On augmented eccentric connectivity index of graphs and trees

Jelena Sedlar
University of Split, Faculty of civil engeneering, architecture and geodesy, Matice hrvatske 15, 21000 Split, Croatia

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Abstract

In this paper we establish all extremal graphs with respect to augmented eccentric connectivity index among all (simple connected) graphs, among trees and among trees with perfect matching. For graphs that turn out to be extremal explicit formulas for the value of augmented eccentric connectivity index are derived.

1 Introduction

Several topological indices based on graph theoretical notion of eccentricity have been recently proposed and/or used in QSAR and QSPR studies. Namely, eccentric connectivity index ([16]), eccentric distance sum ([9]), adjacent eccentric distance sum ([15]) and augmented and super augmented eccentric connectivity index ([3], [2], [7] and [8]). These indices have been shown to be very useful (predicting pharmaceutical properties), therefore their mathematical properties have been studied too. The most extensive study has been conducted for eccentric connectivity index, for which extremal graphs and trees have been established ([6], [18], [11]). Furthermore, the eccentric connectivity index of some special kinds of graphs was studied such as unicyclic graphs and different kinds of hexagonal systems ([1],[4]). For a detailed survey on these and other results concerning eccentric connectivity index we refer the reader to [10]. Recently, mathematical properties of eccentric distance sum started to be investigated too. There are some results on eccentric distance sum of trees and unicyclic graphs ([17]) and of general graphs ([12]). As for the augmented eccentric connectivity index, there are some results with explicit formulas for several classes of graphs, in particular for some open and closed unbranched polymers and nanostructure ([5]). Otherwise, augmented eccentricity index was not very much studied.

In this paper we present the results concerning extremal graphs and values of augmented eccentric connectivity index on class of simple connected graphs, on trees and on trees with perfect matching. The paper is organized as follows. In the second section 'Preliminaries' some basic notions and also the notation are introduced. Also, explicit formulas for the value of augmented eccentric connectivity index for some specific graphs (such as paths, stars, etc.) which will later be proved as extremal are derived. Third section is named 'Extremal trees'. In it we establish all minimal and extremal trees with respect to augmented eccentric connectivity index. Interestingly, it turns out that maximal tree generally is not a star as is the case with other eccentricity based indices, but a specific kind of tree with diameter 4. In fourth section we establish extremal trees among trees with perfect matching. Finally, in fifth section we use the results for trees to establish the extremal graphs in class of general simple connected graphs.

2 Preliminaries

In this paper we consider only simple connected graphs. We will use the following notation: G for graph, $V(G)$ or just V for its set of vertices, $E(G)$ or just E for its set of edges. With n we will denote number of vertices in graph G. For two vertices $u, v \in V$ we define *distance* $d(u, v)$ of u and v as the length of shortest path connecting u and v. Given the notion of distance we can define several other notions based on distance. First, for a vertex $u \in V$ we define *eccentricity* $\varepsilon(u)$ as the maximum of $d(u, v)$ over all $v \in V$. Furthermore, we define *diameter* D of graph G as the maximum of $d(u, v)$ over all pairs of vertices $u, v \in V$. A path P in G connecting vertices u and v is called *diametric* if $d(u, v) = D$. The set of all vertices with minimum eccentricity in G is called *center* of G and such vertices are called *central*. For a vertex $u \in V$ a *degree* $\deg(u)$ is defined as number of vertices from V adjacent to u. Now, we can define *augmented eccentric connectivity index* of a graph G as

$$\xi^{ac}(G) = \sum_{u \in V} \frac{M(u)}{\varepsilon(u)}$$

where $M(u)$ is product of degrees of all neighbors of u and $\varepsilon(u)$ is eccentricity of u. Sometimes, for brevity sake, this index will be called 'augmented ECI'.

Let us now define some special kinds of graphs. First, K_n will denote a *complete graph* on n vertices. Special class of graphs which will be of interest are trees. A *tree* is a graph with no cycles. It is easily seen that tree has only one central vertex if D is even, and two central vertices if D is odd. We say that a vertex in tree T is a leaf if its degree is 1, otherwise we say that a vertex is non-leaf. Also, we say that a vertex in a tree is *branching* if its degree is greater or equal than 3. We say that a tree T is *spanning tree* of graph G if $V(T) = V(G)$ and $E(T) \subseteq E(G)$. Now, P_n will denote a *path* on n vertices and S_n will denote a *star* on n vertices. We will also specially consider trees of diameter 4. Let us therefore introduce some interesting classes of graphs with diameter 4. We say that a tree T is *degree balanced* if its diameter is 4 and all neighbors of (the only) central vertex differ in degree by at most one. With $TB_{n,k}$ we will denote degree balanced tree on n vertices with degree of central vertex being k. Note that there is only one such tree up to isomorphism. Now, from definition follows that neighbors of central vertex in degree balanced tree T can have only two degrees, say $p-1$ and p. Note that p is determined by k and holds

$$p = \left\lceil \frac{n-1}{k} \right\rceil .$$

But, on the other hand k is not determined by p. We have

$$\frac{n-1}{p} \leq k < \frac{n-1}{p-1}.$$

Having this in view, we define (almost) perfect degree balance in a tree. Namely, we say that a degree balance is *perfect* if all neighbors of central vertex have the degree p, we say that balance is

