adding edge $w_1u_1, w_1u_2$ and $d_{G_1}(w_1) - d_{G_1}(v_1)$ pendent edges attached at $w_1$. Then by Lemma 2.4(ii), we have $(G_0; v_1, x) = (G_0; v_1, x, (x))$ for any vertex $x \in V(G_0).$

Case 2. If $r = 1$ and $d_{G_1}(w_1) \geq d_{G_1}(v_1)+1$, let $H_1$ be the graph obtained from $G_1$ by deleting $w_1v_1$ and the edges $w_1u_1, w_1u_2$ on $C_4$ which is adjacent to $w_1, d_{G_1}(w_1) - 3$ pendent edges attached at $w_1$ and $d_{G_1}(v_1) - 2$ pendent edges attached at $v_1$. Then there exists an automorphism $\sigma$ of $H_1$ which interchange $v_1$ and $w_1$, and preserves all other vertices.

Let $H_2 \cong K_1d_{G_1}(v_1) - 3$ with center $v'$ and $G_0 = (H_1(v_1) \circ H_2(v'))(w_1) \circ H_2(v').$ By Lemma 2.4(i), we have $(G_0; w_1, x) = (G_0; w_1, x, (x))$ for any vertex $x \in V(G_0).$ Further, let $G_3$ be the graph obtained from $G_0$ by adding edge $w_1u_1, w_1u_2$ and $d_{G_1}(w_1) - d_{G_1}(v_1)$ pendent edges attached at $w_1$. Then by Lemma 2.4(ii), we have $(G_0; v_1, x) = (G_0; v_1, x, (x))$ for any vertex $x \in V(G_0).$

Case 3. If $r = 1$ and $d_{G_1}(w_1) = d_{G_1}(v_1)$, let $H_1$ be the graph obtained from $G_1$ by deleting the edges $w_1u_1, w_1u_2$ on $C_4$ which is adjacent to $w_1$ and $v_1v_2, d_{G_1}(w_1) - 3$ pendent edges attached at $w_1$ and $d_{G_1}(v_1) - 2$ pendent edges attached at $v_1$. Then there exists an automorphism $\sigma$ of $H_1$ which interchange $v_1$ and $w_1$, and preserves all other vertices.

Let $H_2 \cong K_1d_{G_1}(v_1) - 3$ with center $v'$ and $G_0 = (H_1(v_1) \circ H_2(v'))(w_1) \circ H_2(v').$ By Lemma 2.4(i), we have $(G_0; w_1, x) = (G_0; w_1, x, (x))$ for any vertex $x \in V(G_0).$ Further, let $G_3$ be the graph obtained from $G_0$ by adding edge $w_1u_1, w_1u_2$ and $d_{G_1}(w_1) - d_{G_1}(v_1)$ pendent edges attached at $w_1$. Then by Lemma 2.4(ii), we have $(G_0; v_1, x) = (G_0; v_1, x, (x))$ for any vertex $x \in V(G_0).$

By an argument similar to that in the proof of $B(G_1) \cong G^3_1$, we can also show that $B(G_1) \cong G^3_3$. This completes the proof of Lemma 3.3. □

Lemma 3.4. If $G_1$ be a extremal graph with maximal Estrada index in $\mathcal{F}^4_n$, then there exists a graph $G_2$ in $\mathcal{F}^4_n$ such that $EE(G_2) > EE(G_1)$.

Proof. By Lemma 3.2(ii), we know that $B(G_1) \cong G^3_1$, $j \in \{1, 2\}$. If $B(G_1) \cong G^1_1$, let $uv, v_1v_2, uv_1, w_1w_2 \in E(G_1)$ (as shown in Fig. 2). Then by Lemma 2.4(ii), we have $(G_0; v, x) = (G_0; v, x, (x))$ for any vertex $x \in V(G_0).$ Obviously, $G_1 = G_3 + v_1v_2$. Let $G_2 = G_3 + v_1v_2$, obviously, $G_2 \in \mathcal{F}^6_n$. By Lemma 2.2, we have $EE(G_2) > EE(G_1)$.

