



Research article

On the eccentric connectivity coindex in graphs

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Abstract: The well-studied eccentric connectivity index directly consider the contribution of all edges in a graph. By considering the total eccentricity sum of all non-adjacent vertex, Hua et al. proposed a new topological index, namely, eccentric connectivity coindex of a connected graph. The eccentric connectivity coindex of a connected graph G is defined as

$$\bar{\xi}^c(G) = \sum_{uv \notin E(G)} (\varepsilon_G(u) + \varepsilon_G(v)).$$

Where $\varepsilon_G(u)$ (resp. $\varepsilon_G(v)$) is the eccentricity of the vertex u (resp. v). In this paper, some extremal problems on the $\bar{\xi}^c$ of graphs with given parameters are considered. We present the sharp lower bounds on $\bar{\xi}^c$ for general connecteds graphs. We determine the smallest eccentric connectivity coindex of cacti of given order and cycles. Also, we characterize the graph with minimum and maximum eccentric connectivity coindex among all the trees with given order and diameter. Additionally, we determine the smallest eccentric connectivity coindex of unicyclic graphs with given order and diameter and the corresponding extremal graph is characterized as well.

Keywords: cactus; trees; unicyclic graphs; eccentric connectivity coindex; diameter

Mathematics Subject Classification: 05C12, 05C35, 05C90

1. Introduction

Throughout this paper, all graphs considered are finite, simple, undirected and connected. For a graph $G = (V, E)$ with vertex set $V = V(G)$ and edge set $E = E(G)$. The *degree* of a vertex $v \in V(G)$, denoted by $d_G(v)$, is the number of edges incident with v . For vertices $u, v \in V(G)$, the distance $d(u, v)$ is defined as the length of a shortest path between u and v in G . The *eccentricity* $\varepsilon_G(v)$ or $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex in a graph G . The *diameter* of a connectd graph is the maximum eccentricity of any vertex in the graph. A *pendent vertex* is a vertex of degree 1.

Let P_n , S_n and C_n denote the path, the star and the cycle on n vertices, respectively. By $G - v$ or $G \setminus v$ we denote the graph obtained from G by deleting a vertex $v \in V(G)$. By $G - uv$ we denote the graph obtained from G by deleting an edge $uv \in E(G)$ (This notation is naturally extended if more than one edge are deleted). Similarly, $G + uv$ is obtained from G by adding an edge $uv \notin E(G)$. A path in a connected graph is said to be a *diametrical path*, if this path is of length equal to the diameter. A connected graph is said to be a *tree* if it contains no cycles. Connected graphs in which the number of edges equals the number of vertices are called *unicyclic graphs*. A *cactus* is a connected graph in which any two simple cycles have at most one vertex in common. The set of cacti with n vertices and k cycles is denoted by $C(n, k)$. If $G \in C(n, k)$, then $|E(G)| = n + k - 1$. Other notation and terminology not defined here will conform to those in [4]. In organic chemistry, a molecular graph represents the topology of a molecule. A *topological index* is a function defined on a molecular graph regardless of the labeling of its vertices. Till now, a number of topological indices are introduced and widely used in QSAR/QSPR studies. One of them is the *eccentric connectivity index* (ECI) of graph G , denoted by $\xi^c(G)$, was introduced by Gupta et al. [12], which is defined as

$$\xi^c(G) = \sum_{u \in V(G)} d_G(u) \varepsilon_G(u).$$

The eccentric connectivity index has been shown to give a high degree of predictability properties and may provide leads for the development of safe and potent anti-HIV compounds [5, 13]. Furthermore, the eccentric connectivity index also has a lot of applications in neural science and entropy, see [14, 18]. For the mathematical properties of this index see [1, 9, 11, 17] and the references cited therein.

The eccentric connectivity index of a connected graph G can be rewritten as

$$\xi^c(G) = \sum_{uv \in E(G)} (\varepsilon_G(u) + \varepsilon_G(v)).$$

As is known that the eccentric connectivity index has been used extensively in physical and biological properties. They are defined as sums of contributions dependent on the eccentricity of adjacent vertices over all edges of a graph. By considering analogous contributions from pairs of non-adjacent vertices capturing and quantifying a possible influence of remote pairs of vertices to the molecule's properties, and motivated from [2, 3], Hua and Miao [8] considered the total eccentricity sum of non-adjacent vertex pairs which is defined for a connected graph G as

$$\bar{\xi}^c(G) = \sum_{uv \notin E(G)} (\varepsilon_G(u) + \varepsilon_G(v)), \quad (1)$$

and call this eccentricity-based graph invariant the *eccentric connectivity coindex* $\bar{\xi}^c(G)$. By (1), eccentric connectivity coindex can be rewritten as

$$\bar{\xi}^c(G) = \sum_{u \in V(G)} \varepsilon_G(u)(n - 1 - d_G(u)). \quad (2)$$

The cactus graph has many applications in real life and much work has been done to study the extremal graph according to different index. For more results on the cactus one may be referred to

[6, 7, 10, 15, 16]. In this paper, we continue the above direction of research by considering the extremal problems on the eccentric connectivity coindex.

This paper is compiled as follows. In Section 2, we present the sharp lower bounds on $\bar{\xi}^c$ for general connected graphs. In Section 3, we characterize the extremal graphs with the minimum $\bar{\xi}^c$ among cacti of given order and cycles. In Section 4, we characterize the minimal and maximal $\bar{\xi}^c$ of trees with given order and diameter. In Section 5, we study the minimal $\bar{\xi}^c$ among unicyclic graphs on n vertices with diameter and characterize the extremal graphs.

2. Eccentric connectivity coindex of connected graphs

Hua (2019) characterize all extremal graphs with the maximum and minimum eccentric connectivity coindex among all connected graphs of given order and establish various lower bounds for this index in terms of several other graph parameters. In this section, we continue the investigation along the lines of [8] and present the sharp lower bounds on $\bar{\xi}^c$ for general connected graphs with minimum degree.

Theorem 2.1. *Let $G (\neq K_n)$ be a connected graph of order n with minimum degree δ . Then*

$$\bar{\xi}^c(G) \geq 4(n - 1 - \delta),$$

with equality if and only if $G \cong K_n^\delta$ ($\delta < n - 1$). Where K_n^δ is a connected graph of order n obtained by joining a vertex to the δ vertices in K_{n-1} .

