Leap eccentric connectivity index in graphs with universal vertices

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Abstract

For a graph X, the leap eccentric connectivity index (LECI) is $\sum_{x\in V(X)} d_2(x,X)\varepsilon(x,X)$, where $d_2(x,X)$ is the 2-distance degree and $\varepsilon(x,X)$ the eccentricity of x. We establish a lower and an upper bound for the LECI of X in terms of its order and the number of universal vertices, and identify the extremal graphs. We prove an upper bound on the index for trees of a given order and diameter, and determine the extremal trees. We also determine trees with maximum LECI among all trees of a given order.

Keywords: eccentricity; leap eccentric connectivity index; diameter; universal vertex; tree

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1 Introduction

A large number of topological indices (alias graph invariants) have been defined in mathematical chemistry with the aim of modelling chemical phenomena. Much attention has been paid to the investigation of topological indices that are defined on the basis of the distance function, as well as to indices that are defined as a function of vertex degrees. From here it's just one more step to the indices that combine distances and degrees, which leads us to

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the so-called degree distance based topological indices. To give the reader an initial insight into this topic, we suggest the following selection of recent papers [2, 8, 11, 13, 16, 19]. In particular, the *eccentric connectivity index* of a graph G intertwines the eccentricity of vertices with their degrees as follows:

$$\xi^c(G) = \sum_{v \in V(G)} d(v,G)\varepsilon(v,G)\,.$$

The eccentric connectivity index was introduced back in 1997 by Sharma, Goswami, and Madan [14], see also [5, 7, 17, 18, 20]. In this context we also mention the eccentric distance sum from [4] and the degree distance from [3], where the first index intertwines the eccentricity with the total distance, while the second uses the degrees and the total distance. (For a survey up to 2010 on topological indices based on eccentricity see [9].) Instead of involving vertex degrees $d(v,G)$, we can include into a topological index the 2-*distance degrees* $d_2(v,G) = |\{x : d_G(x,v) = 2\}|$. Now, setting

$$L\xi^c(G) = \sum_{v \in V(G)} d_2(v,G)\varepsilon(v,G)\,,$$

we get the *leap eccentric connectivity index* of G, *LECI* for short, the index of our interest. It was introduced in an (as yet) unpublished manuscript which is available at [12]. There the index is computed for some basic graph families and several bounds are proved. Additional bounds were proved in [15]. In [10], the LECI was studied on some graph operations. The paper [6] deals with the LECI of different classes of thorny graphs, while in [21] the index is determined for transformation graphs of paths.

Our goal is to investigate the extremal values of the LECI of graphs containing cut vertices. In Section 2 we establish a lower and an upper bound for the LECI of G in terms of its order and the number of cut vertices. The extremal graphs are also identified; they can be described as joins of complete graphs with complete graphs minus a perfect matching (for the lower bound), and as joins of complete graphs and edgeless graphs (for the upper bound). In Section 3 we focus on trees. We first prove an upper bound for trees of a given order and diameter; the extremal graphs are brooms. Then we prove that brooms also have the maximum LECI among all trees of a given order. We conclude the paper by conjecturing that brooms also have the maximum LECI among all graphs of a given order. Before moving to our results, notation needed is stated.

1.1 Definitions

Graphs here are finite, simple and connected. Let $G = (V(G), E(G))$ be a graph. The order $|V(G)|$ of a graph G will be denoted by $n(G)$, the open neighbourhood of $u \in V(G)$ by $N_G(u)$, and the degree of u by $d_G(u)$. A vertex of degree $n(G) - 1$ in G is a universal vertex of G. A pendent vertex of G is a vertex of degree 1.

We proceed with metric concepts. The distance between u and v in G is denoted by $d_G(u,v)$. The 2-distance degree $d_2(u,G)$ of u is the number of vertices of G at distance 2 from u. The eccentricity $\varepsilon(u,G)$ of u is the distance to the furthest vertex from u. The diameter diam(G) of G is the maximum eccentricity among its vertices. A *diametral path* of a graph G is a path of length diam(G).

We next list notations for some classes of graphs and some constructions. S_n stands for the star of order n. The graph obtained from the complete graph K_n of even order by removing a perfect matching, will be denoted by K_n^- and the complement of a graph G by $\overline{G}$. If $M \subseteq E(G)$, then $G - M$ is the graph obtained from G by removing all the edges from M. Similarly, $G + M$ is the graph obtained from G by adding to G all the edges from M, where $M \cap E(G) = \emptyset$. If X and Y are disjoint graphs, then the join of Y and Y, denoted by $X \vee Y$, is a graph with $V(X \vee Y) = V(X) \cup V(Y)$ and $E(X \vee Y) = E(X) \cup V(Y) \cup \{xy : x \in V(X), y \in V(Y)\}$. If X is the empty graph, then $X \vee Y = Y$.