Case 2. If $r = 1$ and $d_{G_1}(w_1) \geq d_{G_1}(v_1)+1$, let $H_1$ be the graph obtained from $G_1$ by deleting $w_1u_1, w_1u_2$ and $d_{G_1}(w_1) - 3$ pendent edges attached at $w_1$. Then there exists an automorphism $\sigma$ of $H_1$ which interchange $v_1$ and $w_1$, and preserves all other vertices.

By an argument similar to that in the proof of $B(G_1) \cong G^3_1$, we can also show that $B(G_1) \cong G^3_3$. This completes the proof of Lemma 3.4. □

By Lemmas 3.1–3.4, we have the following corollary.

Corollary 3.5. Let $G^*$ be a graph with maximal Estrada index in $\mathcal{F}_n$, then $B(G^*) \cong G^6_j (j \in \{1, 2, 3\})$ or $B(G^*) \cong G^7_1$.

The internal path of $G$ is a walk $v_0v_1 \ldots v_s$ such that the vertices $v_0, v_1, \ldots, v_s$ are distinct, $d_G(v_0) > 2, d_G(v_s) > 2$, and $d_G(v_i) = 2$, whenever $0 < i < s$.

Lemma 3.6. Let $G \in \mathcal{F}^6_n \cup \mathcal{F}^7_n$, $P^k_i (1 \leq i \leq d_{B(G)}(u))$ be the internal path in $B(G)$ with one end vertex $u$, where $d_{B(G)}(u) \geq 3$ ($u \in B(G)$), if there exist two paths $P^k_i, P^l_j (1 \leq k \leq d_{B(G)}(u))$ with $|P^k_i| \geq 1, |P^l_j| \geq 1$, then there exists a graph $\tilde{G} \in \mathcal{F}^6_n \cup \mathcal{F}^7_n$ such that $|E(B(G))| - |E(B(\tilde{G}))| = 1$ and $EE(\tilde{G}) > EE(G)$.

Proof. Let $P^k_i = uw_1 \ldots u_i, P^l_j = uw_1 \ldots u_j, \eta \geq 1, j \geq 1, t \geq 3$.

Case 1. If $s \geq 2, t \geq 3$, without loss of generality, let $d_G(w_1) \geq d_G(v_1)$.

Let $H_1$ be the graph obtained from $G$ by deleting the edges $w_1w_2$ and $w_1v_1, d_G(v_1) - 2$ pendent edges attached at $v_1$ and $d_G(w_1) - 2$ pendent edges attached at $w_1$. Then there exists an automorphism $\sigma$ of $H_1$ which interchange $v_1$ and $w_1$, and preserves all other vertices.
Let $H_2 \cong K_{1, \delta c(v)} - 2$ with center $v'$ and $G_0 = (H_1(v) \circ H_2(v'))(w_1) \circ H_2(v')$. By Lemma 2.4(i), we have $(G_0; w_1, v) = (G_0; v, \sigma(v))$ for any vertex $v \in V(G_0)$. Further, let $G_1$ be the graph obtained from $G_0$ by adding edge $w_1w_2$ and $d_c(w_1) - d_c(v)$ pendant edges attached at $w_1$. Then by Lemma 2.4(ii), we have $(G_1; w_1, v) \not\cong (G_1; v, \sigma(v))$ for any vertex $v \in V(G_1)$. Obviously, $G = G_1 + v_1v_2$. Let $\tilde{G} = G_1 + w_1v_2$, obviously, $\tilde{G} \in \mathcal{F}_6^{2x} \cup \mathcal{F}_7^{2x}$ and $|E(B(G))| - |E(B(\tilde{G}))| = 1$. By Lemma 2.2, we have $EE(\tilde{G}) > EE(G)$.

Case 2. If $s = 1$, $t \geq 3$, by $d_{B(G)}(u) \geq 3$, let $P_u = u x_1 \ldots x_t$ be the third path with one end vertex $u$, $|P_u| \geq 1$.