Proof. Let v_n be one vertex of degree δ . Denote by $N_G(v_n) = \{v_1, v_2, \dots, v_\delta\}$, also let $S = \{v_{\delta+1}, \dots, v_{n-1}\}$. Since $G \neq K_n$, we have $\delta \leq n - 2$ and $|S| \geq 1$. Thus $V(G) = N_G(v_n) \cup S \cup \{v_n\}$. For $v_i \in N_G(v_n)$, we have $\varepsilon_G(v_i) \geq 1$ and $d_G(v_i) \leq n - 1$. For $v_i \in S$, we have $d_G(v_i) \leq n - 2$ and $\varepsilon_G(v_i) \geq 2$. Moreover, $\varepsilon_G(v_n) \geq 2$ and $d_G(v_n) = \delta$. By the definition of $\bar{\xi}^c(G)$, we have

$$\begin{aligned} \bar{\xi}^c(G) &= \sum_{v \in N_G(v_n)} \varepsilon_G(v)(n - 1 - d_G(v)) + \sum_{v \in S} \varepsilon_G(v)(n - 1 - d_G(v)) + \varepsilon_G(v_n)(n - 1 - \delta) \\ &\geq 0 + 2(n - 1 - (n - 2))(n - \delta - 1) + 2(n - 1 - \delta) \\ &= 4(n - 1 - \delta). \end{aligned}$$

Suppose the equality holds in above equation, then all the inequalities in the above must be equalities. Thus, we have $d_G(v_i) = n - 2$, $\varepsilon_G(v_i) = 2$ for each $v_i \in S$, $d_G(v_i) = n - 1$, $\varepsilon_G(v_i) = 2$ for each $v_i \in N_G(v_n)$ and $d_G(v_n) = \delta$, $\varepsilon_G(v_n) = 2$. Hence, we find that vertex v_n is adjacent to the vertices of degree $n - 1$ and each vertex in S is degree $n - 2$. So $G \cong K_n^\delta$ ($\delta < n - 1$). This completes the proof. \square

3. Eccentric connectivity coindex of cacti

In this section, we turn our attention to eccentric connectivity coindex for cacti and in particular on extremal cacti regarding $\bar{\xi}^c$.

We start with a useful lemma.

Lemma 3.1 ([8]). *Let G be a connected graph of order n , size m and diameter d . Then*

$$\bar{\xi}^c(G) \geq 2n(n - 1) - 4m,$$

with equality if and only if $d \leq 2$.

Let C_n^k be the cactus by adding k independent edges among pendent vertices of S_n (see Figure 1).

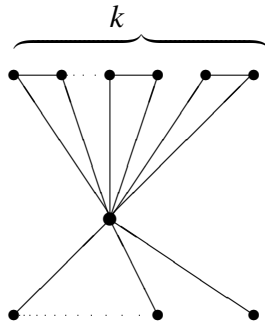


Figure 1. The graph C_n^k with n vertices and k cycles of length 3.

Theorem 3.2. Let G be a cactus on $n \geq 5$ vertices with k cycles. Then

$$\bar{\xi}^c(G) \geq 2n^2 - 6n - 4k + 4.$$

The equality holds if and only if $T \cong C_n^k$.

Proof. Suppose that N is the set of vertices of degree $n-1$. n_0 is the number of elements in N . Assume that $n_0 \geq 2$, let u, v be two vertices in G such that $d_G(u) = d_G(v) = n-1$. Then $\varepsilon_G(u) = \varepsilon_G(v) = 1$. It follows that G is not a cactus. Since there exists cycles sharing common edges in G , then $n_0 = 0$ or $n_0 = 1$. If $n_0 = 1$, then there is a unique vertex v in G such that $d_G(v) = n-1$, thus $\varepsilon_G(v) = 1$, hence each vertex in $G \setminus v$ is adjacent to v . Therefore the cactus G is obtained by introducing k independent edges among pendent vertices of S_n , then $G \cong C_n^k$ and $\bar{\xi}^c(G) = 2n^2 - 6n - 4k + 4$.

Now, we assume that $n_0 = 0$. Let d be the diameter of G . Then $d \geq 3$. Otherwise, if $d \leq 2$, let u be the vertex of maximal degree in G . Then any other vertex of $G \setminus u$ must be adjacent to u , otherwise $d \geq 3$, then $n_0 \geq 1$, a contradiction. By Lemma 3.1,

$$\bar{\xi}^c(G) > 2n(n-1) - 4m = 2n(n-1) - 4(n+k-1) = 2n^2 - 6n + 4 - 4k.$$

Note that, there are exactly $n+k-1$ edges in cactus on n vertices and k cycles. This completes the proof. \square

4. Eccentric connectivity coindex of trees with given diameter

In this section, we shall determine the tree of diameter d with the minimum and maximum $\bar{\xi}^c$ respectively.

The volcano graph $V_{n,d}$ is the graph obtained from a path P_{d+1} and a set S of $n-d-1$ vertices by joining vertex in S to the central vertex of P_{d+1} . Obviously, if d is even, there is only one center of P_{d+1} . If d is odd, there are two central vertices of P_{d+1} (See Figure 2). The caterpillar tree with respect to $P_{d+1} = u_0u_1 \cdots u_d$, denoted by $CP(S_1, \cdots, S_{d-1})$, is the tree obtained from P_d by attaching S_i new vertices to u_i , for $1 \leq i \leq d-1$.

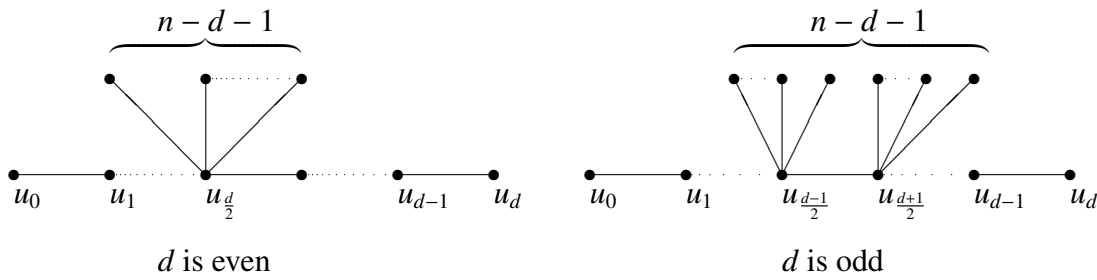


Figure 2. The graph $V_{n,d}$ with d even and d odd.