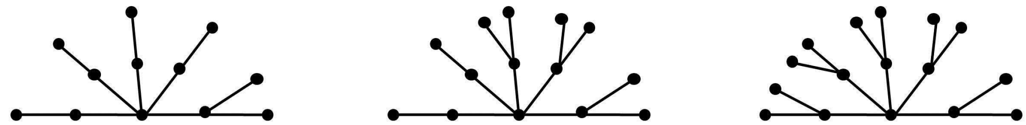

Figure 1: Trees: $TB_{12,5}$ with degree balance, $TB_{14,5}$ with almost perfect degree balance and $TB_{16,5}$ with perfect degree balance.

almost perfect if maximum possible number of neighbors of central vertex have the degree p. Note that degree balanced tree is in (almost) perfect balance if and only if

$$k = \left\lceil \frac{n-1}{p} \right\rceil .$$

An example of tree with degree balance, almost perfect degree balance and perfect degree balance is shown in Figure 1.

Now, we will establish exact values of augmented ECI for some of these graphs, which will later be proved as extremal for some class of graphs. Let us denote $H_n = \sum_{i=1}^{n} \frac{1}{i}$. By direct calculation we obtain the following proposition.

Proposition 1 *For paths P_n on $n \geq 5$ vertices, stars S_n on $n \geq 4$ vertices, degree balanced trees $TB_{n,\lceil \frac{n-1}{3} \rceil}$ on $n \geq 8$ vertices, degree balanced graphs $TB_{n,\frac{n}{2}}$ on $n \geq 6$ vertices where n is even, complete graphs K_n on $n \geq 2$ vertices holds:*

1. $\xi^{ac}(P_n) = \begin{cases} 8(H_{n-1} - H_{\frac{n-2}{2}}) - (\frac{4}{n-1} + \frac{4}{n-2}), & \text{for } n \text{ even}, \\ 8(H_{n-1} - H_{\frac{n-3}{2}}) - (\frac{12}{n-1} + \frac{4}{n-2}), & \text{for } n \text{ odd}, \end{cases}$

2. $\xi^{ac}(S_n) = 1 + \frac{(n-1)^2}{2}$,

3. $\xi^{ac}(TB_{n,\lceil \frac{n-1}{3} \rceil}) = \begin{cases} \frac{3^k}{2} + \frac{k^2}{3} + \frac{3k}{2}, & \text{for } n = 3k+1, \\ 3^{k-1} + \frac{k^2}{3} + \frac{3k}{2} - 1 & \text{for } n = 3k, \\ 2 \cdot 3^{k-2} + \frac{k^2}{3} + \frac{3k}{2} - \frac{1}{2} & \text{for } n = 3k-1. \end{cases}$

4. $\xi^{ac}(TB_{n,\frac{n}{2}}) = 2^{\frac{n}{2}-2} + \frac{1}{12}\left(n^2 + 3n - 6\right)$,

5. $\xi^{ac}(K_n) = n \cdot (n-1)^{n-1}$.

To conclude, we still need the notion of matching. A *matching* in a graph G is collection of edges M from G such that no vertex from G is incident to two edges from M. The *size* of matching is number of edges it contains. We say that matching M is *perfect* if every vertex from G is incident to one edge from M. Obviously, only graphs with even number of vertices can have perfect matching.

3 Extremal trees

In this section we want to establish trees with minimum and maximum value of augmented eccentric connectivity index. First, we will do the minimum. For that purpose we need the following theorem which gives the transformation of tree which increases diameter, but decreases the value of augmented ECI.

Theorem 2 *Let $T \neq P_n$ be a tree on n vertices and let $P = v_0 v_1 \ldots v_D$ be a diametric path in T chosen so that the first branching vertex is furthest possible from v_0. Let v_i be the first branching vertex on P. If $D > 2$ and $i = 1$ and $\deg(v_{i+1}) > 2$ then let $u = v_{i+1}$, else let $u = v_i$. Let $w_1, \ldots, w_k$ be k neighbors of u outside of P $(1 \leq k \leq \deg(u) - 2)$. For tree T' obtained from T by deleting edges $uw_1, \ldots uw_k$ and adding edges $v_0 w_1, \ldots, v_0 w_k$ holds*

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

Proof. Note that this transformation does not decrease eccentricity of any vertex. On the other hand, the only vertex whose degree increases is v_0. Let us denote $m_i = \deg(v_i)$ and $m_{w_i} = \deg(w_i)$. Cases when $D \leq 3$ are easily verified, therefore we distinguish three remaining cases when $D > 3$. Tree transformations from these cases are illustrated with Figure 2.