Case 2.1. If $|P_u| \geq 2$, then the two paths $P_u$, $P_u'$ coincide with the conditions of Case 1, we can obtain a graph with larger Estrada index.

Case 2.2. If $|P_u| = 1$, then $d_{B(G)}(x_1) \geq 3$ and $x_1 \not\in V(P_u)$. Let $x_1$, $x_2$ be two vertex adjacent to $x_1$ in $B(G)$. If $d_{B(G)}(x_1) \geq d_{B(G)}(u)$, let $H_1$ be the graph obtained from $G$ by deleting the edges $w_1w_2$ and $x_1x_1^1$, $x_1x_2^1$, $d_c(w_1) - 2$ pendant edges attached at $w_1$ and $d_c(x_1) - 3$ pendant edges attached at $x_1$. Then there exists an automorphism $\sigma$ of $H_1$ which interchange $w_1$ and $x_1$ and preserves all other vertices.

Let $H_2 \cong K_{1, \delta c(v)} - 2$ with center $v'$ and $G_0 = (H_1(v) \circ H_2(v'))(w_1) \circ H_2(v')$. By Lemma 2.4(i), we have $(G_0; w_1, v) = (G_0; v, \sigma(v))$ for any vertex $v \in V(G_0)$. Further, let $G_1$ be the graph obtained from $G_0$ by adding edge $x_1x_1^1 + x_1x_2^2$ and $d_c(x_1) - d_c(v_1) - 1$ pendant edges attached at $x_1$. Then by Lemma 2.4(ii), we have $(G_1; x_1, v) \not\cong (G_1; x_1, \sigma(v))$ for any vertex $v \in V(G_1)$. Obviously, $G = G_1 + w_1v_2$. Let $\tilde{G} = G_1 + w_2x_1$, obviously, $\tilde{G} \in \mathcal{F}_6^{2x} \cup \mathcal{F}_7^{2x}$ and $|E(B(G))| - |E(B(\tilde{G}))| = 1$. By Lemma 2.2, we have $EE(\tilde{G}) > EE(G)$. □

Similar to the proof of Lemma 3.6, we have the following lemmas.

**Lemma 3.7.** Let $G \in \mathcal{F}_6^{2x} \cup \mathcal{F}_7^{2x}$, $P_u = uv_1v_2$ and $P_u' = uw_1w_2$ be two internal path in $B(G)$, where $d_{B(G)}(u) \geq 3$ ($u \in B(G)$), if $u \neq w_2$, then there exists a graph $\tilde{G} \in \mathcal{F}_6^{2x} \cup \mathcal{F}_7^{2x}$ such that $|E(B(G))| - |E(B(\tilde{G}))| = 1$ and $EE(\tilde{G}) > EE(G)$.

**Lemma 3.8.** Let $G$ be the graph with $B(G) \cong A_4$ (as shown in Fig. 5), then there is a graph $\tilde{G}$ such that $B(\tilde{G}) \cong A_3$ and $EE(\tilde{G}) > EE(G)$.

Let $P_u(1 \leq i \leq d_{B(G)}(u))$ be the internal path in $B(G)$ with one end vertex $u$, where $d_{B(G)}(u) \geq 3$ ($u \in B(G)$) and $P_u$, $P_u'$ ($1 \leq l, k \leq d_{B(G)}(u)$) be two such paths with $|P_u| = s$, $|P_u'| = t$. Note that the complement of the case of $s \geq 1$, $t \geq 3$ is $s \leq 1$, $t \leq 2$. It can be further divided into the three cases:

(i) $s \geq 3$, $t = 2$;  (ii) $s \geq 3$, $t = 1$;  (iii) $s \leq 2$, $t \leq 2$.

If (i) or (ii) holds, by Lemma 3.6, we can obtain a graph $\tilde{G}$ such that $EE(\tilde{G}) > EE(G)$. In order to find the extremal graph with maximal Estrada index, we only need to consider the case $|P_u| \leq 2 (1 \leq i \leq d_{B(G)}(u))$. Further by Lemmas 3.7 and 3.8, we have the following corollary.