Let

$$f_1(n, d) = \begin{cases} \sum_{i=1}^{\frac{d}{2}-1} (d-i)(2n-6) + \frac{n^2d-nd^2-nd+2n^2-6n-4d+3d^2+4}{2} & \text{if } n \text{ is even,} \\ \sum_{i=1}^{\frac{d-1}{2}-1} (d-i)(2n-6) + \frac{n^2d-nd^2+3n^2+3nd-8n+3d^2-4d+1}{2} & \text{if } n \text{ is odd,} \end{cases}$$

Theorem 4.1. Let T be a tree on n ($n \geq 5$) vertices with diameter $d \geq 2$. Then

$$\bar{\xi}^c(T) \geq f_1(n, d).$$

The equality holds if and only if $T \cong V_{n,d}$.

Proof. Let T_0 be a graph chosen among all trees of order n with diameter d such that T_0 has the smallest $\bar{\xi}^c$. First, we have the following claim.

Claim 1. Among all trees T with order n and diameter d , $\min(\bar{\xi}^c(T))$ is achieved on caterpillars.

Proof of Claim 1. Let T be any tree that is not a caterpillar with order n and diameter d . Let P be the diametral path of T , connecting u_0 to u_d . Then the eccentricity of each vertex w of T is equal to $\max\{d(w, u_0), d(w, u_d)\}$. Let $z \notin \{u_0, u_d\}$ be a vertex of P and let T_z be a maximal subtree of T which contains z but no other vertex of P . We may assume that z can be selected such that $\varepsilon_{T_z}(z) = k \geq 2$, for otherwise T is a caterpillar. Let u be vertex of T_z with $d(u, z) = k - 1$ and let v be the neighbor of u with $d(v, z) = k - 2$. Let $S = N(u) \setminus v$ and let $s = |S|$. Note that $s \geq 1$. Let T' be the tree from T by replacing the edges between u and the vertices of S with the edges between v and the vertices of S . Then we have

$$\begin{aligned} \bar{\xi}^c(T) - \bar{\xi}^c(T') &= \sum_{w \in V(T)} \varepsilon_T(w)(n-1-d_T(w)) - \sum_{w \in V(T')} \varepsilon_{T'}(w)(n-1-d_{T'}(w)) \\ &= \varepsilon_T(u)(n-1-d_T(u)) + \varepsilon_T(v)(n-1-d_T(v)) \\ &\quad + \sum_{w \in S} \varepsilon_T(w)(n-1-d_T(w)) - \varepsilon_{T'}(u)(n-1-d_{T'}(u)) \\ &\quad - \varepsilon_{T'}(v)(n-1-d_{T'}(v)) - \sum_{w \in S} \varepsilon_{T'}(w)(n-1-d_{T'}(w)) \end{aligned}$$

$$\geq s(\varepsilon_T(v) - \varepsilon_T(u)) + \sum_{w \in S} (n - 1 - d_T(w)).$$

Note that $\varepsilon_T(u) = \varepsilon_T(v) + 1$, $\varepsilon_T(w) \geq \varepsilon_{T'}(w) + 1$ for $w \in S$ and since $d \geq 2$, we get that $d_T(w) < n - 2$. Hence

$$\begin{aligned} \bar{\xi}^c(T) - \bar{\xi}^c(T') &\geq -s + (n - 1)s - \sum_{w \in S} d_T(w) \\ &= (n - 2)s - \sum_{w \in S} d_T(w) \\ &> (n - 2)s - (n - 2)s = 0. \end{aligned}$$

Therefore,

$$\bar{\xi}^c(T) > \bar{\xi}^c(T').$$

If T' is not a caterpillar, we can repeat the construction as many times as required to arrive at a caterpillar. Since at each step the value of $\bar{\xi}^c(T)$ is decreased. Thus the claim is proven.

Since T_0 is the extremal tree with diametral path $P = u_0 u_1, \dots, u_d$. By claim 1, we conclude that all vertices of $V(T) \setminus V(P)$ must be pendent vertices attached at some vertices of P , we denote this tree T_1 . We now consider the case when d is even, if there exists some vertex u_i ($i \neq \frac{d}{2}$) of P with pendent vertices (say w_1, w_2, \dots, w_t $t \geq 1$) attached. Let

$$T_2 = T_1 - \{u_i w_1, u_i w_2, \dots, u_i w_t\} + \{u_{\frac{d}{2}} w_1, u_{\frac{d}{2}} w_2, \dots, u_{\frac{d}{2}} w_t\}.$$

By the definition of $\bar{\xi}^c$, we have

$$\begin{aligned} \bar{\xi}^c(T_1) - \bar{\xi}^c(T_2) &= \sum_{k=1}^t \varepsilon_{T_1}(w_k)(n - 1 - d_{T_1}(w_k)) + \varepsilon_{T_1}(u_i)(n - 1 - d_{T_1}(u_i)) \\ &\quad + \varepsilon_{T_1}(u_{\frac{d}{2}})(n - 1 - d_{T_1}(u_{\frac{d}{2}})) - \sum_{k=1}^t \varepsilon_{T_2}(w_k)(n - 1 - d_{T_2}(w_k)) \\ &\quad - \varepsilon_{T_2}(u_i)(n - 1 - d_{T_2}(u_i)) - \varepsilon_{T_2}(u_{\frac{d}{2}})(n - 1 - d_{T_2}(u_{\frac{d}{2}})). \end{aligned}$$

As $d_{T_1}(w_k) = d_{T_2}(w_k) = 1$, ($k = 1, 2, \dots, t$) and $\varepsilon_{T_1}(w_k) > \varepsilon_{T_2}(w_k)$, $\varepsilon_{T_1}(u_i) = \varepsilon_{T_2}(u_i) > \varepsilon_{T_1}(u_{\frac{d}{2}}) = \varepsilon_{T_2}(u_{\frac{d}{2}})$, $\varepsilon_{T_1}(w_k) - \varepsilon_{T_2}(w_k) = \varepsilon_{T_1}(u_i) - \varepsilon_{T_2}(u_{\frac{d}{2}})$.

Then, we have

$$\begin{aligned} \bar{\xi}^c(T_1) - \bar{\xi}^c(T_2) &= t\varepsilon_{T_1}(w_k)(n - 2) - t\varepsilon_{T_2}(w_k)(n - 2) - t\varepsilon_{T_1}(u_i) + t\varepsilon_{T_1}(u_{\frac{d}{2}}) \\ &\geq t(n - 2)(\varepsilon_{T_1}(w_k) - \varepsilon_{T_2}(w_k)) - t(\varepsilon_{T_1}(u_i) - \varepsilon_{T_2}(u_{\frac{d}{2}})) \\ &= [(n - 2)t - t](\varepsilon_{T_1}(w_k) - \varepsilon_{T_2}(w_k)) \\ &= (n - 3)t(\varepsilon_{T_1}(w_k) - \varepsilon_{T_2}(w_k)) \end{aligned}$$

> 0 .