Finally, for $n \in \mathbb{N}$ we set $[n] = \{1, \ldots, n\}$.

2 The LECI and universal vertices

Let's start with a lower bound and an upper bound on the LECI of graphs as a function of the number of its universal vertices and its order and detect the extremal graphs. We begin with the lower bound.

Theorem 2.1 *If G contains $\alpha \geq 0$ universal vertices, then*

$$L\xi^c(G) \geq 2(n(G) - \alpha)\,.$$

Equality holds if and only if $G \cong K_\alpha \vee K^-_{n(G)-\alpha}$.

Proof. Suppose first $\alpha = 0$. Then $d_G(v) \leq n(G) - 2$ is true for each $v \in V(G)$ and so we have $u \in V(G)$ such that $d_G(u, v) \geq 2$. Hence $d_2(v, G)\varepsilon(v, G) \geq 2$ holds for each $v \in V(G)$, where the equality holds precisely when $wv \in E(G)$ for each $w \in V(G)\backslash\{v, u\}$. Therefore,

$$L\xi^c(G) = \sum_{v \in V(G)} d_2(v, G)\varepsilon(v, G) \geq 2n(G)\,,$$

and the equality holds if and only if $d_2(v, G)\varepsilon(v, G) = 2$ for each $v \in V(G)$. On the other hand, $d_2(v, G)\varepsilon(v, G) = 2$ holds for each $v \in V(G)$ if and only if $G \cong K^-_{2n} \cong K_0 \vee K^-_{n(G)}$, where K_0 is the empty graph.

Suppose in the rest that $\alpha \geq 1$. Let $v \in V(G)$. If $d_G(v) = n(G) - 1$, then $d_G(u, v) = 1$ for each $u \in V(G)$ and so $d_2(v, G)\varepsilon(v, G) = 0$. Otherwise, $d_G(v) \leq n(G) - 2$ and as above, $d_2(v, G)\varepsilon(v, G) \geq 2$, equality holding precisely when $xv \in V(G)$ for each $x \in V(G)\backslash\{v, w\}$. Setting U to be the set of universal vertices of G, we have

$$\begin{aligned} L\xi^c(G) &= \sum_{v \in V(G)} d_2(v, G)\varepsilon(v, G) \\ &= \sum_{v \in U} d_2(v, G)\varepsilon(v, G) + \sum_{v \in V(G)\backslash U} d_2(v, G)\varepsilon(v, G) \\ &= \sum_{v \in V(G)\backslash U} d_2(v, G)\varepsilon(v, G) \geq \sum_{v \in V(G)\backslash U} 2 = 2(n(G) - \alpha). \end{aligned}$$

The equality holds if and only if $d_2(v,G)\varepsilon(v,G) = 2$ for each $v \in V(G) \setminus U$. On the other hand, $d_2(v,G)\varepsilon(v,G) = 2$ for each $v \in V(G) \setminus U$ if and only if $G \cong K_\alpha \vee K^-_{n(G)-\alpha}$. □

The upper bound reads as follows.

Theorem 2.2 *If G contains $\alpha \geq 1$ universal vertices, then*

$$L\xi^c(G) \leq 2(n(G)-\alpha)(n(G)-\alpha-1)\,.$$

Moreover, equality holds if and only if $G \cong \overline{K_\alpha} \vee K_{n(G)-\alpha}$.

Proof. Let U be the set of all universal vertices of G. By our assumption $U \neq \emptyset$ which implies that $\mathrm{diam}(G) \leq 2$. If $x \in U$, then $\varepsilon(x,G) = 1$ and $d_2(x,G) = 0$. Otherwise, $\varepsilon(x,G) = 2$ and $d_2(x,G) \leq n - \alpha - 1$, equality holding if and only if $xy \notin E(G)$ for each $y \in V(G) \setminus U$. Therefore,

$$\begin{aligned}
L\xi^c(G) &= \sum_{x \in V(G)} d_2(x,G)\varepsilon(x,G) \\
&= \sum_{x \in U} d_2(x,G)\varepsilon(x,G) + \sum_{x \in V(G)\setminus U} d_2(x,G)\varepsilon(x,G) \\
&= \sum_{x \in V(G)\setminus U} d_2(x,G)\varepsilon(x,G) \leq \sum_{x \in V(G)\setminus U} 2(n(G)-\alpha-1) \\
&= 2(n(G)-\alpha)(n(G)-\alpha-1).
\end{aligned}$$

The equality holds if and only if $xy \notin E(G)$ for each $x, y \in V(G) \setminus U$. On the other hand, $xy \notin E(G)$ for each $x, y \in V(G) \setminus U$ if and only if $G \cong \overline{K_\alpha} \vee K_{n(G)-\alpha}$. □

The following result follows immediately from Theorem 2.2, but it is still worth writing down.

