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On the Estrada Indices of Unicyclic Graphs with Fixed Diameters

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Abstract: The Estrada index of a graph G is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. A unicyclic graph is a connected graph with a unique cycle. Let $\mathcal{U}(n,d)$ be the set of all unicyclic graphs with n vertices and diameter d. In this paper, we give some transformations which can be used to compare the Estrada indices of two graphs. Using these transformations, we determine the graphs with the maximum Estrada indices among $\mathcal{U}(n,d)$. We characterize two candidate graphs with the maximum Estrada index if d is odd and three candidate graphs with the maximum Estrada index if d is even.

Keywords: adjacency matrix; Estrada index; unicyclic graph; spectral moment; diameter

Citation: Ning, W.; Wang, K. On the Estrada Indices of Unicyclic Graphs with Fixed Diameters. *Mathematics* **2021**, *9*, 2395. https://doi.org/10.3390/math9192395

Academic Editor: David Dolžan

Received: 4 September 2021
Accepted: 20 September 2021
Published: 26 September 2021

1. Introduction

In this paper, we only consider simple undirected graphs. Let $G = (V(G), E(G))$ be a graph with n vertices and m edges. Let $N_G(v)$ be the set of vertices adjacent to v in G. The degree of v in G, denoted by $d_G(v)$, is equal to $|N_G(v)|$. A vertex of degree one is called a pendant vertex. The edge incident with a pendant vertex is known as a pendant edge. Let $S \neq \emptyset \subseteq V(G)$. Then denote by $G[S]$ the subgraph induced by S. If $D \subseteq E(G)$ (or $D \subseteq V(G)$), then we write $G - D$ for the graph obtained from G by deleting all of its edges (or vertices, resp.) in D. If $D \subseteq E(\overline{G})$, then we denote by $G + D$ the graph obtained from G by adding all of edges in D to the graph.

Let $A(G)$ be the adjacency matrix of G. Denote the eigenvalues of $A(G)$ by $\lambda_1, \lambda_2, \ldots, \lambda_n$ and assume $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. Then λ_1, usually denoted by $\rho(G)$, is called the spectral radius of G. The Estrada index of G is defined as

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

This graph invariant was first proposed as a measure of the degree of folding of a protein [1] and now has been found multiple applications in various fields, such as measurements of the subgraph centrality and the centrality of complex networks [2,3] and the extended molecular branching [4]. Recently, the correlation between the Estrada index and π-electronic energies for benzenoid hydrocarbons was investigated in [5], the results of which warrant its further usage in quantitative structure–activity relationships. Given these prominent applications of the Estrada index, the research on it is of theoretical and practical significance. In the last few decades, some mathematical properties of the Estrada index, including various bounds for it, have been established [6–12].

In 1986, Brualdi and Solheid [13] proposed the following problem concerning the spectral radii of graphs: Given a set $\mathcal{G}$ of graphs, find an upper bound for the spectral radius of graphs in $\mathcal{G}$ and characterize the graphs for which the maximal spectral radius is attained. The corresponding problem of a given graph invariant has been widely studied (see [14–16], for example). Motivated by this, many results have been obtained on characterizing graphs that maximize (or minimize) the Estrada index among a given set of graphs. For example, some interesting results were obtained for the general trees [17], trees with a given matching number [18], trees with a fixed diameter [19], trees with perfect matching and a fixed maximum degree [20], and trees with a fixed number of pendant vertices [21]. Du and Zhou [22] showed a graph with the maximal Estrada index and two candidate graphs with the minimum Estrada index among all unicyclic graphs. Moreover, they determined the unique graphs with maximum Estrada indices among graphs with given parameters [23]. Wang et al. [24] and Zhu et al. [25] characterized the bicyclic graph and the tricyclic graph with maximum Estrada indices, respectively. E. Andrade et al. [26] presented the graph having the largest Estrada index of its line graph among all graphs on n vertices with connectivity less than or equal to a fixed number. For more results on the Estrada index and its variations, the readers may refer to [27–30].

A unicyclic graph is a connected graph with a unique cycle. Let P_n and C_n be the path and the cycle on n vertices, respectively. Denote by $\mathcal{U}(n,d)$ the set of all unicyclic graphs with n vertices and diameter d. In this paper, we characterize the graphs with the maximum Estrada index in $\mathcal{U}(n,d)$.

This paper is organized as follows. In Section 2, we list some transformations which can be used to compare the Estrada indices of two graphs. In Section 3, we determine the graphs with the maximum Estrada index among unicyclic graphs in $\mathcal{U}(n,d)$. We show two candidate graphs with the maximal Estrada index if d is odd and three candidate graphs with the maximal Estrada index if d is even. We also propose a hypothesis on the structure of the extremal graph with the maximum Estrada index in $\mathcal{U}(n,d)$.

2. Preliminaries

In order to obtain the main results of this paper, we give some definitions and lemmas here.

A walk of length k in a graph G is any sequence of vertices and edges in G, $W = v_1e_1v_2e_2\cdots v_ke_kv_{k+1}$, such that $e_i = v_iv_{i+1}$ for every $1 \le i \le k$. For a subsequence $v_ie_iv_{i+1}\cdots v_{j-1}e_{j-1}v_j$ of W, we refer to it as a (v_i, v_j)-section of W. Usually, we write $W = v_1v_2\cdots v_{k+1}$ instead for simplicity and call it a (v_1, v_{k+1})-walk. Let $\overrightarrow{W} = v_{k+1}v_k\cdots v_1$. Then $\overrightarrow{W}$ is called the reverse of W. If $v_1 = v_{k+1}$, then W is called a closed walk.

Let $M_k(G)$ be the kth spectral moment of the graph G defined as $M_k(G) = \sum_{i=1}^{n}\lambda_i^k$. It is well-known that $M_k(G)$ equals the number of closed walks of length k in G; see [31]. Then by the Taylor expansion of the exponential function e^x, we have

$$EE(G) = \sum_{k=0}^{\infty}\frac{M_k(G)}{k!}. \tag{1}$$

Let G and H be two graphs with $x, y \in V(G)$, $u, v \in V(H)$ and $e \in E(G)$. Suppose k is an arbitrary positive integer. Let $W_k(G; x, [e])$ be the set of all (x, x)-walks of length k going through the edge e in G and let $|W_k(G; x, [e])| = M_k(G; x, [e])$. Let $W_k(G; x, y)$ be the set of all (x, y)-walks of length k in G and let $|W_k(G; x, y)| = M_k(G; x, y)$. If $M_k(G; x, y) \le M_k(H; u, v)$ for all positive integers k, then we write $(G; x, y) \preceq (H; u, v)$. If $(G; x, y) \preceq (H; u, v)$, and $M_{k_0}(G; x, y) < M_{k_0}(H; u, v)$ for some positive integer k_0, then we write $(G; x, y) \prec (H; u, v)$. For convenience, let $W_k(G; x) = W_k(G; x, x)$, $M_k(G; x) = M_k(G; x, x)$ and $(G; u) = (G; u, u)$.