Therefore,

$$\bar{\xi}^c(T_1) > \bar{\xi}^c(T_2).$$

Continue this procedure, forming new trees, until all the pendent vertices in T_1 are adjacent to $u_{\frac{d}{2}}$. If d is odd, similarly, the extremal graph must be the graph obtained from a path P_{d+1} by some pendent vertices attached on the center of P_{d+1} . That is to say, $T_0 \cong V_{n,d}$. This completes the proof. \square

For even d ,

$$\begin{aligned} \bar{\xi}^c(V_{n,d}) &= \sum_{i=1}^{\frac{d}{2}-1} (d-i)(2n-6) + \frac{n^2d - nd^2 - nd + 2n^2 - 6n - 4d + 3d^2 + 4}{2} \\ &= \frac{n(n-2)(d+2)}{2} - \frac{(n-2)(d^2+3d+2)}{2} + \frac{d(d-2)(3n-7)}{4} + 2d(n-2). \end{aligned}$$

Let $f(x) = \frac{n(n-2)(x+2)}{2} - \frac{(n-2)(x^2+3x+2)}{2} + \frac{x(x-2)(3n-7)}{4} + 2x(n-2)$, ($x \geq 2$). It remains to determine which value of x minimizes $f(x)$. For this, we use the first and second derivative test. Noting that

$$f'(x) = \frac{n(n-2)}{2} - \frac{(n-2)(2x+3)}{2} + \frac{(x-1)(3n-7)}{2} + 2(n-2).$$

$$f''(x) = -(n-2) + \frac{3n-7}{2} = \frac{n-3}{2} > 0.$$

$f''(x)$ is positive for $x \geq 2$, then $f'(x)$ is an increasing function for $x \geq 2$. So

$$\begin{aligned} f'(x) &> f'(2) = \frac{n(n-2)}{2} - \frac{7(n-2)}{2} + \frac{(3n-7)}{2} + 2(n-2) \\ &= \frac{n^2 - 2n - 1}{2} \\ &= \frac{(n-1)^2 - 2}{2} \\ &> 0. \end{aligned}$$

Therefore, $f(x)$ is an increasing function for $x \geq 2$.

Then

$$\bar{\xi}^c(V_{n,d}) < \bar{\xi}^c(V_{n,d+1}).$$

For odd d , we obtain the same result. Therefore, we obtain the following chain inequality

$$\bar{\xi}^c(P_n) = \bar{\xi}^c(V_{n,n-1}) > \bar{\xi}^c(V_{n,n-2}) > \cdots > \bar{\xi}^c(V_{n,2}) = \bar{\xi}^c(S_n). \quad (3)$$

We denote by $H(p, n, q)$ one double starlike tree which is obtained by attaching the centers of two stars $K_{1,p}$ and $K_{1,q}$ to the ends of path P_{d-2} , respectively, where $p+q = n-d-1$. The broom graph $B_{n,d}$

consists of a path P_{d-1} , together with $n - d$ pendent vertices all adjacent to the same pendent vertex of P_{d-1} , obviously, $B_{n,d} = H(0, n, n - d - 1)$, see Figure 3.

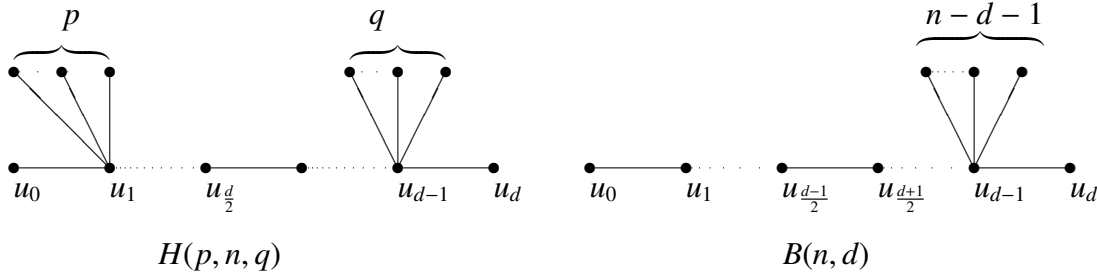


Figure 3. The graphs $H_{p,n,q}$ and $B(n, d)$.

For any tree $T \in H(p, n, q)$, we have $\bar{\xi}^c(T) = \bar{\xi}^c(B_{n,d}) = f_2(n, d)$. Let

$$f_2(n, d) = \begin{cases} \sum_{i=1}^{\frac{d}{2}-1} (d - i)(2n - 6) + \frac{6d^2 - 3nd + 2n^2d - 2nd^2 + 2n - 2 - 7d}{2} & \text{if } n \text{ is even,} \\ \sum_{i=1}^{\frac{d-1}{2}} (d - i)(2n - 6) + 3d^2 - 2nd + n^2d - nd^2 + n - 1 - 2d & \text{if } n \text{ is odd,} \end{cases}$$

Theorem 4.2. *If T is a tree of order n and diameter d , then*

$$\bar{\xi}^c(T) \leq f_2(n, d).$$

The equality holds if and only if $T \cong H(p, n, q)$.

Proof. Let $P = u_0u_1, \dots, u_d$ be a diametral path in T . Assume that T is not the graph $H(p, n, q)$, then there exists a pendent vertex v of T , $v \neq u_0$ such that v is adjacent to a vertex u , where $u \neq u_{d-1}$ and $u \neq u_1$ (It is possible that u lies on P). Denote by $\{v_1, v_2, \dots, v_k\}$ be the set of pendent vertices which are adjacent to u and $v_i \neq u_0$ for $i = 1, 2, \dots, k$. Let

$$T' = T - \{uv_1, uv_2, \dots, uv_k\} + \{u_{d-1}v_1, u_{d-1}v_2, \dots, u_{d-1}v_k\}.$$

Note that T' has the same order and diameter as T . We will show that T' has a larger eccentric connectivity coindex than T .