Case 1: $D > 3$ and $u = v_1$.

Note that in this case $m_2 = 2$ and $m_{w_i} = 1$ for every i. Therefore, the only vertex for which $M(v)$ increases from T to T' is v_1. We have

$$\begin{aligned}
\xi^{ac}(T) - \xi^{\alpha c}(T') &\geq \frac{M(v_1)}{\varepsilon(v_1)} - \frac{M'(v_1)}{\varepsilon'(v_1)} + \frac{M(v_2)}{\varepsilon(v_2)} - \frac{M'(v_2)}{\varepsilon'(v_2)} + \sum_{i=1}^{k} \left(\frac{M(w_i)}{\varepsilon(w_i)} - \frac{M'(w_i)}{\varepsilon'(w_i)} \right) \geq \\
&\geq \frac{2}{D-1} - \frac{2(k+1)}{D-1} + \frac{m_1 \cdot m_3}{D-2} - \frac{(m_1 - k) \cdot m_3}{D-2} + k \left(\frac{m_1}{D} - \frac{k+1}{D} \right) = \\
&= \frac{-2k}{D-1} + \frac{m_3 \cdot k}{D-2} + \frac{k \cdot (m_1 - k - 1)}{D} > [m_3 \geq 2, m_1 \geq k+1] > 0
\end{aligned}$$

Case 2: $D > 3$ and $u = v_2$.

The only vertices for which $M(v)$ possibly increases are v_0 and v_1. We will neutralize increase in $M(v_0)$ by decrease in $M(v_2)$, and also neutralize increase in $M(v_1)$ by decrease in $M(v_3), M(w_1), \ldots, M(w_k)$. Let $m_w = m_{w_1} \cdot \ldots \cdot m_{w_k}$ and $c_2 = M(v_2)/(m_w \cdot m_1)$. Note that $c_2 \geq 2$ because of $m_3 \geq 2$ (which follows from $D > 3$). We have

$$\begin{aligned}
\Delta_1 &= \frac{M(v_0)}{\varepsilon(v_0)} - \frac{M'(v_0)}{\varepsilon'(v_0)} + \frac{M(v_2)}{\varepsilon(v_2)} - \frac{M'(v_2)}{\varepsilon'(v_2)} \geq \frac{m_1}{D} - \frac{m_1 \cdot m_w}{D} + \frac{m_1 \cdot m_w \cdot c_2}{D-2} - \frac{m_1 \cdot c_2}{D-2} = \\
&= -\frac{m_1(m_w - 1)}{D} + \frac{m_1 \cdot c_2 \cdot (m_w - 1)}{D-2} \geq 0.
\end{aligned}$$

Now, let $c_3 = M(v_3)/m_2$. Note that all neighbors of w_i except $u = v_2$ are of degree 1 and therefore $M(w_i) = m_2$ for every i. We have

$$\begin{aligned}
\Delta_2 &= \frac{M(v_1)}{\varepsilon(v_1)} - \frac{M'(v_1)}{\varepsilon'(v_1)} + \frac{M(v_3)}{\varepsilon(v_3)} - \frac{M'(v_3)}{\varepsilon'(v_3)} + \sum_{i=1}^{k} \left(\frac{M(w_i)}{\varepsilon(w_i)} - \frac{M'(w_i)}{\varepsilon'(w_i)} \right) \geq \\
&\geq \frac{m_2}{D-1} - \frac{(m_2 - k)(k+1)}{D-1} + \frac{m_2 \cdot c_3}{\varepsilon(v_3)} - \frac{(m_2 - k) \cdot c_3}{\varepsilon(v_3)} + \sum_{i=1}^{k} \left(\frac{m_2}{D-1} - \frac{k+1}{D-1} \right) = \\
&= -\frac{k(m_2 - k - 1)}{D-1} + \frac{k \cdot c_3}{\varepsilon(v_3)} + \frac{k(m_2 - k - 1)}{D-1} > 0
\end{aligned}$$

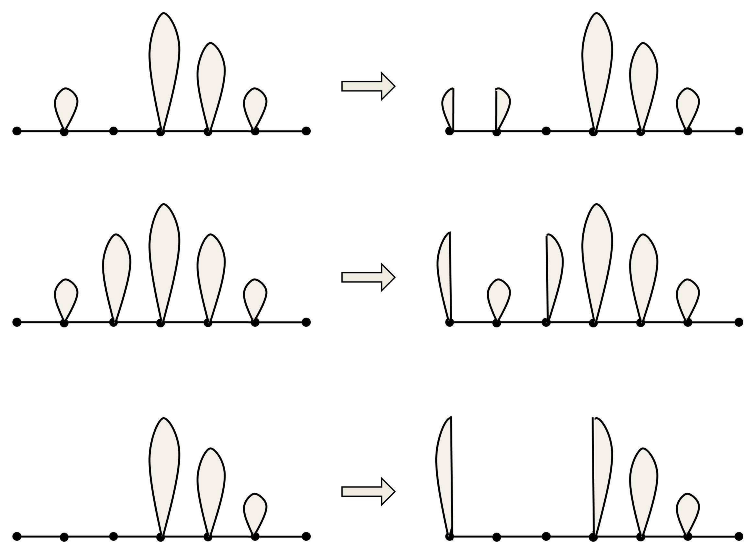

Figure 2: Tree transformations from Cases 1, 2 and 3 of Theorem 2.