The following four results are often used to compare the Estrada indices of two graphs.

Lemma 1 ([28])**.** *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 $1 \le i \le r$. 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 $1 \le i \le r$, then $EE(H_u) < EE(H_v)$.*

Lemma 2 ([32])**.** *Let H_1 and H_2 be two non-trivial graphs with $u, v \in V(H_1)$, $w \in V(H_2)$. Let G_u be the graph obtained from H_1 and H_2 by identifying u with w, and G_v be the graph obtained from H_1 and H_2 by identifying v with w. If $(H_1; v) \prec (H_1; u)$, then $EE(G_v) < EE(G_u)$.*

Lemma 3 ([32])**.** *Let G_1 and G_2 be two connected graphs with $u \in V(G_1)$ and $v \in V(G_2)$. Let G be the graph obtained by joining u and v with and 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 $EE(G) < EE(G')$.*

Theorem 1 ([27])**.** *Let G be a connected graph and $G_{u,v}(p, q)$ be the graph obtained from G by attaching p and q pendant edges to u and v, respectively, where $u, v \in V(G)$ and $p, q \geq 1$. Then $EE(G_{u,v}(p + q, 0)) \geq EE(G_{u,v}(p, q))$ or $EE(G_{u,v}(0, p + q)) \geq EE(G_{u,v}(p, q))$. Furthermore, $EE(G_{u,v}(p + q, 0)) > EE(G_{u,v}(p, q))$ if $d_G(u) \geq d_G(v)$ or $EE(G_{u,v}(0, p + q)) > EE(G_{u,v}(p, q))$ if $d_G(v) \geq d_G(u)$.*

3. Lemmas

In this section, we give some lemmas that can be used to prove $(G; v) \prec (G; u)$ in a graph G, where $u, v \in V(G)$.

Lemma 4. *Let G be a simple graph and $u, v \in V(G)$. If $N_G(v) \subseteq N_G(u)$, then $(G; v) \preceq (G; u)$, and $(G; w, v) \preceq (G; w, u)$ for each $w \in V(G)$. Moreover, if $d_G(v) < d_G(u)$, then $(G; v) \prec (G; u)$.*

Proof of Lemma 4. Since G is simple, $N_G(v) \subseteq N_G(u)$ implies $uv \notin E(G)$. Let $k \geq 0$ and $W \in \mathcal{W}_k(G; v)$. Then W can be written as $W = vw_1 \cdots w_2v$, where $w_1, w_2 \in N_G(v)$. Let $\widehat{W} = uw_1 \cdots w_2u$. Since $N_G(v) \subseteq N_G(u)$ and $uv \notin E(G)$, the map f_k: $\mathcal{W}_k(G; v) \to \mathcal{W}_k(G; u)$, defined as $f_k(W) = \widehat{W}$ is an injection. Thus, $M_k(G; v) \leq M_k(G; u)$. Since $k \geq 0$ is arbitrary, we get $(G; v) \preceq (G; u)$. Note that $d_G(v) = M_2(G; v)$ and $d_G(u) = M_2(G; u)$. Therefore, $(G; v) \prec (G; u)$ if $d_G(v) < d_G(u)$ further holds. Similarly, we can show $(G; w, v) \preceq (G; w, u)$ for each $w \in V(G)$. □

Lemma 5. *Let G be a graph and $H = G + e$ such that $e = uv \in E(\overline{G})$. If $(G; v) \preceq (G; u)$, then $(H; v) \preceq (H; u)$. Moreover, if $(G; v) \prec (G; u)$, then $(H; v) \prec (H; u)$.*

Proof of Lemma 5. For each $z \in \{u, v\}$ and $k \geq 0$, by the definition of $M_k(H; z)$,

$$M_k(H; z) = M_k(G; z) + M_k(H; z, [e]). \tag{2}$$

Since $(G; v) \preceq (G; u)$, we have $M_k(G; v) \leq M_k(G; u)$. Therefore, there exits an injection $f_k : \mathcal{W}_k(G; v) \to \mathcal{W}_k(G; u)$. In order to prove $M_k(H; v) \leq M_k(H; u)$, it suffices to show $M_k(H; v, [e]) \leq M_k(H; u, [e])$.

Let $W \in \mathcal{W}_k(H; v, [e])$. Then either veu or uev must be contained in W. If W does not contain the section uev, or veu appears earlier than uev in W, then W can be decomposed uniquely to $W = W_1eW_2$ such that $W_1 \in \mathcal{W}_{k_1}(G; v)$ for some $k_1 \geq 0$ and $W_2 \in \mathcal{W}_{k_2}(H; u, v)$ for some $k_2 \geq 0$. In this case, we define $h_k(W) = f_{k_1}(W_1)e\overleftarrow{W_2}$. Then $h_k(W) \in \mathcal{W}_k(H; u, [e])$.

If W does not contain the section veu, or uev appears earlier than veu in W, then W can be decomposed uniquely to $W = W_1eW_2e \cdots W_teW_r$, where W_i is a (v, u)-walk in G for each $1 \leq i \leq t$, and W_r is a (v, v)-walk in H. Here, W_r either contains no e, or contains no uev, or veu appears earlier than uev. Without loss of generality, we suppose veu appears earlier than uev in W_r. Then W_r can be decomposed to $W_r = W_{t+1}eW_{t+2}$ such that $W_{t+1} \in \mathcal{W}_{k_{t+1}}(G; v)$ for some $k_{t+1} \geq 0$ and W_{t+2} is a (u, v)-walk in H. In this case, we define $h_k(W) = \overleftarrow{W_1}e\overleftarrow{W_2}e \cdots \overleftarrow{W_t}ef_{k_{t+1}}(W_{t+1})e\overleftarrow{W_{t+2}}$. Then $h_k(W) \in \mathcal{W}_k(H; u, [e])$. Now it is easy to show that the map $h_k : \mathcal{W}_k(H; v, [e]) \leq \mathcal{W}_k(H; u, [e])$ defined as above is an injection. Therefore, $M_k(H; v, [e]) \leq M_k(H; u, [e])$.