**Corollary 3.9.** Let $G^*$ be a graph with maximal Estrada index in $\mathcal{F}_6^{2x} \cup \mathcal{F}_7^{2x}$, then $B(G^*) \cong A_i, i \in \{1, 2, 3, 5, 6, 7\}$ (as shown in Fig. 5).
Lemma 3.10. Let $G^*$ be a extremal graph with maximal Estrada index and $B(G) \cong A_i, i \in \{1, 2, 3, 5, 6, 7\}$ (as shown in Fig. 5), then $G^*$ is obtained from $A_i$ by attaching $n - |V(A_i)|$ pendant vertices at a vertex $w_4$ with maximum degree in $A_i(i \in \{1, 2, 3, 5, 6, 7\})$.

Proof. For the case of $B(G^*) \cong A_1$, let $w_i(i \in \{1, 2, 3, 4, 5\})$ be the vertices of $A_1$ as shown in Fig. 5. Assume each $w_i$ is attached to $m_i$ pendant edges in $G^*$, where $m_i \geq 0$ and $\sum_{i=1}^{5} m_i = n - 5$. For convenience, denote $G^* = A_1(m_1, m_2, m_3, m_4, m_5)$.

Case 1. If at least two of $m_1, m_2, m_3$ are nonzero, say $m_1 > 0, m_2 > 0$, let $H_1$ be the graph obtained from $A_1(m_1, 0, m_3, m_4, m_5)$ by deleting the pendant vertices of $w_1$. Then there exists an automorphism which interchanges $w_1, w_2$ and preserves all other vertices. By Lemma 2.2(ii), we have

$$(A_1(m_1, 0, m_3, m_4, m_5); w_1) \succ (A_1(m_1, 0, m_3, m_4, m_5); w_2).$$

Further by Lemma 2.2,

$$(A_1(m_1, m_2, 0, m_3, m_4, m_5) \succ A_1(m_1, m_2, m_3, m_4, m_5).$$

A contradiction. So at least two of $m_1, m_2, m_3$ are zero, say $m_2 = m_3 = 0$, then $G^* = A_1(m_1, 0, 0, m_4, m_5)$. 

Case 2. If both $m_4, m_5$ are nonzero, similar to the proof of Case 1, we also can obtain a graph with larger Estrada index, a contradiction. So at least one of $m_4, m_5$ are zero, say $m_4 = 0$, then $G^* = A_1(m_1, 0, 0, m_5)$. 

Case 3. If both $m_1, m_5$ are nonzero, let $H_1$ be the graph obtained from $A_1$ by deleting the edges $w_2w_5, w_4w_5$. Then there exists an automorphism which interchanges $w_1, w_3$ and preserves all other vertices. By Lemma 2.4(ii), we have

$$(A_1(0, 0, 0, 0, m_3); w_1) \succ (A_1(0, 0, 0, 0, m_3); w_2).$$

Further by Lemma 2.2,

$$A_1(0, 0, 0, 0, m_1 + m_5) \succ A_1(m_1, 0, 0, 0, m_5),$$

also a contradiction. Then $G^* \cong A_1(0, 0, 0, 0, m_5)$. 

Similarly, we can prove the cases for $B(G^*) \cong A_i(i \in \{2, 3, 5, 6, 7\})$. \hfill \Box

Let $T_i$ be the graph obtained from $A_i$ by attaching $n - |V(A_i)|$ pendant vertices at one of the vertex with maximum degree in $A_i(i \in \{1, 2, 3, 5, 6, 7\})$. By Lemma 2.1, we have

