Research Article

On the Maximal Eccentric Distance Sums of Graphs

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If G is a simple connected graph with vertex $V(G)$, then the eccentric distance sum of G , denoted by $\xi^d(G)$, is defined as $\sum_{v \in V(G)} ec_G(v)D_G(v)$, where $ec_G(v)$ is the eccentricity of the vertex v and $D_G(v)$ is the sum of all distances from the vertex v . Let $n \geq 8$. We determine the n -vertex trees with, respectively, the maximum, second-maximum, third-maximum, and fourth-maximum eccentric distance sums. We also characterize the extremal unicyclic graphs on n vertices with respectively, the maximal, second maximal, and third maximal eccentric distance sums.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d_G(u, v)$ be the distance (or length of a shortest path) between vertices u and v in G . For a vertex $v \in V(G)$, the eccentricity $ec_G(v)$ is the maximum distance from v to any other vertex, and $D_G(v) = \sum_{u \in V(G)} d_G(u, v)$ is the sum of all distances from v . The eccentric distance sum of G (EDS) is defined as

$$\xi^d(G) = \sum_{v \in V(G)} ec_G(v)D_G(v). \quad (1.1)$$

This graph invariant was proposed by Gupta et al. in [1]. Like the Wiener index [2–4] and eccentric connectivity index [5–9], it turned to have high discriminating power and excellent predictability both with regard to biological and physical properties and to provide valuable leads for the development of safe and potent therapeutic agents of diverse nature. So, it is of interest to study the mathematical properties of this invariant.

Yu et al. [10] considered the n -vertex trees and unicyclic graphs with minimal eccentric distance sums, respectively. Ilić et al. [11] proved that path P_n is the unique extremal trees

with n vertices having maximum eccentric distance sum, and provided various lower and upper bounds for the eccentric distance sum. In this paper, we determine the n -vertex trees with, respectively, the maximum, second-maximum, third-maximum, and fourth-maximum eccentric distance sums for $n \geq 8$. We also characterize the extremal unicyclic graphs with the maximal, second maximal, and third maximal eccentric distance sums.

2. The Trees with Maximal Eccentric Distance Sums

Lemma 2.1. *Let u be a vertex of a connected graph G with at least two vertices. Let G^i be the graph obtained by identifying u and a vertex v_i of a path $P_{n+1} = v_0 v_1 \cdots v_{n-1} v_n$, where $1 \leq i \leq \lfloor n/2 \rfloor$. Then, $\xi^d(G^{i-1}) > \xi^d(G^i)$.*

Proof. By the definition of EDS, we have

$$\begin{aligned} \xi^d(G^i) &= \sum_{v \in V(G) \setminus \{u\}} \text{ec}_{G^i}(v) D_{G^i}(v) \\ &+ \sum_{j=0}^{i-1} [\text{ec}_{G^i}(v_j) D_{G^i}(v_j) + \text{ec}_{G^i}(v_{n-j}) D_{G^i}(v_{n-j})] + \sum_{k=i}^{n-i} \text{ec}_{G^i}(v_k) D_{G^i}(v_k). \end{aligned} \quad (2.1)$$

Denoted by A^i , B^i , and C^i respectively, the three sums of right equality above, we only need to prove the following three inequalities: $A^{i-1} > A^i$, $B^{i-1} > B^i$, $C^{i-1} > C^i$.

Note that $\text{ec}_{G^{i-1}}(v) \geq \text{ec}_{G^i}(v)$ for any $v \in V(G)$, and

$$\begin{aligned} D_{G^{i-1}}(v) - D_{G^i}(v) &= \left[\sum_{\omega \in V(G)} d(v, \omega) + \sum_{j=0}^{i-1} (d(u, v) + j) \times 2 + \sum_{j=i}^{n-i+1} (d(u, v) + j) \right] \\ &- \left[\sum_{\omega \in V(G)} d(v, \omega) + \sum_{j=0}^i (d(u, v) + j) \times 2 + \sum_{j=i+1}^{n-i} (d(u, v) + j) \right] \\ &= n - 2i + 1 > 0, \end{aligned} \quad (2.2)$$

and thus, the inequality $A^{i-1} > A^i$ holds.