$$\begin{aligned} \bar{\xi}^c(T') - \bar{\xi}^c(T) &= \sum_{i=1}^k \varepsilon_{T'}(v_i)(n - 1 - d_{T'}(v_i)) + \varepsilon_{T'}(u)(n - 1 - d_{T'}(u)) \\ &\quad + \varepsilon_{T'}(u_{d-1})(n - 1 - d_{T'}(u_{d-1})) - \sum_{i=1}^k \varepsilon_T(v_i)(n - 1 - d_T(v_i)) \\ &\quad - \varepsilon_T(u)(n - 1 - d_T(u)) - \varepsilon_T(u_{d-1})(n - 1 - d_T(u_{d-1})). \end{aligned}$$

As $d_{T'}(v_i) = d_T(v_i) = 1$, ($i = 1, 2, \dots, k$) and $\varepsilon_{T'}(v_i) > \varepsilon_T(v_i)$, $\varepsilon_{T'}(u) = \varepsilon_T(u) < \varepsilon_{T'}(u_{d-1}) = \varepsilon_T(u_{d-1})$, $\varepsilon_{T'}(v_i) - \varepsilon_T(v_i) = \varepsilon_{T'}(u_{d-1}) - \varepsilon_T(u)$. Then, we have

$$\begin{aligned}\bar{\xi}^c(T') - \bar{\xi}^c(T) &= k(n-2)(\varepsilon_{T'}(v_i) - \varepsilon_T(v_i)) - k(\varepsilon_{T'}(u_{d-1}) - \varepsilon_T(u)) \\ &= k(n-2)(\varepsilon_{T'}(v_i) - \varepsilon_T(v_i)) - k(\varepsilon_{T'}(v_i) - \varepsilon_T(v_i)) \\ &= k(n-3)(\varepsilon_{T'}(v_i) - \varepsilon_T(v_i)) \\ &> 0.\end{aligned}$$

Then

$$\bar{\xi}^c(T') > \bar{\xi}^c(T).$$

Continue this procedure, forming new trees until all vertices outside P having degree one are adjacent to x_{d-1} . Thus a tree $H(p, n, q)$ of order n and diameter d is obtained, one has

$$\bar{\xi}^c(B_{n,d}) = \bar{\xi}^c(H(p, n, q)) \geq \bar{\xi}^c(T).$$

This completes the proof. \square

Similar to previous discussion, we have $\bar{\xi}^c(B_{n,d}) < \bar{\xi}^c(B_{n,d+1})$ for any $d \geq 2$. Therefore, it follows that

$$\bar{\xi}^c(P_n) = \bar{\xi}^c(B_{n,n-1}) > \bar{\xi}^c(B_{n,n-2}) > \dots > \bar{\xi}^c(B_{n,2}) = \bar{\xi}^c(S_n). \quad (4)$$

Summarizing theorems 4.1, 4.2 and these inequalities (3), (4), we have the following result.

Theorem 4.3. *Let T be a tree on n vertices. Then*

$$2n^2 - 6n + 4 \leq \bar{\xi}^c(T) \leq f_2(n, n-1).$$

Where $f_2(n, n-1)$ as mentioned in theorem 4.2. The left quality holds if and only if $T \cong S_n$ and the right equality holds if and only if $T \cong P_n$.

5. Eccentric connectivity coindex of unicyclic graphs with given diameter

In this section, we consider the minimum $\bar{\xi}^c$ of unicyclic graphs with given diameter. Let \mathcal{G}_n^d be the unicyclic graph with order n and diameter d . First, for even d , let $V_{n,d}^1$ be the graph obtained from $P_{d+1} = u_0u_1 \dots u_d$ by attaching $n-d-1$ pendent edges to $u_{\frac{d}{2}}$ and adding an edge between $u_{\frac{d}{2}+1}$ and one of the attached pendent vertices of $u_{\frac{d}{2}}$. Let $V_{n,d}^2$ be the graph obtained from $P_{d+1} = u_0u_1 \dots u_d$ by attaching $n-d-1$ pendent edges to $u_{\frac{d}{2}}$ and adding an edge between two attached pendent vertices of $u_{\frac{d}{2}}$, (see Figure 4).

For odd d , let $V_{n,d}^3$ be the unicyclic graphs in which there are s , t ($s+t = n-d-2$) pendent vertices adjacent to $u_{\frac{d-1}{2}}$ and $u_{\frac{d+1}{2}}$ of diametral path respectively. Let $V_{n,d}^4$ be the unicyclic graphs in which there

are p, q ($p + q = n - d - 3$) pendent vertices adjacent to $u_{\frac{d-1}{2}}$ and $u_{\frac{d+1}{2}}$ of diametrel path respectively, (see Figure 4).

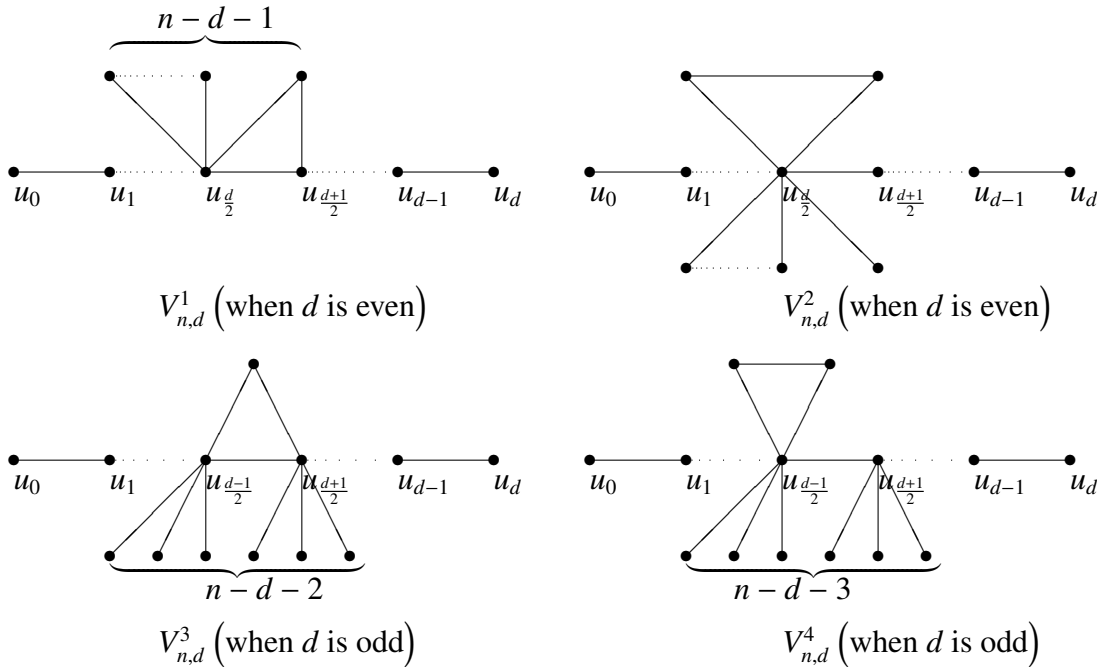


Figure 4. The graphs in Theorem 4.1.