$$\phi(T_1; x) = x^{n-4}[x^4 - (n + 2)x^2 - 6x + 3(n - 5)] = x^{n-4}f_1(x);$$
$$\phi(T_2; x) = x^{n-4}[x^4 - (n + 2)x^2 + 4(n - 6)] = x^{n-4}f_2(x);$$
$$\phi(T_3; x) = x^{n-6}[x^4 - (n + 2)x^2 - 6x^3 + 3(n - 4)x^2 + 2x - (n - 5)] = x^{n-6}f_3(x);$$
$$\phi(T_5; x) = x^{n-5}[x^4 - (n + 2)x^2 - 6x^3 + 3(n - 3)x + 2(n - 4)] = x^{n-5}f_5(x);$$
$$\phi(T_6; x) = x^{n-5}[x^5 - (n + 2)x^3 - 4x^2 + 4(n - 4)x + 4] = x^{n-5}f_6(x);$$
$$\phi(T_7; x) = x^{n-6}[x^6 - (n + 2)x^4 + 5(n - 5)x^2 - 2(n - 8)] = x^{n-6}f_7(x).$$

Theorem 3.11. Let $G$ be a graph in $\mathcal{F}_n$.

(i) If $4 \leq n \leq 9$, $EE(G) \leq EE(T_3)$, the equality holds if and only if $G \cong T_3$.

(ii) If $n \geq 10$, then $EE(G) \leq EE(T_3)$, the equality holds if and only if $G \cong T_3$.

Proof. (i) From Table 1, it is easy to see that the results hold. 

(ii) By a direct calculation, we can see that the results hold for a positive integer $N_0$ larger enough, for example $N_0 = 100$. In the following, let $n \geq N_0$. 

Table 1

<table>
<thead>
<tr>
<th>$n$</th>
<th>$EE(T_1)$</th>
<th>$EE(T_2)$</th>
<th>$EE(T_3)$</th>
<th>$EE(T_5)$</th>
<th>$EE(T_6)$</th>
<th>$EE(T_7)$</th>
</tr>
</thead>
<tbody>
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<td>$-1$</td>
<td>$-1$</td>
<td>$-1$</td>
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<td>$56.25879$</td>
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Firstly, we have
\[
f_1(\sqrt{n - 1}) = -12 - 6\sqrt{n - 1} < 0,
\]
then \(\lambda_1(T_1) > \sqrt{n - 1}\).

It is easy to calculate that the graph \(T_1 - w_4\) has eigenvalues \(\pm \sqrt{3}, 0\) with multiplicity \(n - 3\). By interlacing property of eigenvalues of \(A(T_1 - w_4)\) and \(A(T_1)\), \(\lambda_i(T_1) \geq \lambda_i(T_1 - w_4)\) for \(i = 2, 3, \ldots, n - 1\) [2]. Then
\[
EE(T_1) = \sum_{i=1}^{n} e^{\lambda_i(T_1)} > e^{\lambda_1(T_1)} + \sum_{i=2}^{n-1} e^{\lambda_i(T_1 - w_4)}
\]
\[
> e^{\sqrt{n-1}} + (n - 3) + e^{\sqrt{3}} + e^{-\sqrt{3}} = H_1.
\]
(a) We know that the solutions of \(f_2(x) = 0\) are \(\pm \sqrt{\frac{n+2+\sqrt{n^2-2n+100}}{2}}, \pm \sqrt{\frac{n+2-\sqrt{n^2-2n+100}}{2}}\) and the graph \(T_2 - w_4\) has eigenvalues \(\pm 2, 0\) with multiplicity \(n - 3\). Then by the fact \(\lambda_i(T_2) \leq \lambda_{i-1}(T_2 - w_4)\) for \(i = 2, 3, \ldots, n\),
\[
EE(T_2) = \sum_{i=1}^{n} e^{\lambda_i(T_2)}
\]
\[
= e^{\lambda_1(T_2)} + \sum_{i=2}^{n} e^{\lambda_i(T_2)} \leq e^{\lambda_1(T_2)} + \sum_{i=1}^{n-1} e^{\lambda_i(T_2 - w_4)}
\]
\[
= e^{\sqrt{\frac{n+2+\sqrt{n^2-2n+100}}{2}}} + (n - 3) + e^{2} + e^{-2} = H_2.
\]
Note that \(e^{\sqrt{n-1}} - e^{\sqrt{\frac{n+2+\sqrt{n^2-2n+100}}{2}}} + e^{\sqrt{3}} - e^{2} > 0\) for \(n \geq 24\), then
\[
H_1 - H_2 = e^{\sqrt{n-1}} - e^{\sqrt{\frac{n+2+\sqrt{n^2-2n+100}}{2}}} + e^{\sqrt{3}} + e^{-\sqrt{3}} - e^{2} - e^{-2}
\]
\[
> e^{\sqrt{n-1}} - e^{\sqrt{\frac{n+2+\sqrt{n^2-2n+100}}{2}}} + e^{\sqrt{3}} - e^{2} > 0.
\]
So \(EE(T_1) > EE(T_2)\).