Corollary 2.3 *If G is a graph with $\alpha \geq 1$ universal vertices, then $L\xi^c(G) \leq 2(n(G)-1)(n(G)-2)$. Equality holds if and only if $G \cong S_{n(G)}$.*

3 LECI on trees

The following lemma is well-known, see, e.g., the proof of [1, Theorem 3.1].

Lemma 3.1 *Let x be a vertex of a tree T and let u and v be the end vertices of a diametral path of T. Then $\varepsilon(x,T) = \max\{d_T(x,u), d_T(x,v)\}$.*

Let v be a vertex of a tree T. Then v is a *support vertex* if v has a leaf neighbor. We further say v is a *relatively strong support* if $|\{x \in N_G(v) :\ d_G(x) = 1\}| = d_G(v) - 1$, that is, a support vertex whose all neighbors but one are leaves. For an example consider the tree T depicted in Fig. 1 whose relatively strong support vertices are a, h, n, and m.

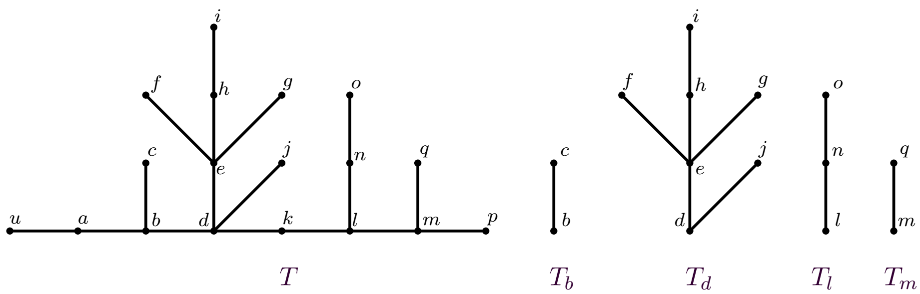

Figure 1: Trees T, T_b, T_d, T_l, and T_m.

Lemma 3.2 *If T be a tree with $\mathrm{diam}(T) \geq 3$, then T has at least two relatively strong support vertices.*

Proof. Let P be a diametral path in T and let u and v be the end-vertices of P. Then $\varepsilon(u,T) = \varepsilon(v,T) = \mathrm{diam}(T) \geq 3$. Let u' and v' be the neighbors of u and v on P, respectively. As $\mathrm{diam}(T) \geq 3$, we have $u' \neq v'$. Then the only non-leaf neighbor of u' is its non-leaf on P, the same holds for v'. Thus u' and v' are two relatively strong support vertices. □

Lemma 3.3 *Let T be a tree and $v_0v_1 \dots v_{\mathrm{diam}(T)}$ its diametral path. If $v \neq v_1, v_{\mathrm{diam}(T)-1}$ is a relatively strong support and u its non-leaf neighbor, then the following holds.*

i. *If $d_T(u) > \frac{d_T(v)+3}{5}$ and $T_1 = (T - \{vx : x \in N_T(v) \backslash \{u\}\}) + \{ux : x \in N_T(v) \backslash \{u\}\}$, then $L\xi^c(T) < L\xi^c(T_1)$.*

ii. *If $T_2 = (T - \{vx : x \in N_T(v) \backslash \{u\}\}) + \{v_1x : x \in N_T(v) \backslash \{u\}\}$, then $L\xi^c(T) < L\xi^c(T_2)$.*

Proof. Let $a \in N_T(v) \backslash \{u\}$, $b \in N_T(u) \backslash \{v\}$, $z \in N_T(v_1)$, and $w \in V(T) \backslash (N_T(v) \cup N_T(u) \cup N_T(v_1))$.

i. Using Lemma 3.1 and the structures of T and T_1, we have:

$$
\begin{gathered}
d_2(v,T_1) = d_2(v,T) + d_T(v) - 1, \;\; d_2(u,T_1) = d_2(u,T) - d_T(v) + 1, \\
d_2(a,T_1) = d_2(a,T) + d_T(u) - 1, \;\; d_2(b,T_1) = d_2(b,T) + d_T(v) - 1, \\
d_2(z,T_1) = d_2(z,T), \;\; d_2(w,T_1) = d_2(w,T), \;\; \varepsilon(v,T_1) = \varepsilon(v,T), \\
\varepsilon(u,T_1) = \varepsilon(u,T), \;\; \varepsilon(a,T_1) = \varepsilon(a,T) - 1, \;\; \varepsilon(b,T_1) = \varepsilon(b,T), \\
\varepsilon(z,T_1) = \varepsilon(z,T), \varepsilon(w,T_1) = \varepsilon(w,T).
\end{gathered}
$$