Note that for any $i \leq k \leq n - i$, $\text{ec}_{G^{i-1}}(v_k) \geq \text{ec}_{G^i}(v_k)$, $D_{G^{i-1}}(v_k) > D_{G^i}(v_k)$, and thus $C_{i-1} > C_i$. So, it suffices to prove $B^{i-1} > B^i$.

Let $\text{ec}_G(u) = s$ and $n_1 = |V(G)|$, and we distinguish the following two cases:

Case 1 ($s \geq n - i + 1$). By direct calculation, it follows that

$$\begin{aligned} B^{i-1} &= \sum_{j=0}^{i-1} \text{ec}_{G^{i-1}}(v_j) D_{G^{i-1}}(v_j) + \text{ec}_{G^{i-1}}(v_{n-j}) D_{G^{i-1}}(v_{n-j}) \\ &= \sum_{j=0}^{i-1} \left\{ [\text{ec}_{G^i}(v_j) - 1] \left[\sum_{v \in V(P_{n+1})} d(v_j, v) + \sum_{v \in V(G) \setminus \{u\}} (d_{G^i}(v_j, u) - 1 + d_G(u, v)) \right] \right\} \end{aligned}$$

$$\begin{aligned}
& + [\text{ec}_{G^i}(v_{n-j}) + 1] \left[\sum_{v \in V(P_{n+1})} d(v_{n-j}, v) + \sum_{v \in V(G) \setminus \{u\}} (d_{G^i}(v_{n-j}, u) + 1 + d_G(u, v)) \right] \Bigg\} \\
& = B_i + \sum_{j=0}^{i-1} \left\{ (n_1 - 1) [\text{ec}_{G^i}(v_{n-j}) - \text{ec}_{G^i}(v_j)] \right. \\
& \quad \left. + \sum_{v \in V(P_{n+1})} [d(v_{n-j}, v) - d(v_j, v)] + (n_1 - 1) [d(v_{n-j}, u) - d(v_j, u)] + 2(n_1 - 1) \right\}.
\end{aligned} \tag{2.3}$$

For $0 \leq j \leq i - 1$, it is easily seen that $\text{ec}_{G^i}(v_{n-j}) > \text{ec}_{G^i}(v_j)$ and $d(v_{n-j}, u) \geq d(v_j, u)$. Furthermore, $\sum_{v \in V(P_{n+1})} [d(v_{n-j}, v) - d(v_j, v)] = 0$, and thus, $B^{i-1} > B^i$.

Case 2 ($s \leq n - i$). For $0 \leq j \leq i - 1$, it is easily seen that $\text{ec}_{G^{i-1}}(v_j) = \text{ec}_{G^i}(v_j)$, $\text{ec}_{G^{i-1}}(v_{n-j}) \geq \text{ec}_{G^i}(v_{n-j})$. Then,

$$\begin{aligned}
B^{i-1} &= \sum_{j=0}^{i-1} [\text{ec}_{G^{i-1}}(v_j) D_{G^{i-1}}(v_j) + \text{ec}_{G^{i-1}}(v_{n-j}) D_{G^{i-1}}(v_{n-j})] \\
&\geq \sum_{j=0}^{i-1} [\text{ec}_{G^i}(v_j) D_{G^{i-1}}(v_j) + \text{ec}_{G^i}(v_{n-j}) D_{G^{i-1}}(v_{n-j})] \\
&= \sum_{j=0}^{i-1} \left\{ \text{ec}_{G^i}(v_j) \left[\sum_{v \in V(P_{n+1})} d(v_j, v) + \sum_{v \in V(G) \setminus \{u\}} (d_{G^i}(v_j, u) - 1 + d_G(u, v)) \right] \right. \\
&\quad \left. + \text{ec}_{G^i}(v_{n-j}) \left[\sum_{v \in V(P_{n+1})} d(v_{n-j}, v) + \sum_{v \in V(G) \setminus \{u\}} (d_{G^i}(v_{n-j}, u) + 1 + d_G(u, v)) \right] \right\} \\
&= B_i + (n_1 - 1) \sum_{j=0}^{i-1} [\text{ec}_{G^i}(v_{n-j}) - \text{ec}_{G^i}(v_j)] \\
&> B^i,
\end{aligned} \tag{2.4}$$