Moreover, if $(G; v) \prec (G; u)$, then $M_{k_0}(G; v) < M_{k_0}(G; u)$ for some $k_0 > 0$. Thus, $M_{k_0}(H; v) < M_{k_0}(H; u)$ by (2), which implies $(H; v) \prec (H; u)$. □

Lemma 6. *Let G be a graph and $P = v_0v_1 \cdots v_m$ be a path in G such that $d_G(v_0) = 1$. Let q and l be two nonnegative integers such that $0 \leq q < l$ and $q + l \leq m$. Suppose $v = v_q$ and $u = v_l$ are two vertices in P such that $d_G(v_i) = 2$ for each $0 < i < \frac{q+l}{2}$. Let $a = \lfloor \frac{q+l}{2} \rfloor$. Then*

(1) $(G; v) \preceq (G; u)$;

(2) *If $q + l < m$, or $q + l = m$ and the condition $\mathcal{C}$ does not hold, then $(G; v) \prec (G; u)$, where $\mathcal{C}$ is: $d_G(v_m) = 1$ and $d_G(v_i) = 2$ for each $a + 1 \leq i \leq m - 1$.*

(3) *If $q + l$ is even, then $(G; w, v) \preceq (G; w, u)$ for each $w \in V(G) \backslash \{v_0, v_1, \ldots, v_{a-1}\}$.*

Proof of Lemma 6. Let $e_i = v_iv_{i+1}$ for each $0 \leq i \leq m - 1$. For each walk W in $G[\{v_0, v_1, \ldots, v_{p+l}\}]$, denote by $\overline{W}$ the walk obtained from W by replacing each vertex v_x with $v_{x'}$ and the corresponding edges, where $x' = q + l - x$. We distinguish the following two cases:

Case 1.$q + l$ is even.

Let $k \geq 0$ and $W \in W_k(G; v)$. Then $v_a = v_{\frac{q+l}{2}}$ has the same distance from v and u in P. If W contains v_a more than once, then it can be decomposed uniquely to $W = W_1W_2W_3$, such that $W_2 \in W_{k_2}(G; v_a)$ which is as long as possible, W_1 is a (v, v_a)-walk in G, and W_3 is a (v_a, v)-walk in G. In this case, let $f_k^{(1)}(W) = \overline{W_1}W_2\overline{W_3}$. Then $f_k^{(1)}(W) \in W_k(G; u)$. If W contains v_a at most once, then let $f_k^{(1)}(W) = \overline{W}$. Obviously, the map $f_k^{(1)} : W_k(G; v) \longrightarrow W_k(G; u)$ defined as above is an injection. Since k is arbitrary, we have $(G; v) \preceq (G; u)$.

If $q + l < m$, then $f_k^{(1)}$ does not cover the walk $v_lv_{l+1} \cdots v_{m-1}v_mv_{m-1} \cdots v_{l+1}v_l$.

Now suppose $q + l = m$ and the condition $\mathcal{C}$ does not hold. Without loss of generality, suppose there exists some $a + 1 \leq j \leq m - 1$ with $d_G(v_j) \neq 2$. Then there exists a vertex $s \neq v_{j-1}, v_{j+1}$ such that $v_js \in E(G)$. If $a + 1 \leq j \leq l - 1$, then $f_k^{(1)}$ does not cover the walk $v_lv_{l-1} \cdots v_{j-1}v_jsv_j \cdots v_{l-1}v_l$. If $l \leq j \leq m - 1$, then $f_k^{(1)}$ does not cover the walk $v_lv_{l+1} \cdots v_jsv_j \cdots v_{l+1}v_l$. Therefore, if $q + l < m$, or $q + l = m$ and the condition $\mathcal{C}$ does not hold, then $M_{k_0}(G; v) < M_{k_0}(G; u)$ for some $k_0 \geq 0$. This implies Lemma 6 (2) holds.

Let $w \in V(G) \backslash \{v_0, v_1, \ldots, v_{a-1}\}$ and $W \in W_k(G; w, v)$. Then W must contain v_a. Thus, W can be decomposed uniquely to $W = W_1W_2$ such that $W_1 \in W_{k_0}(G; w, v_a)$ which is as long as possible and W_2 is a (v_a, v)-walk in G. Then the map g_k: $W_k(G; w, v) \rightarrow W_k(G; w, u)$ defined as $g_k(W) = W_1\overline{W_2}$ is an injection. Therefore, $(G; w, v) \preceq (G; w, u)$.

Case 2. $q + l$ is odd.

Let $k \geq 0$, $W \in W_k(G; v)$, and $e_a = v_av_{a+1}$. If W contains e_a, then it must contain e_a at least twice and can be decomposed uniquely to $W = W_1W_2e_aW_3e_aW_4$, such that $W_1 \in W_{k_1}(G; v, v_a)$, which contains v_a only once; $W_2 \in W_{k_2}(G; v_a)$, which does not contain e_a; $W_3 \in W_{k_3}(G; v_{a+1})$, which is as long as possible; and $W_4 \in W_{k_4}(G; v_a, v)$, which does not contain e_a. In this case, let $f_k^{(2)}(W) = \overline{W_1}W_3e_a\overline{W_2}e_a\overline{W_4}$. If W does not contain e_a, let $f_k^{(2)}(W) = \overline{W}$. Then the map $f_k^{(2)} : W_k(G; v) \longrightarrow W_k(G; u)$ defined as above is an injection. Thus, $(G; v) \preceq (G; u)$.

The proof of (Case 2) when $q + l$ is odd is the same as that of Case 1. □

Remark 1. *Lemma 6 (3) does not hold if $q + l$ is odd. For example, let G be the graph obtained from $P_8 = v_0v_1 \cdots v_7$ and a new vertex w by adding the edge v_3w. Let $v = v_1$ and $u = v_4$. Then $M_3(G; w, v) \geq 1$ and $M_3(G; w, u) = 0$. Thus, $(G; w, v) \preceq (G; w, u)$ does not hold in G.*

4. Graphs with the Maximum Estrada Index in $\mathcal{U}(n, d)$

In this section, we determine the graphs with the maximum Estrada index among $\mathcal{U}(n, d)$.

Let $C_t(n_1, n_2, \ldots, n_t)$ be the graph obtained from the cycle $C_t = v_1v_2 \cdots v_tv_1$ by attaching n_i vertices to v_i for $i = 1, 2, \ldots, l$. Let $C_n^* \cong C_{n-1}(1, 0, \ldots, 0)$ and $X_n \cong C_3(0, 0, n - 3)$. Let $\mathcal{U}(n)$ be the set of all unicyclc graphs of order n.

The following theorem characterizes the graphs with greatest, second-greatest, smallest, and second-smallest Estrada indices among the unicyclic graphs in $\mathcal{U}(n)$.