Then, by the definition of $L\xi^c$,

$$\begin{aligned} L\xi^c(T_1) - L\xi^c(T) &= (d_2(v,T)-1)\varepsilon(v,T) - (d_2(v,T)-1)\varepsilon(u,T) \\ &+ \sum_{a\in N_T(v)\setminus\{u\}} \big[(d_T(u)-1)(\varepsilon(a,T)-1) - d_2(a,T)\big] \\ &+ \sum_{b\in N_T(u)\setminus\{v\}} (d_T(v)-1)\varepsilon(b,T). \qquad (1) \end{aligned}$$

Applying Lemma 3.1 we get $\varepsilon(v,T) = \varepsilon(u,T)+1$. Also, it is clear that $d_2(a,T) = d_T(v)-1$, $\varepsilon(a,T) \ge 4$, and $\varepsilon(b,T) \ge 2$. Thus by (1),

$$L\xi^c(T_1) - L\xi^c(T) \ge 5(d_T(v)-1)(d_T(u)-1) - (d_T(v)-1)(d_T(v)-2)\,.$$

Since we have assumed that $d_T(u) > \frac{d_T(v)+3}{5}$, we conclude that $L\xi^c(T_1) - L\xi^c(T) > 0$.

ii. By the structure of T and T_2, and using Lemma 3.1 we have:

$$\begin{aligned} &d_2(v,T_2) = d_2(v,T),\ \ d_2(u,T_2) = d_2(u,T) - d_T(v) + 1, \\ &d_2(a,T_2) = d_2(a,T) + d_T(v_1) - 1,\ \ d_2(b,T_2) \ge d_2(b,T), \\ &d_2(z,T_2) = d_2(z,T) + d_T(v) - 1,\ \ d_2(w,T_2) = d_2(w,T), \\ &\varepsilon(v,T_1) = \varepsilon(v,T),\ \ \varepsilon(u,T_2) = \varepsilon(u,T),\ \ \varepsilon(a,T_2) \ge \varepsilon(a,T), \\ &\varepsilon(b,T_1) = \varepsilon(b,T),\ \ \varepsilon(z,T_1) = \varepsilon(z,T),\ \ \varepsilon(w,T_1) = \varepsilon(w,T). \end{aligned}$$

Then, by the definition of $L\xi^c$,

$$\begin{aligned} L\xi^c(T_2) - L\xi^c(T) \ge\ & -\varepsilon(u,T)(d_T(v)-1) + \sum_{a\in N_T(v)\setminus\{u\}} \varepsilon(a,T)(d_T(v_1)-1) \\ &+ \sum_{z\in N_T(v_1)} \varepsilon(z,T)(d_T(v)-1). \qquad (2) \end{aligned}$$

By Lemma 3.1, $\varepsilon(a,T) = \varepsilon(u,T)+2$ and $\varepsilon(z,T) \ge \varepsilon(u,T)$. Thus, by (2),

$$\begin{aligned} L\xi^c(T_2) - L\xi^c(T) &\ge \varepsilon(u,T)(d_T(v)-1)\big(d_T(v) + d_T(v_1) - 2\big) \\ &+ 2(d_T(v)-1)(d_T(v_1)-1) > 0\,, \end{aligned}$$

and we are done. □

Let $P: v_0v_1v_2\dots v_{\mathrm{diam}(T)}$ be a diametral path of T. For $i \in [\mathrm{diam}(T)-1]$, let $A(v_i,P) = \{x \in V(T):\ d(x,v_i) < \min\{d(x,v_{i-1}), d(x,v_{i+1})\}\}$. Note that if $d_T(v_i) = 2$, then $A(v_i,P) = \{v_i\}$. Set further $T_{v_i} = T[A(v_i,P)]$. If $d_T(v_i) \ge 3$, then we say that T_{v_i} is a *contracted member* of T with respect to P if $T_{v_i} \cong S_{n((T_{v_i})}$, and a *non-contracted member* otherwise. If $d_T(v_i) = 2$ or $T_{v_i} \cong S_{n(T_{v_i})}$ holds for every $i \in [\mathrm{diam}(T)-1]$, then T is a *caterpillar*. For an example let's return to Fig. 1. Consider the following diametral path of T: $P: uabdklmq$. Then $A(b,P) = \{b,c\}$, $A(d,P) = \{d,e,f,g,h,i,j\}$, $A(l,P) = \{l,n,o\}$, and $A(m,P) = \{m,q\}$. Further, $T[A(b,P)] = T_b$, $T[A(d,P)] = T_d$, $T[A(l,P)] = T_l$, and $T[A(m,P)] = T_m$. Moreover, T_d and T_l are non-contracted members of T with respect to P.

Let $P: v_0v_1v_2\dots v_{\mathrm{diam}(T)}$ be a diametral path of a caterpillar T. Then T is a *broom* if precisely one of v_1 and $v_{\mathrm{diam}(T)-1}$ is of degree at least 3, while all the other inner vertices of T are of degree 2. Let $\mathcal{B}_{n,d}$ denote a broom of order n and diameter d, see Fig. 2.