where the last inequality follows as $\text{ec}_{G^i}(v_{n-j}) > \text{ec}_{G^i}(v_j)$ for $0 \leq j \leq i - 1$. $\square$

By Lemma 2.1 the inequality $\xi^d(G^i) < \xi^d(G^0)$ follows easily. Note that G^i has the number of pendent vertices greater than that of G^0 . Let T be a tree with at least i pendent vertices, where $3 \leq i \leq n - 1$, by applying the above transformation to T repeatedly, then we can obtain a new tree with exactly $i - 1$ pendent vertices, which has larger eccentric distance sum. So it is easy to prove the following result, which is also obtained by Ilić et al. in [11].

Theorem 2.2. *Among all trees with n vertices, P_n has the maximal eccentric distance sum.*

Let $T_{n,i}$ be the tree obtained from $P_{n-1} = v_0 v_1 \cdots v_{n-2}$ by attaching a pendent vertex v_{n-1} to v_i , where $1 \leq i \leq \lfloor (n - 2)/2 \rfloor$.

Lemma 2.3. Let $n \geq 8$. Then,

$$\xi^d(T_{n,1}) - \xi^d(T_{n,2}) > 2n - 4, \quad \xi^d(T_{n,2}) - \xi^d(T_{n,3}) > 4n - 10. \quad (2.5)$$

Proof. Suppose that $T_{n,i}$ has the same vertex labeling as the above definition. We have two cases based on the parity of n . If $n \geq 8$ is even, then

$$\begin{aligned} \xi^d(T_{n,1}) - \xi^d(T_{n,2}) &= \sum_{i=0}^{n-1} [\text{ec}_{T_{n,1}}(v_i)D_{T_{n,1}}(v_i) - \text{ec}_{T_{n,2}}(v_i)D_{T_{n,2}}(v_i)] \\ &= (n-2) \cdot (-1) + (n-3) \cdot (-1) + (n-4) \cdot 1 + \cdots + \frac{n}{2} \cdot 1 \\ &\quad + \left(\frac{n}{2} - 1\right) \cdot 1 + \frac{n}{2} \cdot 1 + \cdots + (n-3) \cdot 1 \\ &\quad + (n-2) \cdot 1 + \frac{1}{2}(3n^2 - 19n + 36) \\ &= \frac{1}{4}(9n^2 - 62n + 116) \\ &= 2(n-2)\left(\frac{9}{8}n - \frac{44}{8}\right) + 7 \\ &> 2(n-2), \\ \xi^d(T_{n,2}) - \xi^d(T_{n,3}) &= \sum_{i=0}^{n-1} [\text{ec}_{T_{n,2}}(v_i)D_{T_{n,2}}(v_i) - \text{ec}_{T_{n,3}}(v_i)D_{T_{n,3}}(v_i)] \\ &= (n-2) \cdot (-1) + (n-3) \cdot (-1) + (n-4) \cdot (-1) + (n-5) \cdot 1 \\ &\quad + \cdots + \frac{n}{2} \cdot 1 + \left(\frac{n}{2} - 1\right) \cdot 1 + \frac{n}{2} \cdot 1 + \cdots + (n-3) \cdot 1 + (n-2) \cdot 1 \\ &\quad + \frac{1}{2}(3n^2 - 27n + 72) \\ &= \frac{1}{4}(9n^2 - 86n + 220) \\ &= (4n-10)\left(\frac{9}{16}n - \frac{127}{32}\right) + \frac{227}{16} \\ &> 4n - 10. \end{aligned} \quad (2.6)$$