Theorem 2 ([33]). *Among the unicyclic graphs in $\mathcal{U}(n)$,*

(i) *According to references [22,34], the cycle C_n has smalles tindex and the graph C_n^* has second-smallest Estrada index;*
(ii) *According to references [22,34], the graph X_n has the greatest Estrada index;*
(iii) *The graph $C_3(0,1,n-4)$ has the second-greatest Estrada index.*

For $G \in \mathcal{U}(n,d)$, we have $n \geq 3$ and $1 \leq d \leq n-2$. If $d = 1$, then $G = C_3$. By Theorem 2, the graphs with the maximum Estrada indices among the graphs in $\mathcal{U}(n,2)$ and $\mathcal{U}(n,3)$ are X_n and $C_3(0,1,n-4)$, respectively. Therefore, we assume $d \geq 4$ and $n \geq 6$ in the following. Now we give some lemmas.

Lemma 7. *Let $P = v_0 v_1 \cdots v_{d-1} v_d$ be a path, where $d \geq 4$ is even. Let H be the graph obtained from P and a new vertex v_{d+1} by adding the edges $v_{\frac{d}{2}-1} v_{d+1}$ and $v_{\frac{d}{2}} v_{d+1}$; see Figure 1. Then $(H; v_{\frac{d}{2}-1}) \prec (H; v_{\frac{d}{2}})$.*

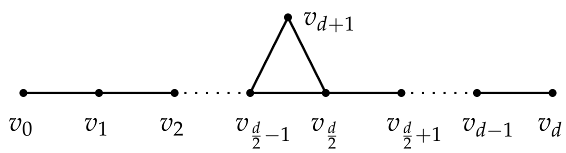

Figure 1. Graph H in Lemma 7.

Proof of Lemma 7. Let $e_i = v_i v_{i+1}$ for each $0 \leq i \leq d-1$. Let $e = v_{\frac{d}{2}-1} v_{d+1}$ and $\bar{e} = v_{\frac{d}{2}} v_{d+1}$. For each walk W in $H[\{v_0, v_1, \ldots, v_{\frac{d}{2}-1}, v_{d+1}\}]$ and each $0 \leq i \leq \frac{d}{2} - 1$, denote by $\overline{W}$ the walk obtained from W by replacing v_i with v_{d-1-i} and the corresponding edges. Let $k \geq 0$ and $W \in W_k(H; v_{\frac{d}{2}-1})$. If W does not contain $v_{\frac{d}{2}}$, then define $f_k(W) = \overline{W}$. If W contains $v_{\frac{d}{2}}$, then W can be decomposed uniquely to $W = W_1 W_2 W_3 W_4 W_5$, such that $W_1 \in W_{k_1}(G; v_{\frac{d}{2}-1})$ for some $k_1 \geq 0$, $W_5 \in W_{k_5}(H; v_{\frac{d}{2}-1})$ for some $k_5 \geq 0$, $W_3 \in W_{k_3}(H; v_{\frac{d}{2}})$ which is as long as possible, $W_2 = e_{\frac{d}{2}-1}$ or $e v_{d+1} \bar{e}$, $W_4 = e_{\frac{d}{2}-1}$ or $\bar{e} v_{d+1} e$. Obviously, neither W_1 nor W_5 contains $v_{\frac{d}{2}}$. In this case, we define $f_k(W) = W_3 W_4 W_5 W_2 \overline{W_1}$. Then it is easy to show that the map $f_k : W_k(H; v_{\frac{d}{2}-1}) \longrightarrow W_k(H; v_{\frac{d}{2}})$ defined as above is an injection. Since f_k does not cover the walk $v_{\frac{d}{2}} v_{\frac{d}{2}+1} \cdots v_{d-1} v_d v_{d-1} \cdots v_{\frac{d}{2}+1} v_{\frac{d}{2}}$, we have $(H; v_{\frac{d}{2}-1}) \prec (H; v_{\frac{d}{2}})$. $\square$

Lemma 8. *Let $C_4 = xvyux$ be a 4-cycle. Denote by H the graph obtained from C_4 by attaching two paths $P_p = v_1 v_2 \cdots v_p$ and $P_q = u_1 u_2 \cdots u_q$ at vertices v and u, respectively; see Figure 2. If $0 \leq p < q$, then $(H; v) \prec (H; u)$.*

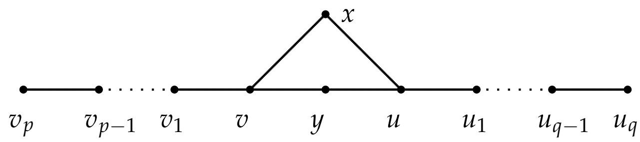

Figure 2. Graph H in Lemmas 8 and 9.

Proof of Lemma 8. For each walk W in $H[\{x, y, v, v_1, \ldots, v_p\}]$ and each $1 \leq i \leq p$, denote by $\overline{W}$ the walk obtained from W by replacing v_i with u_i, v with u and the corresponding edges. Let $k \geq 0$ and $W \in W_k(H; v)$. If W contains neither x nor y, then let $f_k(W) = \overline{W}$. If W contains x or y, then W can be decomposed uniquely to $W = W_1 W_2 W_3$, such that W_1 is a (v,s)-walk; W_2 is a (s,t)-walk which is as long as possible, where $s, t \in \{x, y\}$; and W_3 is a (t,v)-walk. It is obvious that both of W_1 and W_3 are walks in $H[\{x, y, v, v_1, \ldots, v_p\}]$. In this case, we define $f_k(W) = \overline{W_1} W_2 \overline{W_3}$. Then it is easy to show that the map $f_k : W_k(H; v) \longrightarrow W_k(H; u)$ defined as above is an injection. Since $p < q$, f_k does not cover the walk $uu_1 \cdots u_{q-1}u_q u_{q-1} \cdots u_1 u$. Therefore, we have $(H; v) \prec (H; u)$. □

Lemma 9. *Let H be the graph depicted in Figure 2. If $0 \leq p \leq q$ and $q \geq 1$, then $(H; y) \prec (H; u)$.*

Proof of Lemma 9. Let $k \geq 0$ be an arbitrary integer. By the definition of the walk, we have

$$\begin{aligned} M_k(H; y) &= M_{k-1}(H; y, u) + M_{k-1}(H; y, v) \\ &= M_{k-1}(H; u, y) + M_{k-1}(H; y, v) \\ &= M_{k-1}(H; u, y) + M_{k-1}(H; x, v) \end{aligned}$$

and

$$\begin{aligned} M_k(H; u) &= M_{k-1}(H; u, y) + M_{k-1}(H; u, x) + M_{k-1}(H; u, u_1) \\ &= M_{k-1}(H; u, y) + M_{k-1}(H; x, u) + M_{k-1}(H; u, u_1). \end{aligned}$$

Since $M_{k-1}(H; u, u_1) \geq 0$, in order to prove $M_k(H; y) \leq M_k(H; u)$, it suffices to show $M_{k-1}(H; x, v) \leq M_{k-1}(H; x, u)$, i.e., $M_k(H; x, v) \leq M_k(H; x, u)$ for each $k \geq 0$. We prove this by induction on k.