Therefore,

$$\xi^{ac}(T) - \xi^{\alpha c}(T') \geq \Delta_1 + \Delta_2 > 0.$$

Case 3: $D > 3$ and $u = v_i$ $(i \geq 3)$.

The only vertices for which $M(v)$ possibly increases are v_0 and v_1. We will neutralize increase in $M(v_0)$ by decrease in $M(v_i)$, and also neutralize increase in $M(v_1)$ by decrease in $M(v_{i-1})$. Let $m_w = m_{w_1} \cdot \ldots \cdot m_{w_k}$ and let $c_i = M(v_i) / (m_{i-1} \cdot m_w)$ We have

$$\Delta_1 = \frac{M(v_0)}{\varepsilon(v_0)} - \frac{M'(v_0)}{\varepsilon'(v_0)} + \frac{M(v_i)}{\varepsilon(v_i)} - \frac{M'(v_i)}{\varepsilon'(v_i)} \geq \frac{2}{D} - \frac{2 \cdot m_w}{D} + \frac{m_{i-1} \cdot m_w \cdot c_i}{\varepsilon(v_i)} - \frac{m_{i-1} \cdot c_i}{\varepsilon(v_i)} =$$

$$= -\frac{2\,(m_w - 1)}{D} + \frac{m_{i-1} \cdot c_i \cdot (m_w - 1)}{\varepsilon(v_i)} \overset{m_{i-1}=2}{\geq} 0.$$

Also, from $i \geq 3$ we know that $v_1 \neq v_i$, so we have

$$\Delta_2 = \frac{M(v_1)}{\varepsilon(v_1)} - \frac{M'(v_1)}{\varepsilon'(v_1)} + \frac{M(v_{i-1})}{\varepsilon(v_{i-1})} - \frac{M'(v_{i-1})}{\varepsilon'(v_{i-1})} \geq \frac{2}{D-1} - \frac{2(k+1)}{D-1} + \frac{2 \cdot m_i}{\varepsilon(v_{i-1})} - \frac{2\,(m_i - k)}{\varepsilon(v_{i-1})} =$$

$$= -\frac{2k}{D-1} + \frac{2k}{\varepsilon(v_{i-1})} > [\varepsilon(v_{i-1}) < D - 1] > 0$$

Therefore, we conclude

$$\xi^{ac}(T) - \xi^{\alpha c}(T') \geq \Delta_1 + \Delta_2 > 0.$$

■

Corollary 3 *Let $T \neq P_n$ be a tree on n vertices. Then*

$$\xi^{ac}(T) > \xi^{ac}(P_n).$$

Proof. Note that transformation of tree from Theorem 2 increases diameter of the tree. Therefore, applying that transformation consecutively on T we obtain in the end path P_n which by that Theorem has smaller value of ξ^{ac} then T. ■

Now that we found a tree with minimum value of augmented ECI, we want to find a tree with maximum value of augmented ECI. One could expect a star S_n to have maximum value of augmented ECI, as that was the case of other eccentricity based indices. But, comparing the value of S_{16} and $TM_{16,5}$ we obtain

$$\xi^{ac}(S_{16}) = 1 + 15 \cdot \frac{15}{2} = \frac{227}{2} = 113.5,$$
$$\xi^{ac}(TB_{16,5}) = \frac{3^5}{2} + 5 \cdot \frac{5}{3} + 10 \cdot \frac{3}{4} = \frac{412}{3} = 137.33,$$

which clearly indicates that S_n is not maximal tree with respect to value of augmented ECI. Now, we want to establish which trees are maximal. For that purpose, we need the following theorem.