If $n \geq 9$ is odd, then we make a similar calculation as above and obtain that

$$\begin{aligned} \xi^d(T_{n,1}) - \xi^d(T_{n,2}) &= 2(n-2)\left(\frac{9}{8}n - \frac{44}{8}\right) + \frac{29}{4} > 2(n-2), \\ \xi^d(T_{n,2}) - \xi^d(T_{n,3}) &= (4n-10)\left(\frac{9}{16}n - \frac{143}{32}\right) + \frac{149}{16} > 4n - 10. \end{aligned} \quad (2.7)$$

These complete the proof. $\square$

Lemma 2.4. Among all trees on n vertices, where $n \geq 8$, $T_{n,3}$ has the maximal eccentric distance sum except P_n , $T_{n,1}$, and $T_{n,2}$.

Proof. suppose that T is an n -vertex tree different from P_n , $T_{n,1}$, and $T_{n,2}$. Let p be the number of pendent vertices of T , then $p \geq 3$.

If $p = 3$, then T is a tree obtained by identifying three pendent vertices of three paths. Denote by r, s , and t , respectively, the lengths of the three paths, where $r \geq s \geq t \geq 1$ and $r+s+t+1 = n$. Here, we denote it by $T_n(r, s, t)$. Clearly, $T_n(n-i-2, i, 1) \cong T_{n,i}$ ($1 \leq i \leq \lfloor (n-2)/2 \rfloor$). Suppose first that $t = 1$. Then, $T = T_{n,i}$ with $i \geq 3$. For $3 \leq i \leq \lfloor (n-4)/2 \rfloor$, by Lemma 2.1, we have $\xi^d(T_{n,i+1}) < \xi^d(T_{n,i})$, and thus, $\xi^d(T) \leq \xi^d(T_{n,3})$ with equality if and only if $T \cong T_{n,3}$. Now suppose that $t \geq 2$, then $r \geq 3$ for $n \geq 8$, and by Lemma 2.1, we can obtain a new tree $T_n(r, s+t-1, 1)$ or $T_n(s+t-1, r, 1)$, which is not isomorphic to $T_{n,1}$, $T_{n,2}$, and $T_{n,3}$ and has larger eccentric distance sum.

If $p \geq 5$ by applying transformation of Lemma 2.1 to T repeatedly, we can obtain a new tree with exactly four pendant vertices and larger eccentric distance sum. Thus, it suffices to consider the case $p = 4$.

Now, suppose that $p = 4$. In this case, T has at most two vertices with degree more than 2.

Case 1. If T has exactly two vertices with degree more than 2, say u and v , then $d(u) = d(v) = 3$. Suppose that the length of path connecting u and v is a , the lengths of pendent paths at u are b, c , and the lengths of pendent paths at v are d, f . We denote this tree by $T_n(a; b, c; d, f)$, where $a \geq 1, b \geq c, d \geq f$ and $a + b + c + d + f + 1 = n$. If $b \geq 3$, then $b, d + f + a \geq 3$, and by Lemma 2.1 and above proof, we have $\xi^d(T_n(a; b, c; d, f)) < \xi^d(T_n(b, d + f + a, c)) < \xi^d(T_{n,3})$, where we suppose that $b \geq d + f + a \geq c$. If $b = c = 2$, then by Lemma 2.1 and the result above we have $\xi^d(T_n(a; 2, 2; d, f)) < \xi^d(T_n(a; 3, 1; d, f)) < \xi^d(T_{n,3})$. If $b = 2, c = 1$ or $b = 1, c = 1$. Applying similar proof of Lemma 2.3, it is easily proven that $\xi^d(T_n(n-6; 1, 1; 2, 1)) - \xi^d(T_n(n-7; 2, 1; 2, 1)) > 0$, $\xi^d(T_n(n-5; 1, 1; 1, 1)) - \xi^d(T_n(n-6; 1, 1; 2, 1)) > 0$, and thus, we only need to prove that $\xi^d(T_n(n-5; 1, 1; 1, 1)) < \xi^d(T_{n,3})$.