If $k = 1$, $M_k(H; x, v) = M_k(H; x, u) = 1$. If $k = 2$, $M_k(H; x, v) = M_k(H; x, u) = 0$. Now suppose $k \geq 3$ and let $W \in W_k(H; x, v)$. We consider the edge e preceding the last vertex v in W. If $e = (x, v)$, then W can be written as $W = W_1(x, v)v$. In this case, let $f_k(W) = W_1(x, u)u$. If $e = (y, v)$, then W can be written as $W = W_1(y, v)v$. In this case, let $f_k(W) = W_1(y, u)u$. If $e = v_1 v$, then W can be uniquely decomposed to $W_1 W_2$, such that $W_1 \in W_{k_1}(x, v)$ for some $0 \leq k_1 < k$ which is as large as possible, and $W_2 \in W_{k_2}(v, v)$ for some $k_2 \geq 0$. Obviously, W_2 is a walk in $H[\{v, v_1, \ldots, v_p\}]$. Define $\overline{W_2}$ the walk obtained from W_2 by replacing v_i with u_i for each $1 \leq i \leq p$, v with u, and the corresponding edges. By the inductive hypothesis, there is an injection $f_{k_1} : W_{k_1}(H; x, v) \to W_{k_1}(H; x, u)$. In this case, let $f_k(W) = f_{k_1}(W_1)\overline{W_2}$. Then it is easy to show that the map $f_k : W_k(H; x, v) \longrightarrow W_k(H; x, u)$ defined as above is an injection. Therefore, $M_k(H; x, v) \leq M_k(H; x, u)$.

Since $q \geq 1$, $M_2(H; y) = d_H(y) = 2 < 3 = d_H(u) = M_2(H; u)$. Thus, $(H; y) \prec (H; u)$. This completes the proof. □

Let $P = v_0 v_1 \cdots v_d$ be a path of length d with $d \geq 2$. Let Δ_n^d be the graph obtained from P and a new vertex v_{d+1} by adding the edges $v_{\lfloor \frac{d}{2} \rfloor} v_{d+1}$ and $v_{\lfloor \frac{d}{2} \rfloor + 1} v_{d+1}$, and attaching $n - d - 2$ pendant edges at the vertex $v_{\lfloor \frac{d}{2} \rfloor}$ (see Figure 3).

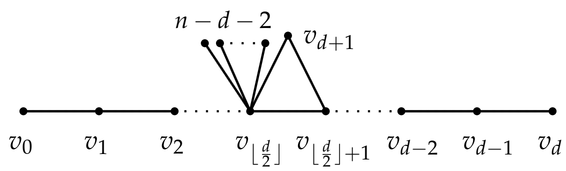

Figure 3. Graph Δ_n^d.

Lemma 10. *Let $P = v_0 v_1 \cdots v_d$ be a path of length $d \geq 4$. Let $G_{v_k, v}$ be the graph with diameter d obtained from P and a new vertex v_{d+1} by adding the edges $v_k v_{d+1}$ and $v_{k+1} v_{d+1}$, and attaching $n - d - 2$ pendant edges at one vertex $v \in V(P) \cup \{v_{d+1}\}$, where $0 \leq k \leq d - 1$ and $n - d - 2 \geq 0$. Then $EE(G_{v_k, v}) \leq EE(\Delta_n^d)$, with equality if and only if $G_{v_k, v} \cong \Delta_n^d$, where Δ_n^d is depicted in Figure 3.*

Proof of Lemma 10. Denote by $\mathcal{B}$ the set of all graphs $G_{v_k, v}$. Let G^* be the graph in $\mathcal{B}$ with the maximum Estrada index. Then there exists some $0 \leq k \leq d - 1$ such that G^* is obtained from P and v_{d+1} by adding the edges $v_k v_{d+1}$ and $v_{k+1} v_{d+1}$, and attaching $n - d - 2$ pendant edges at a vertex v for some vertex $v \in V(P) \cup \{v_{d+1}\}$. We show that $v_k = v = v_{\lfloor \frac{d}{2} \rfloor}$, i.e.,

$G^* \cong \Delta_n^d$. For each vertex v_i in P, let $\overline{N_{G^*}(v_i)} = N_{G^*}(v_i) \cap (V(G^*) \setminus V(P))$. We distinguish the following two cases.

Case 1. d is odd.

We show that for each $v_i \in V(P) \setminus \{v_{\lfloor \frac{d}{2} \rfloor}, v_{\lfloor \frac{d}{2} \rfloor+1}\}$, we have $\overline{N_{G^*}(v_i)} = \emptyset$.

Let t be the minimum index with $\overline{N_{G^*}(v_t)} \neq \emptyset$. Suppose $\overline{N_{G^*}(v_t)} = \{w_1, w_2, \dots, w_s\}$. If $t < \lfloor \frac{d}{2} \rfloor$, then $t + (t+2) < d$ and $t + (t+2)$ is even. Let $G_0 = G^* - \{v_t w_i \mid 1 \leq i \leq s\}$. By Lemma 6, $(G_0; v_t) \prec (G_0; v_{t+2})$, and for each $1 \leq i \leq s$, $(G_0; w_i, v_t) \preceq (G_0; w_i, v_{t+2})$. Define $G' = G_0 + \{v_{t+2} w_i \mid 1 \leq i \leq s\}$. Then $G' \in \mathcal{B}$ and $EE(G^*) < EE(G')$ by Lemma 1, a contradiction to the choice of G^*. Therefore, $t \geq \lfloor \frac{d}{2} \rfloor$, i.e., $\overline{N_{G^*}(v_i)} = \emptyset$ for each $i < \lfloor \frac{d}{2} \rfloor$. Similarly, we have $\overline{N_{G^*}(v_i)} = \emptyset$ for each $i > \lfloor \frac{d}{2} \rfloor + 1$. Thus, $v_k = v_{\lfloor \frac{d}{2} \rfloor}$ and $v \in \{v_{\lfloor \frac{d}{2} \rfloor}, v_{\lfloor \frac{d}{2} \rfloor+1}, v_{d+1}\}$.