Theorem 4 *Let T be a tree on n vertices with diameter $D \geq 5$ and let $P = v_0 v_1 \ldots v_D$ be a diametric path such that $M(v_2)/\deg(v_1) \leq M(v_{D-2})/\deg(v_{D-1})$. Let $w_1, \ldots, v_k$ be all pendent vertices of v_1. For a tree T' obtained from T by deleting edges $v_1w_1, \ldots, v_1w_k$ and adding vertices $v_{D-1}w_1, \ldots, v_{D-1}w_k$ holds*

$$\xi^{ac}(T) < \xi^{ac}(T').$$

Proof. Note that by this transformation eccentricities of vertices do not increase. The only vertex for which $M(v)$ decreases is v_2. We will neutralize this decrease by increase for v_{D-1}. For the simplicity sake, let $m_i = \deg(v_i)$ for $v_i \in P$. Taking into account that $\varepsilon(v) \geq \varepsilon'(v)$ for every $v \in T$ we have

$$\begin{aligned}
\xi^{ac}(T) - \xi^{ac}(T') &\leq \frac{M(v_2)}{\varepsilon(v_2)} - \frac{M'(v_2)}{\varepsilon'(v_2)} + \frac{M(v_{D-2})}{\varepsilon(v_{D-2})} - \frac{M'(v_{D-2})}{\varepsilon'(v_{D-2})} \leq \\
&\leq \frac{(m_1 - 1) \cdot M(v_2)/m_1}{\varepsilon'(v_2)} + \frac{(m_{D-1} - m_{D-1} - m_1 + 1) \cdot M(v_{D-1})/m_{D-1}}{\varepsilon'(v_{D-2})} = \\
&= \frac{(m_1 - 1) \cdot M(v_2)/m_1}{\varepsilon'(v_2)} - \frac{(m_1 - 1) \cdot M(v_{D-1})/m_{D-1}}{\varepsilon'(v_{D-2})}
\end{aligned}$$

Since $\varepsilon'(v_2) \geq \varepsilon'(v_{D-2})$ by construction and since

$$M(v_2)/m_1 \leq M(v_{D-1})/m_{D-1}$$

by assumption of the Theorem, we conclude $\xi^{ac}(T) - \xi^{ac}(T') \leq 0$. Since also obviously

$$\frac{M(v_0)}{\varepsilon(v_0)} - \frac{M'(v_0)}{\varepsilon'(v_0)} < 0$$

we obtain $\xi^{ac}(T) - \xi^{ac}(T') < 0$. ■

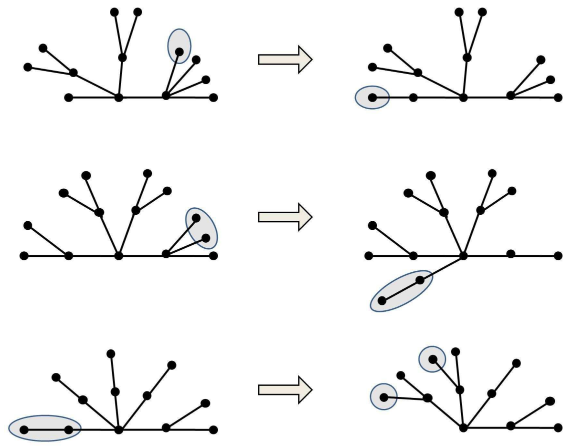

Figure 3: Tree transformations from Lemmas 6, 7 and 8 respectively.

Note that in every tree T there must exist a diametric path which satisfies conditions of Theorem 4, for either the condition holds for diametric path P or for the same path with vertices labeled in reverse order. Applying this transformation repeatedly on a tree with diameter greater than 5, we will finally obtain a tree of diameter 4 with greater value of augmented ECI.

Therefore, a tree with maximum value of augmented ECI lies among trees with $D \leq 4$. Let us now consider such trees.

Lemma 5 *Let $T \neq S_n$ be a tree on n vertices with diameter $D \leq 4$ such that central vertices have at most two non-leaf neighbors. Then $\xi^{ac}(T) < \xi^{ac}(S_n)$.*

Proof. This lemma is corollary of Theorem 2, since every tree T satisfying conditions of this lemma can be obtained from S_n by applying once (if $D = 3$) or twice (if $D = 4$) the transformation of tree from that theorem. ■

As a consequence of this lemma, we can conclude that the "problem" are trees with diameter 4 and at least three non-leaf neighbors of central vertex. Let us now consider such trees. Before we proceed, let us note that tree transformations from some of the following Lemmas are illustrated in Figure 3.

Lemma 6 *Let T be a tree on n vertices with diameter $D = 4$ such that central vertex u has at least three non-leaf neighbors. Let $v_1, \ldots v_k$ be all neighbors of u labeled so that* $\deg(v_1) \leq \ldots \leq \deg(v_k)$. *If* $\deg(v_k) - \deg(v_1) \geq 2$ *than for a tree T' obtained from T by deleting a pending vertex of v_k and adding pending vertex to v_1 holds*

$$\xi^{ac}(T) < \xi^{ac}(T').$$

Proof. Note that eccentricities of vertices remain the same after this transformation. The only vertex whose degree decreases is v_k, therefore $M(v)$ decreases possibly for u and pending vertices of v_k. Let us denote $m_i = \deg v_i$ and $c = M(u)/\,(m_1 \cdot m_k)$. Note that $c \geq 2$ because central vertex has at least three non-leaf neighbors. Considering vertex u and pending vertices of v_1 and v_k we obtain

$$\begin{aligned}\xi(T)-\xi(T') &= \frac{m_1\cdot c\cdot m_k}{2}-\frac{(m_1+1)\cdot c\cdot(m_k-1)}{2}+(m_1-1)\left(\frac{m_1}{4}-\frac{m_1+1}{4}\right)+\\ &+(m_k-2)\left(\frac{m_k}{4}-\frac{m_k-1}{4}\right)+\left(\frac{m_k}{4}-\frac{m_1+1}{4}\right)\\ &=\frac{1}{2}(c-1)(m_1-m_k+1)\leq\frac{1}{2}(c-1)(-2+1)<0.\end{aligned}$$