Here, we write T_n instead of $T_n(n-5; 1, 1; 1, 1)$. Then, T_n is a tree obtained from the path $v_0v_1 \cdots v_{n-4}v_{n-3}$ by joining an isolated vertex v_{n-2} to v_{n-4} and an isolated vertex v_{n-1} to v_1 . Let $T_{n,1}$ be a tree obtained from T_n by deleting the edge v_1v_{n-1} and adding the edge v_0v_{n-1} . If $n \geq 8$ is odd, then

$$\begin{aligned}
 & ec_{T_{n,1}}(v_0)D_{T_{n,1}}(v_0) - ec_{T_n}(v_0)D_{T_n}(v_0) = -(n-3), \\
 & ec_{T_{n,1}}(v_1)D_{T_{n,1}}(v_1) - ec_{T_n}(v_1)D_{T_n}(v_1) = n-4, \\
 & ec_{T_{n,1}}(v_{n-1})D_{T_{n,1}}(v_{n-1}) - ec_{T_n}(v_{n-1})D_{T_n}(v_{n-1}) \\
 & \quad = (n-2)(D_{T_n}(v_{n-1}) + n-3) - (n-3)D_{T_n}(v_{n-1}) \\
 & \quad = \frac{3n^2 - 13n + 16}{2}, \\
 & ec_{T_{n,1}}(v_{n-3})D_{T_{n,1}}(v_{n-3}) - ec_{T_n}(v_{n-3})D_{T_n}(v_{n-3}) \\
 & \quad = ec_{T_{n,1}}(v_{n-2})D_{T_{n,1}}(v_{n-2}) - ec_{T_n}(v_{n-2})D_{T_n}(v_{n-2}) \\
 & \quad = (n-2)(D_{T_n}(v_{n-2}) + 1) - (n-3)D_{T_n}(v_{n-2}) \\
 & \quad = \frac{n^2 - n}{2},
 \end{aligned}$$

$$\begin{aligned}
& \text{ec}_{T_{n,1}}(v_{(n-3)/2})D_{T_{n,1}}(v_{(n-3)/2}) - \text{ec}_{T_n}(v_{(n-3)/2})D_{T_n}(v_{(n-3)/2}) \\
&= \left(\frac{n-3}{2} + 1\right)(D_{T_n}(v_{(n-3)/2}) + 1) - \frac{n-3}{2}D_{T_n}(v_{(n-3)/2}) \\
&= \frac{n^2 + 2n - 11}{4},
\end{aligned} \tag{2.8}$$

for $2 \leq i \leq (n-5)/2$, $\text{ec}_{T_{n,1}}(v_i)D_{T_{n,1}}(v_i) - \text{ec}_{T_n}(v_i)D_{T_n}(v_i) = n-3-i$; for $(n-1)/2 \leq i \leq n-4$,

$$\begin{aligned}
& \text{ec}_{T_{n,1}}(v_i)D_{T_{n,1}}(v_i) - \text{ec}_{T_n}(v_i)D_{T_n}(v_i) = (i+1)(D_{T_n}(v_i) + 1) - iD_{T_n}(v_i) \\
&= i^2 - (n-4)i + \frac{n^2 - 3n + 2}{2}.
\end{aligned} \tag{2.9}$$