Obviously, $G^* \cong \Delta_n^d$ if $n - d - 2 = 0$. Now we suppose $n - d - 2 > 0$. Then $d_{G^*}(v) \geq 3$. Suppose $v = v_{d+1}$. Let $G_0 = G^* - v_{\lfloor \frac{d}{2} \rfloor - 1} v_{\lfloor \frac{d}{2} \rfloor}$ and $G_1 = G_0 - v_{\lfloor \frac{d}{2} \rfloor} v_{d+1}$. Then $N_{G_1}(v_{\lfloor \frac{d}{2} \rfloor}) \subseteq N_{G_1}(v_{d+1})$ and $d_{G_1}(v_{\lfloor \frac{d}{2} \rfloor}) = 1 < 2 \leq d_{G_1}(v_{d+1})$. Thus, we have $(G_1; v_{\lfloor \frac{d}{2} \rfloor}) \prec (G_1; v_{d+1})$ by Lemma 4 and $(G_0; v_{\lfloor \frac{d}{2} \rfloor}) \prec (G_0; v_{d+1})$ by Lemma 5. Note that for each $k \geq 0$, $M_k(G_0; v_{\lfloor \frac{d}{2} \rfloor - 1}, v_{\lfloor \frac{d}{2} \rfloor}) = M_k(G_0; v_{\lfloor \frac{d}{2} \rfloor - 1}, v_{d+1}) = 0$. By Lemma 1, we get $EE(G^*) < EE(\Delta_n^d)$, a contradiction to the choice of G^*. Therefore, $v \neq v_{d+1}$, i.e., $G^* \cong \Delta_n^d$.

Case 2. d is even.

By an argument similar to that of Case 1, we have $\overline{N_{G^*}(v_i)} = \emptyset$ for each $i < \lfloor \frac{d}{2} \rfloor - 1$ and $i > \lfloor \frac{d}{2} \rfloor + 1$. Thus, $v_k = v_{\lfloor \frac{d}{2} \rfloor - 1}$ or $v_{\lfloor \frac{d}{2} \rfloor}$, and $v \in \{v_{\lfloor \frac{d}{2} \rfloor - 1}, v_{\lfloor \frac{d}{2} \rfloor}, v_{\lfloor \frac{d}{2} \rfloor + 1}, v_{d+1}\}$. Without loss of generality, we may suppose $v_k = v_{\lfloor \frac{d}{2} \rfloor}$. Then $G^* \cong \Delta_n^d$ if $n - d - 2 = 0$. Now suppose $n - d - 2 > 0$. By an argument similar to that in Case 1, we have $v \neq v_{d+1}$. Suppose $v = v_{\lfloor \frac{d}{2} \rfloor - 1}$ or $v_{\lfloor \frac{d}{2} \rfloor + 1}$. Let $\{u_1, u_2, \dots, u_{n-d-2}\}$ be the set of all pendant vertices adjacent to v and $G_0 = G^* - \{v u_i \mid 1 \leq i \leq n - d - 2\}$. Then by Lemmas 6 and 7, $(G_0; v) \prec (G_0; v_{\lfloor \frac{d}{2} \rfloor})$, and for each $1 \leq i \leq n - d - 2$, $(G_0; u_i, v) \preceq (G_0; u_i, v_{\lfloor \frac{d}{2} \rfloor})$. By Lemma 1, $EE(G^*) < EE(\Delta_n^d)$, a contradiction to the choice of G^*. Therefore, $v = v_{\lfloor \frac{d}{2} \rfloor}$, i.e., $G^* \cong \Delta_n^d$. This completes the proof. □

Lemma 11. *Let $P = v_0 v_1 \cdots v_d$ be a path of length $d \geq 4$. Let $G_{k,t}$ be the graph with diameter d obtained from P and a new vertex v_{d+1} by adding the edges $v_k v_{d+1}$ and $v_{k+2} v_{d+1}$, and attaching $n - d - 2$ pendant edges at v_t, where $0 \leq k \leq d - 2$, $1 \leq t \leq d - 1$ and $n - d - 2 \geq 0$. Let $G_1 = G_{\lfloor \frac{d}{2} \rfloor, \lfloor \frac{d}{2} \rfloor}$ and $G_2 = G_{\lfloor \frac{d}{2} \rfloor - 1, \lfloor \frac{d}{2} \rfloor - 1}$ be depicted in Figure 4.*

(i) *If d is odd, then $EE(G_{k,t}) \leq EE(G_1)$, with equality if and only if $G_{k,t} \cong G_1$.*
(ii) *If d is even, then $EE(G_{k,t}) \leq \max\{EE(G_1), EE(G_2)\}$, with equality if and only if $G_{k,t}$ is isomorphic to the graph with a larger Estrada index between G_1 and G_2.*

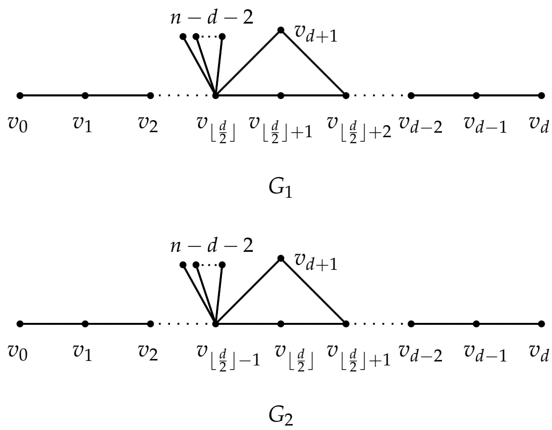

Figure 4. Graphs G_1 and G_2.

Proof of Lemma 11. Denote by $\mathcal{B}$ the set of all graphs $G_{k,t}$. Let G^* be the graph in $\mathcal{B}$ with the maximum Estrada index. Then there exists some $0 \le k \le d-2$ and $1 \le t \le d-1$ such that G^* is obtained from P and v_{d+1} by adding the edges $v_k v_{d+1}$ and $v_{k+2}v_{d+1}$, and attaching $n-d-2$ pendant edges at the vertex v_t. We distinguish the following two cases.

Case 1. d is odd.

Without loss of generality, we suppose $n-d-2>0$. Let $\{u_1, u_2, \dots, u_{n-d-2}\}$ be the set of all pendant vertices adjacent to v_t. Let $H = G^* - \{v_t u_i \mid 1 \le i \le n-d-2\}$. We show in the following that either $k = t-2 = \lfloor \frac{d}{2} \rfloor - 1$, or $k = t = \lfloor \frac{d}{2} \rfloor$.