(b) By a direct calculation, the graph \(T_6 - w_4\) has eigenvalues \(\pm 2, 0\) with multiplicity \(n - 3\). For \(n \geq 101\),
\[
f_6\left(\sqrt{\frac{n - 3}{2}}\right) = \frac{(2n - 43)}{4} \sqrt{\frac{n - 3}{2}} - 4n + 10 > 0 \quad (3.2)
\]
\[
f_6(\sqrt{n - 2}) = -8\sqrt{n - 2} - 4n + 12 < 0 \quad (3.3)
\]
\[
f_6(1) = 3n - 13 > 0 \quad (3.4)
\]
By interlacing property of eigenvalues of \(T_6 - w_4\) and \(T_6, \lambda_2(T_6) \leq \lambda_1(T_6 - w_4) = 2\). Further by \(3.2\)–\(3.4\), we have \(2 < \lambda_1(T_6) < \sqrt{\frac{n - 3}{2}}\). Similarly, by the fact \(\lambda_i(T_6) \leq \lambda_{i-1}(T_6 - w_4)\) for \(i = 2, 3, \ldots, n\),
\[
EE(T_6) = \sum_{i=1}^{n} e^{\lambda_i(T_6)} \leq e^{\lambda_1(T_6)} + \sum_{i=1}^{n-1} e^{\lambda_i(T_6 - w_4)}
\]
\[
< e^{\sqrt{n-1}} + (n - 3) + e^{2} + e^{-2} = H_6.
\]
Note that \(e^{\sqrt{n-1}} - e^{\sqrt{\frac{n-3}{2}}} + e^{\sqrt{3}} - e^{2} > 0\) for \(n \geq 11\), then
\[
H_1 - H_6 = e^{\sqrt{n-1}} - e^{\sqrt{\frac{n-3}{2}}} + e^{\sqrt{3}} + e^{-\sqrt{3}} - e^{2} - e^{-2}
\]
\[
> e^{\sqrt{n-1}} - e^{\sqrt{\frac{n-3}{2}}} + e^{\sqrt{3}} - e^{2}.
\]
So \(EE(T_1) > EE(T_6)\).

Note that for \(n \geq 14\),
\[
f_7\left(\sqrt{\frac{n - 3}{2}}\right) = \left(n - \frac{3}{2}\right) \left(\frac{3}{2} n - \frac{79}{4}\right) - 2n + 16 > 0.
\]
Similar to processes of \(b\), we can prove \(EE(T_1) > EE(T_7)\).
Secondly, we know that $f_1(x) = x^4 - (n + 2)x^2 + 3(n - 5) - 6\sqrt{n - 1} + 6\sqrt{n - 1} - 6x$, then the maximum solution $x_1$ of $x^4 - (n + 2)x^2 + 3(n - 5) - 6\sqrt{n - 1} = 0$ is

$$\sqrt{\frac{1}{2}(n + 2 + \sqrt{n^2 - 8n + 64 + 24\sqrt{n - 1}})}.$$ 

It is easy to see that

$$n^2 - 8n + 64 + 24\sqrt{n - 1} = (n - 4)^2 + 48 + 24\sqrt{n - 1} < (n - 4)^2,$$

$$\sqrt{\frac{1}{2}(n + 2 + \sqrt{n^2 - 8n + 64 + 24\sqrt{n - 1}})} < \sqrt{n - 1},$$

$$f_1(x_1) = 6\sqrt{n - 1} - 6\sqrt{\frac{1}{2}(n + 2 + \sqrt{n^2 - 8n + 64 + 24\sqrt{n - 1}})} < 0,$$

then

$$\lambda_1(T_1) > \sqrt{\frac{1}{2}(n + 2 + \sqrt{n^2 - 8n + 64 + 24\sqrt{n - 1}})}.$$ 