It follows that

$$\begin{aligned}
& \xi^d(T_{n,1}) - \xi^d(T_n(n-5; 1, 1; 1, 1)) \\
&= \frac{5n^2 - 15n + 14}{2} + \sum_{i=2}^{(n-5)/2} (n-3-i) + \frac{n^2 + 2n - 11}{4} + \sum_{i=(n-1)/2}^{n-4} \left[i^2 - (n-4)i + \frac{n^2 - 3n + 2}{2} \right] \\
&= \frac{25n^2 - 48n + 111}{8} + \frac{(n-5)(n+3)(2n-5)}{12} = \frac{4n^3 + 57n^2 - 304n + 337}{24} \\
&> \frac{18n^2 - 148n + 337}{4} = \xi^d(T_{n,1}) - \xi^d(T_{n,3}).
\end{aligned} \tag{2.10}$$

Thus, $\xi^d(T_{n,3}) > \xi^d(T_n(n-5; 1, 1; 1, 1))$.

Similarly, for even n , we have

$$\begin{aligned}
& \xi^d(T_{n,1}) - \xi^d(T_n(n-5; 1, 1; 1, 1)) \\
&= \frac{5n^2 - 15n + 14}{2} + \sum_{i=2}^{n/2-2} (n-3-i) + \sum_{i=n/2-1}^{n-4} \left[i^2 - (n-4)i + \frac{n^2 - 3n + 2}{2} \right] \\
&> \frac{18n^2 - 148n + 256}{4} = \xi^d(T_{n,1}) - \xi^d(T_{n,3}),
\end{aligned} \tag{2.11}$$

and the inequality $\xi^d(T_{n,3}) > \xi^d(T_n(n-5; 1, 1; 1, 1))$ also holds.

Case 2. If T has an unique vertex of degree greater than 2, say w , then $d(w) = 4$, and T is a tree obtained by identifying four pendent vertices of four paths. Denote by $T_n(r, s, t, l)$ this tree, where r, s, t, l are the lengths of the four pendent paths respectively and $r \geq s \geq t \geq l \geq 1$, $r+s+t+l+1 = n$. If $t = 2$, by Lemma 2.1, we have $\xi^d(T_n(r, s, t, l)) < \xi^d(T_n(r+1, s+1, l)) < \xi^d(T_{n,3})$. Similarly, we can show the result for $t = l = 1$ and $r \geq 2$. In the following, we will prove that $\xi^d(T_n(n-4, 1, 1, 1)) < \xi^d(T_{n,3})$. We label the vertices of $T_n(n-4, 1, 1, 1)$ and $T_{n,3}$ such

that $T_n(n-4, 1, 1, 1)$ can be viewed as obtained from the path $v_0v_1 \cdots v_{n-4}$ by joining three isolated vertices v_{n-3} , v_{n-2} and v_{n-1} to v_{n-4} , and $T_{n,3}$ can be viewed as obtained from the path $v_0v_1 \cdots v_{n-2}$ by joining an isolated vertex v_{n-1} to v_{n-5} . Clearly, $ec_{T_{n,3}}(v_i) \geq ec_{T_n(n-4,1,1,1)}(v_i)$ for $0 \leq i \leq n-3$, $D_{T_{n,3}}(v_i) = D_{T_n(n-4,1,1,1)}(v_i)$ for $0 \leq i \leq n-5$ and $i = n-3$, and $D_{T_{n,3}}(v_{n-4}) = D_{T_n(n-4,1,1,1)}(v_{n-4}) + 2$. Note that