By direct calculation, for even d ,

$$\bar{\xi}^c(V_{n,d}^1) = \bar{\xi}^c(V_{n,d}^2) = \sum_{i=1}^{\frac{d}{2}-1} (d-i)(2n-6) + 2d(n-2) + \frac{d(d-2)}{2} + \frac{(d+2)((n-2)(n-d)-n)}{2}.$$

For odd d , any $G \in V_{n,d}^3$, we have

$$\bar{\xi}^c(G) = \sum_{i=1}^{\frac{d-1}{2}-1} (d-i)(2n-6) + 2d(n-2) + \frac{(d+1)(2n+d-9)}{2} + \frac{(n-2)(d+3)(n-d-2)}{2}.$$

If $G_1 \in V_{n,d}^3$ and $G_2 \in V_{n,d}^4$. By direct calculation we find that, $\bar{\xi}^c(G_1) < \bar{\xi}^c(G_2)$. Let

$$f_3(n, d) = \begin{cases} \sum_{i=1}^{\frac{d}{2}-1} (d-i)(2n-6) + \frac{3d^2-6d+n^2d-nd^2+2n^2-6n-nd}{2} & \text{if } n \text{ is even,} \\ \sum_{i=1}^{\frac{d-1}{2}-1} (d-i)(2n-6) + \frac{3d^2-nd-6d-10n+n^2d-nd^2+3n^2+3}{2} & \text{if } n \text{ is odd.} \end{cases}$$

Theorem 5.1. Let G be a unicyclic graph on n (≥ 7) vertices with diameter $d \geq 2$. Then

$$\bar{\xi}^c(G) \geq f_3(n, d).$$

The equality holds if and only if $G \cong V_{n,d}^1$ or $G \cong V_{n,d}^2$ for even d and $G \cong V_{n,d}^3$ for odd d .

Proof. Choose G_0 in \mathcal{G}_n^d such that $\bar{\xi}^c(G_0)$ is as small as possible. Let $P_{d+1} = u_0u_1, \dots, u_d$ be a diametral path and C_k be the unique cycle in G_0 . Similar as the proof of theorem 4.1 all vertices in $V(G_0) \setminus \{V(P) \cup V(C_k)\}$ must be pendent vertices and adjacent to some vertices of $V(P) \cup V(C_k)$, we denote it by G^* . First, we consider when the diameter d is even, we proceed by considering the following possible cases.

Case 1. $|V(C_k) \cap V(P_{d+1})| = 1$.

In this case, let $V(C_k) \cap V(P_{d+1}) = u_i$. In the following, we show three facts.

Fact 1. All vertices in $V(G^*) \setminus \{V(P) \cup V(C_k)\}$ must be adjacent to $u_{\frac{d}{2}}$ of P .

Proof of Fact 1. If there exists a vertex u_s (with $s \neq \frac{d}{2}$) of P with pendent vertices, say w_1, w_2, \dots, w_k attached in G^* . Let

$$G_1 = G^* - \{u_s w_1, u_s w_2, \dots, u_s w_k\} + \{u_{\frac{d}{2}} w_1, u_{\frac{d}{2}} w_2, \dots, u_{\frac{d}{2}} w_k\}.$$

By a similar approach in the proof of theorem 4.1, we get $\bar{\xi}^c(G^*) > \bar{\xi}^c(G_1)$, a contradiction to our choice of G^* . Similarly, we conclude that there is no pendent vertices attached the vertex of cycle C_k in G^* other than u_i . That is to say, each of the vertices other u_i on cycle C_k in G^* is of degree 2. This completes the proof of fact 1.

Fact 2. The length of the cycle C_k is equal to 3, i.e., $k = 3$ in G^* .

Proof of Fact 2. If the length of the cycle $k \neq 3$.

Let $C_k = u_i v_1 v_2, \dots, v_{k-1} u_i$ and $N_{G^*}(u_i) \cap V(C_k) = \{v_1, v_{k-1}\}$. Let

$$G_2 = G^* - E(C_k) + v_1 v_{k-1} + \{u_i v_1, u_i v_2, \dots, u_i v_{k-1}\}.$$

Clearly, G_2 is in \mathcal{G}_n^d and C_3 is the unique cycle in G_2 . It is routine to check that

$$\begin{aligned} \bar{\xi}^c(G^*) - \bar{\xi}^c(G_2) &= \sum_{j=2}^{k-2} \varepsilon_{G^*}(v_j)(n-1-d_{G^*}(v_j)) + \varepsilon_{G^*}(u_i)(n-1-d_{G^*}(u_i)) \\ &\quad + \varepsilon_{G^*}(v_1)(n-1-d_{G^*}(v_1)) + \varepsilon_{G^*}(v_{k-1})(n-1-d_{G^*}(v_{k-1})) \\ &\quad - \sum_{j=2}^{k-2} \varepsilon_{G_2}(v_j)(n-1-d_{G_2}(v_j)) - \varepsilon_{G_2}(u_i)(n-1-d_{G_2}(u_i)) \\ &\quad - \varepsilon_{G_2}(v_1)(n-1-d_{G_2}(v_1)) - \varepsilon_{G_2}(v_{k-1})(n-1-d_{G_2}(v_{k-1})). \end{aligned}$$

Note that $\varepsilon_{G^*}(u_i) = \varepsilon_{G_2}(u_i)$, $\varepsilon_{G^*}(v_1) = \varepsilon_{G_2}(v_1)$, $\varepsilon_{G^*}(v_{k-1}) = \varepsilon_{G_2}(v_{k-1})$ and $\varepsilon_{G^*}(v_j) \geq \varepsilon_{G_2}(v_j) > \varepsilon_{G^*}(u_i)$ for $j = 2, \dots, k-2$ and $\varepsilon_{G^*}(v_2) = \varepsilon_{G^*}(u_i) + 2$, $\varepsilon_{G_2}(v_2) = \varepsilon_{G_2}(u_i) + 1$.