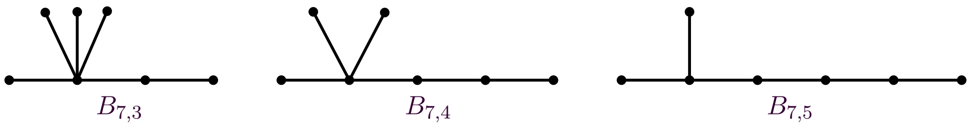

Figure 2: Brooms of order 7.

Theorem 3.4 *If T is a tree of order $n \geq 4$ and diameter d, then*

$$L\xi^c(T) \leq \begin{cases} 2(n-1)(n-2); & d=2, \\ 3n^2-16n+26; & d=3, \\ d^3-\frac{1}{2}(4n-1)d^2+\frac{1}{2}(2n^2+2n-4)d-2n+4; & d \geq 4 \text{ even}, \\ d^3-\frac{1}{2}(4n-1)d^2+\frac{1}{2}(2n^2+2n-4)d-2n+\frac{9}{2}; & d \geq 3 \text{ odd}. \end{cases}$$

Moreover, equality holds if and only if $T \cong B_{n,d}$.

Proof. Let $P_d : v_0v_1v_2 \dots v_d$ be a diametral path of T. We distinguish five cases.

Case 1. T is not a caterpillar.
Then, there exists $i \in [d-1]$ such that $T_{v_i} = T[A(v_i, P_d)]$ is a non-contracted member of T with respect to P_d. Thus, by Lemma 3.2, T_{v_i} has two relatively strong support vertices. Hence, there exists a relatively strong support vertex v in $V(T_{v_i})\backslash\{v_i\}$. Then, by Lemma 3.3, we have a tree T_2 of order n and diameter d such that $L\xi^c(T_2) > L\xi^c(T)$.

Case 2. T is a caterpillar, $d \geq 4$, and $d_T(v_2) \geq 3$.
Set $T_3 = (T - \{xv_2 : x \in N_T(v_2)\backslash\{v_1, v_3\}\}) + \{xv_1 : x \in N_T(v_2)\backslash\{v_1, v_3\}\}$. So, if $x \in N_T(v_1)\backslash\{v_0, v_2\}$, $y \in N_T(v_2)\backslash\{v_1, v_3\}$, and $w \in V(T)\backslash(N_T(v_1) \cup N_T(v_2))$, then by the the structure of T and T_3,

$$\begin{aligned} d_2(v_0, T_3) &= d_2(v_0, T) + d_T(v_2) - 2,\ d_2(v_1, T_3) = d_2(v_1, T) - d_T(v_2) + 2, \\ d_2(v_2, T_3) &= d_2(v_2, T) + d_T(v_2) - 2,\ d_2(v_3, T_3) = d_2(v_3, T) - d_T(v_2) + 2, \\ d_2(x, T_3) &= d_2(x, T) + d_T(v_2) - 2,\ d_2(y, T_3) = d_2(y, T) + d_T(v_1) - 2, \\ d_2(w, T_3) &= d_2(w, T),\ \varepsilon(y, T_3) = \varepsilon(y, T) + 1,\ \varepsilon(v_3, T) \leq (d-1), \\ d_2(y, T) &= d_T(v_2) - 1. \end{aligned}$$

Also, $\varepsilon(z, T_3) = \varepsilon(z, T)$ for $z \in V(T)\backslash(N_T(v_2)\backslash\{v_1, v_3\})$. Thus,

$$\begin{aligned} L\xi^c(T_3) - L\xi^c(T) \geq\ & (d_T(v_2) - 2)d - (d_T(v_2) - 2)(d-1) \\ & + (d_T(v_2) - 2)(d-2) - (d_T(v_2) - 2)(d-1) \\ & + \sum_{x \in N_T(v_1)\backslash\{v_0, v_2\}} (d_T(v_2) - 2)d \\ & + \sum_{y \in N_T(v_2)\backslash\{v_1, v_3\}} \big[(d_T(v_1) - 2)d + (d_T(v_2) - 1)\big] \end{aligned}$$

$$= 2(d_T(v_1)-2)(d_T(v_2)-2)d$$
$$+ (d_T(v_2)-2)(d_T(v_2)-1) > 0.$$

So, T_3 is a caterpillar of order n and diameter d such that $L\xi^c(T_3) > L\xi^c(T)$.