$$\begin{aligned}
 & ec_{T_{n,3}}(v_{n-2})D_{T_{n,3}}(v_{n-2}) - ec_{T_n(n-4,1,1,1)}(v_{n-2})D_{T_n(n-4,1,1,1)}(v_{n-2}) \\
 &= (n-2)[D_{T_n(n-4,1,1,1)}(v_{n-2}) + n-2] - (n-3)D_{T_n(n-4,1,1,1)}(v_{n-2}) \\
 &= (n-2)(n-2) + \frac{1}{2}(n-2)(n-3) + 4 \\
 &= \frac{3n^2 - 13n + 22}{2}, \\
 & ec_{T_{n,3}}(v_{n-1})D_{T_{n,3}}(v_{n-1}) - ec_{T_n(n-4,1,1,1)}(v_{n-1})D_{T_n(n-4,1,1,1)}(v_{n-1}) \\
 &= (n-4)[D_{T_n(n-4,1,1,1)}(v_{n-2}) - n + 8] - (n-3)D_{T_n(n-4,1,1,1)}(v_{n-2}) \\
 &= -(n-2)(n-8) - \frac{1}{2}(n-2)(n-3) - 4 \\
 &= -\frac{3n^2 - 25n + 46}{2},
 \end{aligned} \tag{2.12}$$

then

$$\xi^d(T_{n,3}) - \xi^d(T_n(n-4, 1, 1, 1)) > \frac{3n^2 - 13n + 22}{2} - \frac{3n^2 - 25n + 46}{2} > 0, \tag{2.13}$$

and this completes the proof. $\square$

From Lemmas 2.1 and 2.4, We have the following

Theorem 2.5. *If $n \geq 8$, then $T_{n,1}$, $T_{n,2}$, and $T_{n,3}$ are the unique trees with the second-maximal, third-maximal, and fourth-maximal eccentric distance sums among the trees on n vertices.*

3. The Unicyclic Graphs with Maximal Eccentric Distance Sums

Let U_n be the graph obtained from a path $P_{n-1} = v_0v_1 \cdots v_{n-3}v_{n-2}$ by joining the vertex v_{n-1} to v_{n-3} and v_{n-2} . Let Q_n be the graph obtained from a path $P_{n-1} = v_0v_1 \cdots v_{n-3}v_{n-2}$ by joining the vertex v_{n-1} to v_{n-4} and v_{n-2} , and B_n be obtained by joining v_{n-1} to v_{n-4} and v_{n-3} .

Theorem 3.1. *Let G be a graph with n vertices and n edges; that is, G is an unicyclic graph, where $n \geq 8$. Then, $\xi^d(G) \leq \xi^d(U_n)$, with equality if and only if $G \cong U_n$.*

Proof. If $G \not\cong C_n$ and $G \not\cong U_n$, then we can always find an edge e of G such that $G - e$ is a tree with at least three pendent vertices and $G - e \not\cong T_{n,1}, P_n$. It follows from Lemma 2.3 that

$$\xi^d(G) < \xi^d(G - e) \leq \xi^d(T_{n,2}) < \xi^d(T_{n,1}) - 2(n-2) = \xi^d(U_n). \tag{3.1}$$

Suppose that $G \cong C_n$ and v is any vertex of C_n . If $n \geq 8$ is even, then

$$ec(v)D(v) = \frac{n}{2} \left[\left(1 + 2 + \cdots + \frac{n}{2} - 1 \right) \times 2 + \frac{n}{2} \right] = \frac{n^3}{8}. \quad (3.2)$$

By the definition of EDS, we have

$$\begin{aligned} \xi^d(U_n) &= (ec(v_0)D(v_0) + ec(v_{n/2-1})D(v_{n/2-1})) \\ &\quad + (ec(v_{n/2-2})D(v_{n/2-2}) + ec(v_{n/2})D(v_{n/2})) + \sum_{i \neq 0, n/2-1, n/2-2, n/2} ec(v_i)D(v_i). \end{aligned} \quad (3.3)$$