Therefore,

$$\bar{\xi}^c(G^*) - \bar{\xi}^c(G_2) > (k-3)\varepsilon_{G^*}(u_i) + \sum_{j=2}^{k-2} \varepsilon_{G^*}(v_j)(n-3) - \sum_{j=2}^{k-2} \varepsilon_{G_2}(v_j)(n-2)$$

$$\begin{aligned}
&> (k-3)\varepsilon_{G^*}(u_i) + (k-3)(n-3)\varepsilon_{G^*}(v_2) - (k-3)(n-2)\varepsilon_{G_2}(v_2) \\
&= (k-3)\varepsilon_{G^*}(u_i) + (k-3)(n-3)(\varepsilon_{G^*}(u_i) + 2) \\
&\quad - (k-3)(n-2)(\varepsilon_{G^*}(u_i) + 1) \\
&= (k-3)\varepsilon_{G^*}(u_i) + (k-3)(-\varepsilon_{G^*}(u_i) + n-4) \\
&= (k-3)(n-4) \\
&> 0.
\end{aligned}$$

Then $\bar{\xi}^c(G^*) > \bar{\xi}^c(G_2)$, a contradiction. This completes the proof of fact 2.

Fact 3. u_i is the center of the diametral path P in G^* .

Proof of Fact 3. Based on fact 2, we know that $P_{d+1} = u_0u_1, \dots, u_d$ and $C_k = u_iv_1v_{k-1}$. If $u_i \neq u_{\frac{d}{2}}$, we assume without loss of generality that $d_{G^*}(u_0, u_i) < \frac{d}{2}$, that is to say, $d_{G^*}(u_0, u_i) < d_{G^*}(u_{i+1}, u_d)$. Move the triangle and all the pendent edges from u_i to $u_{\frac{d}{2}}$ in G^* and denote the result graph by G_3 . It is routine to check that G_3 in \mathcal{G}_n^d . Since

$$\varepsilon_{G^*}(u_i) - \varepsilon_{G^*}(u_{\frac{d}{2}}) = \varepsilon_{G^*}(v_1) - \varepsilon_{G_3}(v_1) = \varepsilon_{G^*}(v_{k-1}) - \varepsilon_{G_3}(v_{k-1}) = \varepsilon_{G^*}(v_2) - \varepsilon_{G_3}(v_2).$$

We have

$$\begin{aligned}
\bar{\xi}^c(G^*) - \bar{\xi}^c(G_3) &= \varepsilon_{G^*}(u_i)(n-1-d_{G^*}(u_i)) + \varepsilon_{G^*}(u_{\frac{d}{2}})(n-1-d_{G^*}(u_{\frac{d}{2}})) \\
&\quad + \sum_{i=1}^{k-1} \varepsilon_{G^*}(v_i)(n-1-d_{G^*}(v_i)) - \varepsilon_{G_3}(u_i)(n-1-d_{G_3}(u_i)) \\
&\quad - \varepsilon_{G_3}(u_{\frac{d}{2}})(n-1-d_{G_3}(u_{\frac{d}{2}})) - \sum_{i=1}^{k-1} \varepsilon_{G_3}(v_i)(n-1-d_{G_3}(v_i)) \\
&> (k-1)(\varepsilon_{G^*}(u_{\frac{d}{2}}) - \varepsilon_{G^*}(u_i)) + (n-3)\varepsilon_{G^*}(v_1) \\
&\quad + (n-3)\varepsilon_{G^*}(v_{k-1}) + (k-3)(n-2)\varepsilon_{G^*}(v_2) - (n-3)\varepsilon_{G_3}(v_1) \\
&\quad - (n-3)\varepsilon_{G_3}(v_{k-1}) - (k-3)(n-2)\varepsilon_{G_3}(v_2) \\
&= \left[-(k-1) + 2(n-3) + (n-2)(k-3) \right] (\varepsilon_{G^*}(u_i) - \varepsilon_{G^*}(u_{\frac{d}{2}})) \\
&> (k-1)(n-4)(\varepsilon_{G^*}(u_i) - \varepsilon_{G^*}(u_{\frac{d}{2}})) \\
&> 0.
\end{aligned}$$

Then $\bar{\xi}^c(G^*) > \bar{\xi}^c(G_3)$, a contradiction again. This completes the proof of fact 3.

Case 2. P and C_k are vertex and edge disjoint.

Let $Q = u_iz_1z_2, \dots, z_{s-1}z_s$ be a path connecting path P and C_k . By the similar approach in the proof of theorem 4.1, we can contract the whole path Q (i.e., u_i and z_s coincide and then attaching suitable number of pendent vertices at u_i) to get a new graph G_4 with P and C_k having exactly one vertex in common. So the following procedure similar as case 1.

By the discussion as above, we obtain that for all G in \mathcal{G}_n^d . If the unique cycle and the diameter in G have no edges in common, then the extremal graph is $V_{n,d}^2$ when d is even. When d is even, the diameter path has only one center, while when d is odd, the diameter path has two centers. In either case, the pendent vertices in the minimum graph except the endpoints of the diameter path are all adjacent to the center of the diameter path, the proof process is exactly the same. Here we omit the proof when d is odd. Hence, the extremal graph is $V_{n,d}^4$ when d is odd. As is depicted in Figure 4.

Case 3. $|V(C_k) \cap V(P_{d+1})| \geq 2$.

If there exist common edges between P_{d+1} and C_k , then we get that all vertices in $V(G_0) \setminus \{V(P) \cup V(C_k)\}$ must be adjacent to $u_{\frac{d}{2}}$ of P similar as case 1. We denote it by G^* . Let $P_{d+1} = u_0u_1, \dots, u_d$ and $C_k = u_iu_{i+1}, \dots, u_jy_1y_2, \dots, y_mu_i$. In this case, we first show that the unique cycle C_k contained in G^* is just C_3 , that is to say, $k = 3$, otherwise, we assume that $k \geq 4$. First we consider the diameter d is even. Let

$$G_5 = G^* - \{u_iy_m, y_my_{m-1}, \dots, y_2y_1, y_1u_j\} + \{u_{\frac{d}{2}}y_m + u_{\frac{d}{2}}y_{m-1}, \dots, u_{\frac{d}{2}}y_2, u_{\frac{d}{2}}y_1\} + \{u_{\frac{d}{2}+1}y_1\}.$$