■

Note that Lemma 6 holds even for trees with only two non-pendant neighbors of central vertex. But then we do not necessarily have strict inequality (constant c from proof can be 1). Lemma 6 can be applied repeatedly until we obtain degree balanced tree. Therefore, we conclude that among trees on n vertices with $D=4$ and central vertex u with given degree $\deg(u)=m$ degree balanced tree $TB_{n,m}$ has maximum value of ξ^{ac}. Now, we can obtain the increase in ξ^{ac} by changing the degree of central vertex. For that purpose we need following lemma.

Lemma 7 *Let T be a tree on n vertices with diameter $D=4$ such that central vertex u has at least three non-leaf neighbors. Let $v_1,\ldots v_k$ be all neighbors of u labeled so that $\deg(v_1)\leq\ldots\leq\deg(v_k)$. If $\deg(v_k)-\deg(v_1)\leq 1$ and $\deg(v_k)\geq 4$ than for a tree T' obtained from T by deleting two pendant vertices of v_k and adding pendant path of length 2 to u holds*

$$\xi^{ac}(T)<\xi^{ac}(T').$$

Proof. Let us denote $k=\deg(u)$, $m_i=\deg(v_i)$ and $c=M(u)/m_k$. Considering $u,v_1,\ldots,v_k$ and pendant vertices of v_k we obtain

$$\begin{aligned}\xi(T)-\xi(T') &= \frac{c\cdot m_k}{2}-\frac{2\cdot c\cdot(m_k-2)}{2}+k\left(\frac{k}{3}-\frac{k+1}{3}\right)+\\ &+(m_k-3)\left(\frac{m_k}{4}-\frac{m_k-2}{4}\right)+\left(2\cdot\frac{m_k}{4}-\left(\frac{k+1}{3}+\frac{2}{4}\right)\right)\\ &=-\frac{c}{2}(m_k-4)-\frac{2}{3}k+m_k-\frac{7}{3}\leq[c\geq 6]\leq\\ &\leq\frac{29}{3}-2m_k-\frac{2}{3}k\leq[m_k\geq 4,k\geq 3]\leq-\frac{1}{3}<0\end{aligned}$$

which concludes the proof. ■

By combining Lemmas 6 and 7, we can conclude that we have restricted our search for trees with extremal ξ^{ac} to S_n or degree balanced trees $TB_{n,k}$ with

$$p=\left\lceil\frac{n-1}{k}\right\rceil\leq 3.$$

Now we will consider separately cases when $p=2$ and $p=3$. First we will consider case when $p=3$. For that purpose we need the following lemma.

Lemma 8 *Let T be a tree on n vertices with diameter $D = 4$ such that central vertex u has at least three non-leaf neighbors. If $T = TB_{n,k}$ where $p = \left\lceil \frac{n-1}{k} \right\rceil = 3$ then*

$$\xi^{ac}(T) \leq \xi^{ac}(TB_{n,\left\lceil \frac{n-1}{3} \right\rceil})$$

with equality if and only if $k = \left\lceil \frac{n-1}{3} \right\rceil$.

Proof. From $p = 3$ follows that all neighbors of u are of degree 3 and possibly 2. Suppose $p \neq \left\lceil \frac{n-1}{3} \right\rceil$. That means there are at least three neighbors of u of degree 2. Let us denote all neighbors of u with $v_1, \ldots, v_k$ so that $m_1 \leq m_2 \leq \ldots \leq m_k$ where m_i denotes $\deg(v_i)$. Let w_1 be a pendant vertex of v_1. Now, let T' be a tree obtained from T by deleting edges uv_1, v_1w_1 and adding edges v_2v_1, v_3w_1. We will show that ξ^{ac} has increased by this transformation. For that purpose let $c = M(u)/8$. Considering vertices $u, v_1, \ldots, v_k$ and pendant vertices of v_1, v_2 and v_3 we obtain

$$\begin{aligned}
\xi^{ac}(T) - \xi^{ac}(T') &\leq \left(\frac{c \cdot 8}{2} - \frac{c \cdot 9}{2}\right) + (k-1)\left(\frac{k}{3} - \frac{k-1}{3}\right) + \left(\frac{k}{3} - \frac{3}{4}\right) + 3\left(\frac{2}{4} - \frac{3}{4}\right) \\
&= \frac{2}{3}k - \frac{1}{2}c - \frac{11}{6} \leq [c \geq 2^{k-3}] \leq \\
&\leq \frac{2}{3}k - 2^{k-4} - \frac{11}{6} \leq \frac{2}{3}3 - 2^{3-4} - \frac{11}{6} = -\frac{1}{3} < 0.
\end{aligned}$$