Suppose $k < \lfloor \frac{d}{2} \rfloor - 1$. Then $k + (k+4) < d$ and $k + (k+4)$ is even. Moreover, $(H; v_i) \prec (H; v_k)$ for each $1 \le i < k$ by Lemma 6, $(H; v_k) \prec (H; v_{k+2})$ and $(H; v_{k+1}) \prec (H_1; v_{k+2})$ by Lemmas 8 and 9. Thus, $t \ge k+2$ by Lemma 1. Now let $G' = G^* - v_k v_{d+1} + v_{k+4}v_{d+1}$. Then $G' \in \mathcal{B}$ and $EE(G^*) < EE(G')$ by Lemmas 1 and 6, a contradiction to the choice of G^*. Therefore, $k \ge \lfloor \frac{d}{2} \rfloor - 1$. Similarly, $k \le \lfloor \frac{d}{2} \rfloor$. Thus, $k = \lfloor \frac{d}{2} \rfloor - 1$ or $\lfloor \frac{d}{2} \rfloor$. Suppose $k = \lfloor \frac{d}{2} \rfloor - 1$. Then $(H; v_i) \prec (H; v_{\lfloor \frac{d}{2} \rfloor + 1})$ for each $i \ne \lfloor \frac{d}{2} \rfloor + 1$ with $1 \le i \le d-1$ by Lemmas 6, 8, and 9. Thus, $t = \lfloor \frac{d}{2} \rfloor + 1$ from the choice of G^*. Similarly, $t = \lfloor \frac{d}{2} \rfloor$ if $k = \lfloor \frac{d}{2} \rfloor$. Since d is odd, we get $G^* \cong G_1$.

Case 2. d is even.

By a similar argument to that in Case 1, we can show that either $k = t-2 = \lfloor \frac{d}{2} \rfloor - 2$, or $k = t-2 = \lfloor \frac{d}{2} \rfloor - 1$, or $k = t = \lfloor \frac{d}{2} \rfloor - 1$, or $k = t = \lfloor \frac{d}{2} \rfloor$. Note that G^* has a maximum among $\mathcal{B}$. Therefore, G^* is isomorphic to the graph between G_1 and G_2 with a larger Estrada index. □

Now we give our main results.

Theorem 3. *Let G be the graph with the maximum Estrada index among $\mathcal{U}(n,d)$. Let Δ_n^d, G_1 and G_2 be depicted in Figures 3 and 4. Then $G \in \{\Delta_n^d, G_1\}$ if d is odd, and $G \in \{\Delta_n^d, G_1, G_2\}$ otherwise.*

Proof of Theorem 3. If $d=1$, then $G \cong C_3$. If $d = 2$ or 3, then $G \cong \Delta_n^d$ by Theorem 2. Thus, the result holds when $d \le 3$. We assume $n-2 \ge d \ge 4$ below.

By Theorem 2, $G \ncong C_n$. Let $P_d = v_0 v_1 \cdots v_d$ be an induced path of length d and C_q be the unique cycle in G. Since $G \ncong C_n$, $\min\{d(v_0), d(v_d)\} = 1$—say, $d(v_0) = 1$. Thus, we can make some claims.

Claim 1. $V(P_d) \cap V(C_q) \ne \emptyset$.

Proof of Claim 1. Otherwise, since G is connected, there exists a shortest path $Q = v_i u_k u_{k+1} \cdots u_{l-1} u_l$ connecting C_q and P_d, where $u_l \in V(C_q)$ and $v_i \in V(P_d)$, and $u_k, u_{k+1}, \dots$ and $u_{l-1} \in V(G) \setminus (V(C_q) \cup V(P_d))$. Denote by G_1 and G_2 the connected components containing v_i and u_k in $G - v_i u_k$, respectively. Let G' be the graph obtained from G_1 and G_2 by identifying v_i with u_k, and attaching a pendant vertex to the common vertex. Then $G' \in \mathcal{U}_n^d$ and $EE(G) < EE(G')$ by Lemma 3, a contradiction. □

By Claim 1, $V(C_q) \cap V(P_d) \ne \emptyset$. Denote $C_q = v_k v_{k+1} \cdots v_{l-1} v_l v_{d+1} v_{d+2} \cdots v_s v_k$, where $s \ge d+1$, $\{v_k, v_{k+1}, \dots, v_{l-1}, v_l\} = V(C_q) \cap V(P_d)$ and $\{v_{d+1}, v_{d+2}, \dots, v_s\} = V(C_q) \setminus V(P_d)$. By a similar argument, we have

Claim 2. $d(v) = 1$ *for each vertex* $v \in V(G) \setminus (V(C_q) \cup V(P_d))$.

By Theorem 1, we have

Claim 3. *All pendant vertices except v_0 and v_d in G are adjacent to one common vertex v.*

Claim 4. $k \ne l$.

Proof of Claim 4. Suppose $k = l$. Then $s \geq d+2$ and $k \neq 0, d$. Since $d \geq 4$, we can assume $k \geq 2$ (otherwise, relabel the vertices in P_d). Let $N_G(v_{d+1}) \setminus \{v_k, v_{d+2}\} = \{w_1, w_2, \ldots, w_t\}$, $H = G - \{v_{d+1}v_{d+2}\} \cup \{v_{d+1}w_i \mid 1 \leq i \leq t\}$ and $G' = H + \{v_{k-1}v_{d+2}\} \cup \{v_{k-1}w_i \mid 1 \leq i \leq t\}$. Then $N_H(v_{d+1}) \subseteq N_H(v_{k-1})$, $d_H(v_{d+1}) = 1 < d_H(v_{k-1})$ and $G' \in \mathcal{U}_n^d$. By Lemma 4, we have $(H; v_{d+1}) \prec (H; v_{k-1})$ and for each vertex $w \in \{v_{d+2}, w_1, w_2, \ldots, w_t\}$, $(H; w, v_{d+1}) \preceq (H; w, v_{k-1})$. Thus, $EE(G) < EE(G')$ by Lemma 1, a contradiction. □

Claim 5. *If $l = k+1$, then $s = d+1$; and if $l \geq k+2$, then $l = k+2$ and $s = d+1$.*

Proof of Claim 5. Suppose $l = k+1$. If $s \geq d+3$, by letting $N_G(v_{d+1}) \setminus \{v_{k+1}, v_{d+2}\} = \{w_1, w_2, \ldots, w_t\}$, $H = G - \{v_{d+1}v_{d+2}\} \cup \{v_{d+1}w_i \mid 1 \leq i \leq t\}$ and $G' = H + \{v_k v_{d+2}\} \cup \{v_k w_i \mid 1 \leq i \leq t\}$, then $N_H(v_{d+1}) \subseteq N_H(v_k)$, $d_H(v_{d+1}) = 1 < d_H(v_k)$ and $G' \in \mathcal{U}_n^d$. Moreover, $(H; v_{d+1}) \prec (H; v_k)$ and $(H; w, v_{d+1}) \preceq (H; w, v_k)$ for each vertex $w \in \{v_{d+2}, w_1, w_2, \cdots, w_t\}$ by Lemma 4. Thus, $EE(G) < EE(G')$ by Lemma 1, a contradiction. Hence, $s = d+2$ or $d+1$. □