By the definition of $\bar{\xi}^c$ and bearing in mind that it is possible $u_{j-1} = u_i$. As $\varepsilon_{G^*}(y_i) \geq \varepsilon_{G_5}(y_i)$, $i = 1, \dots, m$ and $\varepsilon_{G_5}(y_1) = \varepsilon_{G_5}(y_2) = \varepsilon_{G_5}(y_3) = \dots = \varepsilon_{G_5}(y_m)$. $\varepsilon_{G_5}(u_i) = \varepsilon_{G^*}(u_i)$ and $\varepsilon_{G_5}(u_{j+1}) = \varepsilon_{G^*}(u_{j+1})$, $\varepsilon_{G_5}(y_i) \geq \varepsilon_{G_5}(u_{\frac{d}{2}}) + 1$, $\varepsilon_{G^*}(y_i) \geq \varepsilon_{G^*}(u_{\frac{d}{2}}) + 2$, $\varepsilon_{G_5}(u_{\frac{d}{2}}) = \varepsilon_{G^*}(u_{\frac{d}{2}})$, $\varepsilon_{G_5}(u_{\frac{d}{2}+1}) = \varepsilon_{G^*}(u_{\frac{d}{2}+1})$,

Moreover, $d_{G^*}(y_i) = 2$, $d_{G_5}(y_i) = 1$, $i = 2, \dots, m$

$d_{G^*}(y_1) = 2$, $d_{G_5}(y_1) = 2$ and $d_{G_5}(u_{\frac{d}{2}}) = d_{G^*}(u_{\frac{d}{2}}) + m$, $d_{G_5}(u_{\frac{d}{2}+1}) = d_{G^*}(u_{\frac{d}{2}+1}) + 1$

It follows that

$$\begin{aligned} \bar{\xi}^c(G^*) - \bar{\xi}^c(G_5) &= \sum_{i=2}^m \varepsilon_{G^*}(y_i)(n-3) + \varepsilon_{G^*}(y_1)(n-3) \\ &\quad + \varepsilon_{G^*}(u_i)(n-4) + \varepsilon_{G^*}(u_j)(n-4) + \varepsilon_{G^*}(u_{\frac{d}{2}})(n-1-d_{G^*}(u_{\frac{d}{2}})) \\ &\quad + \varepsilon_{G^*}(u_{\frac{d}{2}+1})(n-1-d_{G^*}(u_{\frac{d}{2}+1})) \\ &\quad - \sum_{i=2}^m \varepsilon_{G_5}(y_i)(n-2) - \varepsilon_{G_5}(y_1)(n-3) - \varepsilon_{G_5}(u_i)(n-3) \\ &\quad - \varepsilon_{G_5}(u_j)(n-3) - \varepsilon_{G_5}(u_{\frac{d}{2}})(n-1-d_{G_5}(u_{\frac{d}{2}})) \\ &\quad - \varepsilon_{G_5}(u_{\frac{d}{2}+1})(n-1-d_{G_5}(u_{\frac{d}{2}+1})) \\ &= \sum_{i=2}^m [\varepsilon_{G^*}(y_i)(n-3) - \varepsilon_{G_5}(y_i)(n-2)] - \varepsilon_{G^*}(u_i) \\ &\quad - \varepsilon_{G^*}(u_j) + m\varepsilon_{G^*}(u_{\frac{d}{2}}) + \varepsilon_{G^*}(u_{\frac{d}{2}+1}) \\ &> (m-1)[(\varepsilon_{G^*}(u_{\frac{d}{2}}) + 2)(n-3) - (n-2)(\varepsilon_{G^*}(u_{\frac{d}{2}}) + 1)] \\ &\quad - \varepsilon_{G^*}(u_i) - \varepsilon_{G^*}(u_j) + (m-1)\varepsilon_{G^*}(u_{\frac{d}{2}}) + \varepsilon_{G^*}(u_{\frac{d}{2}}) + \varepsilon_{G^*}(u_{\frac{d}{2}+1}) \\ &> (m-1)(n-4 - \varepsilon_{G^*}(u_{\frac{d}{2}})) + d \\ &\quad - \varepsilon_{G^*}(u_i) - \varepsilon_{G^*}(u_j) + (m-1)\varepsilon_{G^*}(u_{\frac{d}{2}}) \end{aligned}$$

$$\begin{aligned}
&= (m-1)(n-4) + d - (\varepsilon_{G^*}(u_i) + \varepsilon_{G^*}(u_j)) \\
&> (m-1)(n-4) + d - 2d \\
&= (m-1)(n-4) - d \\
&> (m-1)(n-4) - (n-2) \\
&> 2(n-4) - (n-2) = n-6 \\
&> 0.
\end{aligned}$$

Therefore,

$$\bar{\xi}^c(G^*) > \bar{\xi}^c(G_5),$$

which contradicts the choice of G^* .

Hence, the structure of G^* can be described as follows: its unique cycle C_3 and its diametral path $P_{d+1} = u_0u_1, \dots, u_d$ have only one edge $u_{\frac{d}{2}}u_{\frac{d}{2}+1}$ in common and there are some pendent edges attached to $u_{\frac{d}{2}}$ in G^* .

Summarizing the discussion as in case 3, we obtain that for all G in \mathcal{G}_n^d , if the unique cycle and the diameter in G have edge in common. When d is even, then the graph say $V_{n,d}^1$ with the minimum $\bar{\xi}^c$ and when d is odd, we can similarly get that the extremal graph belongs to $V_{n,d}^3$.

Summarizing cases 1–3, when d is odd, for any $G_1 \in V_{n,d}^3$ and $G_2 \in V_{n,d}^4$, we can easily obtain that $\bar{\xi}^c(G_1) < \bar{\xi}^c(G_2)$. Therefore, $V_{n,d}^3$ achieved the minimum $\bar{\xi}^c$ for d is odd.

When d is even, $\bar{\xi}^c(V_{n,d}^1) = \bar{\xi}^c(V_{n,d}^2)$, $V_{n,d}^1$ and $V_{n,d}^2$ obtain the minimum value of Eccentric connectivity coindex at the same time (See Figure 4).

This completes the proof. \square

6. Conclusions

In this paper, we first present the sharp lower bounds on $\bar{\xi}^c$ for general connecteds graphs and present a structure of the extremal graphs for eccentric connectivity coindex over cacti graphs with n vertices and k cycles, then characterize the extremal trees with given order and diameter on the eccentric connectivity coindex. Moreover, we optimize the extremal structure of unicyclic graphs with given order and diameter. Along this line, some other interesting extremal problems on the eccentric connectivity coindex are valuable to be considered.

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Conflict of interest

All authors in the paper have no conflict of interest.

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