Repeating this transformation, we obtain $TB_{n,\left\lceil \frac{n-1}{3} \right\rceil}$ which proves the lemma. ■

Now, we want to address trees $TB_{n,k}$ with $p = \left\lceil \frac{n-1}{k} \right\rceil = 2$.

Lemma 9 *Let T be a tree on n vertices with diameter $D = 4$ such that central vertex u has at least three non-leaf neighbors. If $T = TB_{n,k}$ where $p = \left\lceil \frac{n-1}{k} \right\rceil = 2$. Then*

$$\xi^{\alpha c}(T) < \xi^{ac}(S_n) \quad or \quad \xi^{\alpha c}(T) < \xi^{ac}(TB_{n,\left\lceil \frac{n-1}{3} \right\rceil})$$

Proof. Note that it has to be $n \geq 7$ for a tree T to be able to satisfy conditions of lemma. From $p = \left\lceil \frac{n-1}{k} \right\rceil = 2$ follows that neighbors of central vertex have degree 1 or 2. Let u be a central vertex in T and let t neighbors of u have degree 2. First note that $2 \leq t \leq \frac{n-1}{2}$. Also, note that

$$\begin{aligned}
n &= 1 + 2t + (k - t) = 1 + t + k, \\
k &= n - t - 1.
\end{aligned}$$

Now we have

$$\xi^{\alpha c}(TB_{n,k}) = \frac{2^t}{2} + k \cdot \frac{k}{3} + t \cdot \frac{2}{4} = 2^{t-1} + \frac{(n-t-1)^2}{3} + \frac{t}{2} = f(t).$$

Let us analyze obtained function $f(t)$. We have

$$f'(t) = 2^{t-1} \cdot \ln 2 + \frac{2}{3}t + \frac{7}{6} - \frac{2}{3}n$$

This is obviously increasing function in k, therefore from

$$\begin{aligned}
f'(2) &= 2^{2-1} \cdot \ln 2 + \frac{2}{3} \cdot 2 + \frac{7}{6} - \frac{2}{3}n < 0 \text{ for } n \geq 7. \\
f'(\frac{n-1}{2}) &= 2^{\frac{n-1}{2}-1} \cdot \ln 2 + \frac{2}{3} \cdot \frac{n-1}{2} + \frac{7}{6} - \frac{2}{3}n > 0 \text{ for } n \geq 7,
\end{aligned}$$

we conclude that maximum of $f(t) = \xi^{\alpha c}(TB_{n,k})$ is obtained for $t = 2$ or $t = \left\lfloor \frac{n-1}{2} \right\rfloor$. If $t = 2$ then by Lemma 5 we conclude that $\xi^{\alpha c}(T) < \xi^{ac}(S_n)$. If $t = \left\lfloor \frac{n-1}{2} \right\rfloor$ and n is odd then by Lemma 5 we conclude that $\xi^{\alpha c}(T) < \xi^{ac}(TM_{n,3})$. If $t = \left\lfloor \frac{n-1}{2} \right\rfloor$ and n is odd, then before we can apply Lemma 5, we have to prove that tree T with $t = \left\lfloor \frac{n-1}{2} \right\rfloor$ has smaller ξ^{ac} than tree T' obtained from it by deleting last pending vertex of central vertex and adding one pending vertex to one neighbor of central vertex. We have

$$\xi^{ac}(T) - \xi^{ac}(T') = \left(\frac{2^t}{2} + \frac{(t+1)^2}{3} + \frac{t}{2}\right) - \left(\frac{3 \cdot 2^{t-1}}{2} + \frac{t^2}{3} + \frac{t-1}{2} + 2 \cdot \frac{3}{4}\right) =$$

$$= \frac{2}{3}t - \frac{1}{4}2^t - \frac{2}{3} \leq -\frac{1}{3} < 0$$

which completes the proof. ■

Therefore, a tree with extremal value of augmented ECI must be either S_n or $TB_{n, \lceil \frac{n-1}{3} \rceil}$. To decide which is it, we need following lemma.

Lemma 10 *Holds*

$$\xi^{ac}(TB_{n, \lceil \frac{n-1}{3} \rceil}) > \xi^{ac}(S_n).$$

if and only if $n \geq 16$.