Suppose $s = d+2$ when $l = k+1$. Since $d \geq 4$, we can assume $k \geq 2$ (otherwise, relabel the vertices in P_d). Let $N_G(v_{d+2}) \setminus \{v_k, v_{d+1}\} = \{w_1, w_2, \ldots, w_t\}$, $H = G - \{v_{d+2}v_{d+1}\} \cup \{v_{d+2}w_i \mid 1 \leq i \leq t\}$ and $G' = H + \{v_{k-1}v_{d+1}\} \cup \{v_{k-1}w_i \mid 1 \leq i \leq t\}$. Then $N_H(v_{d+2}) \subseteq N_H(v_{k-1})$, $d_H(v_{d+2}) = 1 < d_H(v_{k-1})$ and $G' \in \mathcal{U}_n^d$. By Lemma 4, $(H; v_{d+2}) \prec (H; v_{k-1})$ and for each vertex $w \in \{v_{d+1}, w_1, w_2, \ldots, w_t\}$, $(H; w, v_{d+2}) \preceq (H; w, v_{k-1})$. Thus, $EE(G) < EE(G')$ by Lemma 1, a contradiction. This implies $s = d+1$ if $l = k+1$.

Now suppose $l \geq k+2$. Suppose $s \geq d+2$. Let $N_G(v_s) \setminus \{v_k, v_{s-1}\} = \{w_1, \ldots, w_t\}$, $H = G - \{v_s v_{s-1}\} \cup \{v_s w_i \mid 1 \leq i \leq t\}$ and $G' = H + \{v_{k+1}v_{s-1}\} \cup \{v_{k+1}w_i \mid 1 \leq i \leq t\}$. Then $N_H(v_s) \subseteq N_H(v_{k+1})$, $d_H(v_s) = 1 < d_H(v_{k+1})$ and $G' \in \mathcal{U}_n^d$. By Lemma 4, $(H; v_s) \prec (H; v_{k+1})$ and for each vertex $w \in \{v_{s-1}, w_1, w_2, \ldots, w_t\}$, $(H; w, v_s) \preceq (H; w, v_{k+1})$. Thus, $EE(G) < EE(G')$ by Lemma 1, a contradiction. Therefore, $s = d+1$. Since $s - d + 1 \geq l - k$, we have $l = k+2$.

By Claims 5 and 3, if $l = k+1$, then G is the unicyclic graph with maximum Estrada index of diameter d obtained from P_d and v_{d+1} by adding the edges $v_k v_{d+1}$ and $v_{k+1}v_{d+1}$, and attaching $n-d-2$ pendant edges at one vertex $v \in V(P) \cup \{v_{d+1}\}$ for some $1 \leq k \leq d-1$. By Lemma 10, we get

Claim 6. *If $l = k+1$, then $G \cong \Delta_n^d$.*

By Claims 5 and 3, if $l = k+1$, then G is the unicyclic graph with the maximum Estrada index of diameter d obtained from P_d and v_{d+1} by adding the edges $v_k v_{d+1}$ and $v_{k+2}v_{d+1}$, and attaching $n-d-2$ pendant edges at one vertex $v \in V(P)$ for some $1 \leq k \leq d-2$. By Lemma 11, we get

Claim 7. *If $l = k+2$, then $G \cong G_1$ if d is odd, and $G \in \{G_1, G_2\}$ if d is even.*

Now the proof is complete. □

By Theorem 3, we can easily obtain the following corollary.

Corollary 1. *Let G be a graph in $\mathcal{U}(n,d)$. If the girth of G is odd, then $EE(G) \leq EE(\Delta_n^d)$, with equality if and only if $G \cong \Delta_n^d$.*

Liu et al. in [35] showed the following result on the spectral radii of unicyclic graphs.

Theorem 4 ([35])**.** *Let G be a graph in $\mathcal{U}(n,d)$, $d \geq 1$. Then $\rho(G) \leq \rho(\Delta_n^d)$, and equality holds if and only if $G \cong \Delta_n^d$.*

Based on Theorems 3 and 4 and previous results on extremal values of Estrada index and spectral radius, we propose the following hypothesis.

Hypothesis 1. *Let G be a graph in $\mathcal{U}(n,d)$. Then $EE(G) \le EE(\Delta_n^d)$, with equality if and only if $G \cong \Delta_n^d$.*

Remark 2. *To prove Hypothesis 1, it suffices to show that $EE(\Delta_n^d) > EE(G_1)$ and $EE(\Delta_n^d) > EE(G_2)$ by Theorem 3. To show this, by previous methods and (1), it suffices to show that for $i = 1,2$, the inequality $M_k(\Delta_n^d) \ge M_k(G_i)$ holds for each $k \ge 0$ and is strict for some $k_0 > 0$. However, this can not happen since $M_4(\Delta_n^d) = 2\sum_{j=1}^{n} d_{\Delta_n^d}(v_j)^2 - 2m = 2\sum_{j=1}^{n} d_{G_i}(v_j)^2 - 2m < 2\sum_{j=1}^{n} d_{G_i}(v_j)^2 - 2m + 8 = M_4(G_i)$ for $i = 1,2$. Notice that G_1 and G_2 are both bipartite graphs. The hypothesis is true if we can show that for $i = 1,2$, $\frac{M_{2k-1}(\Delta_n^d)}{(2k-1)!} + \frac{M_{2k}(\Delta_n^d)}{(2k)!} \ge \frac{M_{2k}(G_i)}{(2k)!}$ holds for all $k > 0$ and is strict for some $k_0 > 0$.*

5. Conclusions

In [1], Estrada proposed a graph invariant (the Estrada index) based on a Taylor series expansion of spectral moments. In this paper, we gave some transformations that can be used to compare the Estrada indices of two graphs. As applications, we determined the graphs with the maximum Estrada indices among all unicyclic graphs with fixed diameter d. We showed two candidate extremal graphs if d is odd and three candidate extremal graphs if d is even. For future research, it would be interesting to study Hypothesis 1.

Author Contributions: Methodology, W.N. and K.W.; investigation, W.N. and K.W.; writing—original draft preparation, K.W.; writing—review and editing, W.N.; funding acquisition, W.N. All authors have read and agreed to the published version of the manuscript.

Funding: This study was supported by the National Natural Science Foundation of China (number 11801568).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

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