Case 3. T is a caterpillar, $d \geq 5$, $d_T(v_2) = 2$, and $d_T(v_3) \geq 3$.
Set, $T_4 = (T - \{xv_3 : x \in N_T(v_3)\backslash\{v_2, v_4\}\}) + \{xv_1 : x \in N_T(v_2)\backslash\{v_2, v_4\}\}$. Thus, if $x \in N_T(v_1)\backslash\{v_0, v_2\}$, $y \in N_T(v_3)\backslash\{v_2, v_4\}$, and $w \in (V(T)\backslash(N_T(v_1) \cup N_T(v_3))) \cup \{v_1, v_2, v_3\}$, then by the structure of T and T_4,

$$d_2(v_0, T_4) = d_2(v_0, T) + d_T(v_3) - 2,\ d_2(v_4, T_4) = d_2(v_4, T) - d_T(v_3) + 2,$$
$$d_2(x, T_4) = d_2(x, T) + d_T(v_3) - 2,\ d_2(y, T_4) = d_2(y, T) + d_T(v_1) - 2,$$
$$d_2(w, T_4) = d_2(w, T),\ \varepsilon(y, T_4) \geq \varepsilon(y, T) + 1,\ \varepsilon(v_4, T) \leq (d-1).$$

Also, $\varepsilon(z, T_3) = \varepsilon(z, T)$ for $z \in V(T)\backslash(N_T(v_3)\backslash\{v_2, v_4\})$. Therefore,

$$L\xi^c(T_4) - L\xi^c(T) = (d_T(v_3)-2)d - (d_T(v_3)-2)(d-1)$$
$$+ \sum_{x \in N_T(v_1)\backslash\{v_0,v_2\}} (d_T(v_3)-2)d$$
$$+ \sum_{y \in N_T(v_3)\backslash\{v_2,v_4\}} \big[(d_T(v_1)-2)d + (d_T(v_3)-1)\big]$$
$$= 2(d_T(v_1)-2)(d_T(v_3)-2)d$$
$$+ (d_T(v_3)-2)d_T(v_3) > 0.$$

So, T_4 is a caterpillar of diameter d and order n with $L\xi^c(T_4) > L\xi^c(T)$.

Case 4. T is a caterpillar, and there exists $i \geq 4$ such that $d \geq i+2$, $d_T(v_2) = d_T(v_3) = \cdots = d_T(v_{i-1}) = 2$, and $d_T(v_i) \geq 3$.
Set $T_5 = (T - \{xv_i : x \in N_T(v_i)\backslash\{v_{i-1}, v_{i+1}\}\}) + \{xv_1 : x \in N_T(v_i)\backslash\{v_{i-1}, v_{i+1}\}\}$. Thus, if $x \in N_T(v_1)\backslash\{v_0, v_2\}$, $y \in N_T(v_i)\backslash\{v_{i-1}, v_{i+1}\}$, and $w \in V(T)\backslash(N_T(v_1) \cup N_T(v_i))$, then by the structure of T and T_5,

$$d_2(v_0, T_5) = d_2(v_0, T) + d_T(v_i) - 2,\ d_2(v_2, T_5) = d_2(v_2, T) + d_T(v_i) - 2,$$
$$d_2(v_{i-1}, T_5) = d_2(v_{i-1}, T) - d_T(v_i) + 2,\ d_2(v_{i+1}, T_5) = d_2(v_{i+1}, T) - d_T(v_i) + 2,$$
$$d_2(x, T_5) = d_2(x, T) + d_T(v_i) - 2,\ d_2(y, T_5) = d_2(y, T) + d_T(v_1) - 2,$$
$$d_2(w, T_5) = d_2(w, T),\ \varepsilon(y, T_5) = \varepsilon(y, T) + 1,\ \varepsilon(v_{i-1}, T) \leq (d-3),$$
$$\varepsilon(v_{i+1}, T) \leq (d-1).$$

Also, $\varepsilon(z, T_5) = \varepsilon(z, T)$ for $z \in V(T)\backslash(N_T(v_i)\backslash\{v_{i-1}, v_{i+1}\})$. Then

$$L\xi^c(T_3) - L\xi^c(T) \geq (d_T(v_i)-2)d + (d_T(v_i)-2)(d-2)$$
$$- (d_T(v_i)-2)(d-3) - (d_T(v_i)-2)(d-1)$$
$$+ \sum_{x \in N_T(v_1)\backslash\{v_0,v_2\}} (d_T(v_i)-2)d$$

$$+ \sum_{y \in N_T(v_2)\setminus\{v_1,v_3\}} \big[(d_T(v_1)-2)d + (d_T(v_i)-1)\big]$$
$$= 2(d_T(v_i)-2) + 2(d_T(v_1)-2)(d_T(v_i)-2)d$$
$$+ (d_T(v_i)-2)(d_T(v_i)-1) > 0.$$

Therefore there exists a tree T_5 of order n and diameter d such that $L\xi^c(T_5) > L\xi^c(T)$.

Case 5. T is a caterpillar, $d \geq 3$, $d_T(v_1) \geq 3$, $d_T(v_{d-1}) \geq 3$, and $d_T(v_i) = 2$ for $i \in [d-1]\setminus\{1, d-1\}$.