It is easily checked that

$$\begin{aligned} ec(v_0)D(v_0) + ec(v_{n/2-1})D(v_{n/2-1}) &> \frac{n^3}{4}, \\ ec(v_{n/2-2})D(v_{n/2-2}) + ec(v_{n/2})D(v_{n/2}) &= \frac{n^3}{4}, \end{aligned} \quad (3.4)$$

and for $i \neq 0, n/2-1, n/2-2, n/2$, $ec(v_i) \geq n/2+1$, $D(v_i) > n^2/4$. Then,

$$\xi^d(U_n) > \frac{n^3}{4} + \frac{n^3}{4} + (n-4) \left(\frac{n}{2} + 1 \right) \frac{n^2}{4} = \frac{n^4}{8} + \frac{3}{8}n^2(n-2) > \frac{n^4}{8} = \xi^d(C_n). \quad (3.5)$$

We can prove the result for odd number n similarly, and thus complete the proof. $\square$

Theorem 3.2. Let $n \geq 8$. Then, B_n , Q_n are the graph with, respectively, the second-maximal and third-maximal eccentric distance sums among all unicyclic graphs on n vertices.

Proof. If G has a spanning tree T such that $T \not\cong P_n, T_{n,1}, T_{n,2}$, then

$$\xi^d(G) < \xi^d(T) \leq \xi^d(T_{n,3}) < \xi^d(T_{n,2}) - 4n + 10 = \xi^d(Q_n). \quad (3.6)$$

Now suppose that any spanning tree of G is one of $\{P_n, T_{n,1}, T_{n,2}\}$. Then, G must be isomorphic to C_n , Q_n or B_n . It can be proven easily that $\xi^d(C_n) < \xi^d(Q_n)$ by similar proof of Theorem 3.1. And by directed computation, we obtain that $\xi^d(B_n) = \xi^d(Q_n) + 1$. Thus, the result follows. $\square$

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References

- [1] S. Gupta, M. Singh, and A. K. Madan, "Eccentric distance sum: a novel graph invariant for predicting biological and physical properties," *Journal of Mathematical Analysis and Applications*, vol. 275, no. 1, pp. 386–401, 2002.
- [2] A. A. Dobrynin, R. Entringer, and I. Gutman, "Wiener index of trees: theory and applications," *Acta Applicandae Mathematicae*, vol. 66, no. 3, pp. 211–249, 2001.
- [3] I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, Germany, 1986.
- [4] I. Gutman, S. Klavžar, and B. Mohar, Eds., *Fifty Years of the Wiener Index*, A. Kerber, Bayreuth, Germany, 1997.
- [5] V. Sharma, R. Goswami, and A. K. Madan, "Eccentric connectivity index: a novel highly discriminating topological descriptor for structure-property and structure-activity studies," *Journal of Chemical Information and Computer Sciences*, vol. 37, no. 2, pp. 273–282, 1997.
- [6] M. J. Morgan, S. Mukwembi, and H. C. Swart, "On the eccentric connectivity index of a graph," *Discrete Mathematics*, vol. 311, no. 13, pp. 1229–1234, 2011.
- [7] A. R. Ashrafi, M. Saheli, and M. Ghorbani, "The eccentric connectivity index of nanotubes and nanotori," *Journal of Computational and Applied Mathematics*, vol. 235, no. 16, pp. 4561–4566, 2011.
- [8] A. Ilić and I. Gutman, "Eccentric connectivity index of chemical trees," *MATCH. Communications in Mathematical and in Computer Chemistry*, vol. 65, pp. 731–744, 2011.
- [9] B. Zhou and Z. Du, "On eccentric connectivity index," *MATCH. Communications in Mathematical and in Computer Chemistry*, vol. 63, no. 1, pp. 181–198, 2010.
- [10] G. Yu, L. Feng, and A. Ilić, "On the eccentric distance sum of trees and unicyclic graphs," *Journal of Mathematical Analysis and Applications*, vol. 375, no. 1, pp. 99–107, 2011.
- [11] A. Ilić, G. Yu, and L. Feng, "On the eccentric distance sum of graphs," *Journal of Mathematical Analysis and Applications*, vol. 381, no. 2, pp. 590–600, 2011.