Further by the continuity of $f_1(x)$, there exists a positive number $\epsilon_0$ such that

$$\lambda_1(T_1) \geq \sqrt{\frac{1}{2}(n + 2 + \sqrt{n^2 - 8n + 64 + 24\sqrt{n - 1}}) + \epsilon_0}.$$ 

Then

$$EE(T_1) = \sum_{i=1}^{n} e^{\lambda_i(T_1)} > e^{\lambda_1(T_1)} + \sum_{i=1}^{n-1} e^{\lambda_i(T_1 - w_4)} \geq e^{\sqrt{\frac{1}{2}(n+2+\sqrt{n^2-8n+64+24\sqrt{n-1}})+\epsilon_0}} + (n-3) + e^{\sqrt{3}} + e^{\sqrt{3}} = H'_1.$$ 

For $n \geq 12$,

$$f_3(x_1) = 6\sqrt{\frac{1}{2}(n + 2 + \sqrt{n^2 - 8n + 64 + 24\sqrt{n - 1}}) - 2n - 16 - 4\sqrt{n^2 - 8n + 64 + 24\sqrt{n - 1}}} > 0$$

$$f_3(\sqrt{n - 1}) = -(6n - 8)\sqrt{n - 1} - 10n + 14 < 0$$

$$f_3(1) = n - 12 > 0.$$ 

By a direct calculation, the graph $T_5 - w_4$ has eigenvalues $2, -1$ with multiplicity $2$ and $0$ with multiplicity $n - 4$. By interlacing property of eigenvalues of $T_5 - w_4$ and $T_5$, $\lambda_2(T_5) \leq \lambda_1(T_5 - w_4) = 2$. Further by (3.6)–(3.8), we have

$$2 < \lambda_1(T_5) < \sqrt{\frac{1}{2}(n + 2 + \sqrt{n^2 - 8n + 64 + 24\sqrt{n - 1}})}.$$ 

Similarly, by the fact $\lambda_i(T_5) \leq \lambda_{i-1}(T_5 - w_4)$ for $i = 2, 3, \ldots, n$,

$$EE(T_5) = \sum_{i=1}^{n} e^{\lambda_i(T_5)} \leq e^{\lambda_1(T_5)} + \sum_{i=1}^{n-1} e^{\lambda_i(T_5 - w_4)} < e^{\sqrt{\frac{1}{2}(n+2+\sqrt{n^2-8n+64+24\sqrt{n-1}})+\epsilon_0}} + (n-4) + e^2 + 2e^{-1} = H_5.$$ 

For $n \geq N_1(\epsilon_0)$ (where $N_1(\epsilon_0)$ is some positive integer), we have

$$H'_1 - H_5 = e^{\sqrt{\frac{1}{2}(n+2+\sqrt{n^2-8n+64+24\sqrt{n-1}})+\epsilon_0}} - e^{\sqrt{\frac{1}{2}(n+2+\sqrt{n^2-8n+64+24\sqrt{n-1}})}} + 1 + e^{\sqrt{3}} + e^{\sqrt{3}} - e^2 - 2e^{-1}$$

$$> e^{\sqrt{\frac{1}{2}(n+2+\sqrt{n^2-8n+64+24\sqrt{n-1}})+\epsilon_0}} - e^{\sqrt{\frac{1}{2}(n+2+\sqrt{n^2-8n+64+24\sqrt{n-1}})}} + e^{\sqrt{3}} + e^{\sqrt{3}} - e^2 > 0.$$ 

So $EE(T_1) > EE(T_3)$.

Similarly, we can prove $EE(T_1) > EE(T_3)$. \(\Box\)

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References