Now, set

$$T_6 = (T - \{xv_{d-1} : x \in N_T(v_{d-1})\setminus\{v_{d-2}, v_d\}\}) + \{xv_1 : x \in N_T(v_{d-1})\setminus\{v_{d-2}, v_d\}\}.$$

It is clear that $\varepsilon(v, T_6) = \varepsilon(v, T)$ for $v \in V(T)$. Using similar arguments as in previous cases we get:

$$L\xi^c(T_6) - L\xi^c(T) = \sum_{x \in N_T(v_1)\setminus\{v_0,v_2\}} d(d_T(v_{d-1})-2)$$
$$+ \sum_{y \in N_T(v_{d-1})\setminus\{v_{d-2},v_d\}} d(d_T(v_1)-2)$$
$$= 2d(d_T(v_{d-1})-2)(d_T(v_1)-2) > 0.$$

Thus, in this case there exists a broom $T_6 \cong B_{n,d}$ such that $L\xi^c(T_6) > L\xi^c(T)$.

By cases 1-5 we conclude that if T has maximum value of $L\xi^c$ among all trees of order n and diameter d, then $T \cong B_{n,d}$. Moreover, according to the definition of the structure of $B_{n,d}$, we conclude that if $d = 2$, then

$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = n-2,\ \ \varepsilon(x, B_{n,d}) = 2\}| = n-1,$$
$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 0,\ \ \varepsilon(x, B_{n,d}) = 1\}| = 1. \tag{3}$$

If $d = 3$, then

$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = n-3,\ \ \varepsilon(x, B_{n,d}) = 3\}| = n-3,$$
$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 1,\ \ \varepsilon(x, B_{n,d}) = 2\}| = 1,$$
$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = n-3,\ \ \varepsilon(x, B_{n,d}) = 2\}| = 1,$$
$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 1,\ \ \varepsilon(x, B_{n,d}) = 3\}| = 1. \tag{4}$$

If $d \geq 4$ is even, then

$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 1,\ \ \varepsilon(x, B_{n,d}) = d\}| = 1,$$
$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 1,\ \ \varepsilon(x, B_{n,d}) = d-1\}| = 2,$$
$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = n-d+1,\ \ \varepsilon(x, B_{n,d}) = d-2\}| = 1,$$
$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = n-d,\ \ \varepsilon(x, B_{n,d}) = d\}| = n-d, \tag{5}$$

and if $d \geq 6$ is even, then

$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 2,\ \ \varepsilon(x, B_{n,d}) = d-2\}| = 1,$$
$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 2,\ \ \varepsilon(x, B_{n,d}) = \frac{d}{2}\}| = 1. \tag{6}$$

Also, for $i \in \{3, \dots, \frac{d}{2}-1\}$ we have,

$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 2,\ \ \varepsilon(x, B_{n,d}) = d-i\}| = 2. \tag{7}$$

If $d \geq 5$ is odd, then

$$\begin{aligned}
&|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 1,\ \ \varepsilon(x, B_{n,d}) = d\}| = 1,\\
&|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 1,\ \ \varepsilon(x, B_{n,d}) = d-1\}| = 2,\\
&|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = n-d+1,\ \ \varepsilon(x, B_{n,d}) = d-2\}| = 1,\\
&|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 2,\ \ \varepsilon(x, B_{n,d}) = d-2\}| = 1,\\
&|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = n-d,\ \ \varepsilon(x, B_{n,d}) = d\}| = n-d,
\end{aligned} \tag{8}$$

and if $d \geq 7$, then for $i \in \{3, \dots, \frac{d-1}{2}\}$,

$$|\{x \in V(B_{n,d}) : d_2(x, B_{n,d}) = 2,\ \ \varepsilon(x, B_{n,d}) = d-i\}| = 2. \tag{9}$$

From (3)-(9) we conclude that

$$L\xi^c(B_{n,d}) = \begin{cases} 2(n-1)(n-2); & d = 2,\\ 3n^2 - 16n + 26; & d = 3,\\ d^3 - \frac{1}{2}(4n-1)d^2 + \frac{1}{2}(2n^2+2n-4)d - 2n + 4; & d \neq 2,\ 2 \mid d,\\ d^3 - \frac{1}{2}(4n-1)d^2 + \frac{1}{2}(2n^2+2n-4)d - 2n + \frac{9}{2}; & d \neq 3,\ 2 \nmid d. \end{cases} \tag{10}$$

and we are done. □

Theorem 3.5 *If $n \geq 3$, then $B_{n,d}$ has the maximum value of $L\xi^c$ among all trees of order n, where*

$$d = \begin{cases} 2; & n \in \{3,4,5,6\},\\ 3; & n \in \{7,8,9\},\\ \lfloor \frac{n}{3} \rfloor + 1; & n \geq 10. \end{cases}$$

Proof. If the theorem holds for brooms of order $n \geq 3$, then by Theorem 3.4 the assertion is valid in general. Thus, we prove that if

$$d = \begin{cases} 2; & n \in \{3,4,5,6\},\\ 3; & n \in \{7,8,9\},\\ \lfloor \frac{n}{3} \rfloor + 1; & n \geq 10. \end{cases}$$

then $B_{n,d}$ has maximum value of $L\xi^c$ among all brooms of order n. By (10), the assertion of the theorem is true for $3 \leq n \leq 10$. Let $n \geq 11$ and for $x \in [4, n-1]$ set

$$f(x) = x^3 - \frac{1}{2}(4n-1)x^2 + \frac{1}{2}(2n^2+2n-4)x - 2n.$$

Then,

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

By a simple calculation, $f(\frac{n+2}{3}) > \max\{f(4), f(n-1)\}$. Thus, function f has maximum in $\frac{n+2}{3}$. Moreover, we have $f(\frac{n+2}{3}) > \max\{2(n-1)(n-2), 3n^2 - 16n + 26\}$. Then, by (10) and the fact that d is an integer, we conclude that $B_{n,\lfloor \frac{n+2}{3} \rfloor}$ or $B_{n,\lceil \frac{n+2}{3} \rceil}$ has the maximum value of $L\xi^c$ among all brooms of order $n \geq 11$. To complete the proof we have to investigate all possible cases for $\lfloor \frac{n+2}{3} \rfloor$ and $\lceil \frac{n+2}{3} \rceil$.

Case 1. If $3 \mid n$, then $\lfloor \frac{n+2}{3} \rfloor = \frac{n}{3}$ and $\lceil \frac{n+2}{3} \rceil = \frac{n}{3} + 1$. Also, clearly the parity of $\lfloor \frac{n+2}{3} \rfloor = \frac{n}{3}$ and of $\lceil \frac{n+2}{3} \rceil = \frac{n}{3} + 1$ is not the same. Then by (10), $L\xi^c(B_{n,\lfloor \frac{n+2}{3} \rfloor}) - L\xi^c(B_{n,\lceil \frac{n+2}{3} \rceil}) = -\frac{n}{3}$ or $L\xi^c(B_{n,\lfloor \frac{n+2}{3} \rfloor}) - L\xi^c(B_{n,\lceil \frac{n+2}{3} \rceil}) = -\frac{n}{3} + 1$. Then, in this case, $B_{n,\frac{n}{3}+1}$ has the maximum value of $L\xi^c$.

Case 2. If $3 \mid n - 1$, then $\lfloor \frac{n+2}{3} \rfloor = \lceil \frac{n+2}{3} \rceil = \frac{n-1}{3} + 1$. Thus, in this case, $B_{n,\frac{n-1}{3}+1}$ has the maximum value of $L\xi^c$.

Case 3. If $3 \mid n - 2$, then $\lfloor \frac{n+2}{3} \rfloor = \frac{n-2}{3} + 1$ and $\lceil \frac{n+2}{3} \rceil = \frac{n+1}{3} + 1$. On the other hand, it is clear that the parity of $\lfloor \frac{n+2}{3} \rfloor = \frac{n-2}{3} + 1$ and of $\lceil \frac{n+2}{3} \rceil = \frac{n+1}{3} + 1$ is not the same. Then by (10), $L\xi^c(B_{n,\lfloor \frac{n+2}{3} \rfloor}) - L\xi^c(B_{n,\lceil \frac{n+2}{3} \rceil}) = \frac{n-5}{3}$ or $L\xi^c(B_{n,\lfloor \frac{n+2}{3} \rfloor}) - L\xi^c(B_{n,\lceil \frac{n+2}{3} \rceil}) = \frac{n-2}{3} + 1$. Thus, in this case, $B_{n,\frac{n-2}{3}+1}$ has the maximum value of $L\xi^c$. □

Based on proven results and some computer experiments we conclude the paper with:

Conjecture 3.6 *If $n \geq 3$, then $B_{n,d}$ has the maximum value of $L\xi^c$ among all graphs of order n, where*

$$d = \begin{cases} 2; & n \in \{3, 4, 5, 6\}, \\ 3; & n \in \{7, 8, 9\}, \\ \lfloor \frac{n}{3} \rfloor + 1; & n \geq 10. \end{cases}$$

Here we pose a related problem.

Problem 3.7 *Let n and k be two natural numbers such that $n \geq k + 1$. Then*

(a) *characterize the minimum trees with respect to LECI among all trees of order n.*
(b) *characterize the minimum trees with respect to LECI among all trees of order n and diameter k.*
(c) *characterize the minimum trees with respect to LECI among all trees of order n with k pendant vertices.*
(d) *characterize the maximum trees with respect to LECI among all trees of order n with k pendant vertices.*

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