Proof. Let $T = TB_{n, \lceil \frac{n-1}{3} \rceil}$ and let $k = \left\lceil \frac{n-1}{3} \right\rceil$ be the degree of central vertex in T. From the value of k follows that neighbors of central vertex have degrees 3 or 3 and 2. Let k_2 be number of neighbors of central vertex with degree 2 and let k_3 be number of neighbors of central vertex with degree 3. Obviously $k_2 \leq 2$ and $k_2 + k_3 = k$. We have

$$n = 1 + k_2 + k_3 + k_2 + 2k_3 = 1 + 3k - k_2.$$

We distinguish three cases. Given the exact formula from Proposition 1 we have

$$\xi^{ac}(T) - \xi^{ac}(S_n) = \begin{cases} \frac{1}{2}3^k - \left(\frac{25}{6}k^2 - \frac{3}{2}k + 1\right) & \text{for } n = 3k+1, \\ 3^{k-1} - \left(\frac{25}{6}k^2 - \frac{9}{2}k + \frac{5}{2}\right) & \text{for } n = 3k, \\ \frac{2}{9}3^k - \left(\frac{25}{6}k^2 - \frac{15}{2}k + \frac{7}{2}\right) & \text{for } n = 3k-1. \end{cases}$$

Since exponential function grows faster then polynomial, from analyzing obtained expressions we conclude that difference $\xi^{ac}(T) - \xi^{ac}(S_n)$ is strictly positive:

- for $k \geq 5$ ($n \geq 16$) in the case of $n = 3k+1$,
- for $k \geq 6$ ($n \geq 18$) in the case od $n = 3k$,
- for $k \geq 6$ ($n \geq 17$) in the case of $n = 3k-1$.

Otherwise, the difference is strictly negative. That concludes the proof. ■

Now, we can summarize our results in the following theorem.

Theorem 11 *Let T be a tree on n vertices. Then*

$$\xi^{ac}(T) \leq \begin{cases} \xi^{ac}(S_n) & \text{if } n \leq 15, \\ \xi^{ac}(TB_{n, \lceil \frac{n-1}{3} \rceil}) & \text{if } n \geq 16, \end{cases}$$

with equality holding id and only if $T = S_n$ for $n \leq 15$ and $T = \xi^{ac}(TB_{n, \lceil \frac{n-1}{3} \rceil})$ for $n \geq 16$.

4 Extremal trees with perfect matching

In this section we assume n to be even since only trees with even n can have perfect matching. Also, tree with a perfect matching can obviously have at most one pendant vertex on every vertex in it. Furthermore, if $P = v_0 v_1 \ldots v_D$ is diametric path in a tree with a perfect matching then v_1 and v_{D-1} must be of degree 2 since they already have one pendent vertex and can't have more.

Path P_n on n vertices obviously has perfect matching, therefore the problem of finding a tree with perfect matching and minimum ξ^{ac} is trivial - it is P_n. But star S_n and degree balanced tree $TB_{n,\lceil \frac{n-1}{3} \rceil}$ do not have a perfect matching. Therefore finding a tree with perfect matching and maximum ξ^{ac} is a nontrivial one. In order to find such tree, we will introduce transformation of a tree which preserves existence of perfect matching and increases ξ^{ac}. But before that, note that for every integer $m \geq 2$ the following inequalities hold

$$m \leq 2^{m-1}, \tag{1}$$

$$2^{m-2} - m + 1 \geq 0. \tag{2}$$

Also, for every integer $m \geq 4$ holds

$$m \leq 2^{m-2}. \tag{3}$$

Now, we can state the following theorem.

Theorem 12 *Let T be a tree on n vertices with a perfect matching and $D \geq 5$. Let $P = v_0 v_1 \ldots v_D$ be a diametric path in T and let $w_1, \ldots, w_k$ be all vertices from $V \setminus \{v_3\}$ adjacent to v_2 and of degree 2. Let T' be a tree obtained from T by deleting edges $v_2w_1, \ldots, v_2w_k$ and adding edges $v_3w_1, \ldots, v_3w_k$. Then T' is a tree on n vertices which has perfect matching and*

$$\xi^{ac}(T) < \xi^{ac}(T').$$

Proof. First note that $k \geq 1$ since at least v_1 is included among $w_1, \ldots, w_k$. Let m_i denote a degree of $v_i \in P$. Note that $m_2 - 2 \leq k \leq m_2 - 1$ since all neighbors of v_2 are of degree 2 except possibly v_3 (which is not counted in k by construction) and one pendant vertex. Now, eccentricities of all vertices do not increase by this transformation. The only vertices whose $M(v)$ possibly decreases are v_2, v_3 and a pendent vertex of v_2 (if such exists). We distinguish three cases.

Case 1. v_2 has one pendent vertex and v_3 has one pendent vertex.

Let us denote with u_2 and u_3 pendant vertices of v_2 and v_3 respectively. In this case $k = m_2 - 2$. We have

$$\Delta_1 = \frac{M(v_2)}{\varepsilon(v_2)} - \frac{M'(v_2)}{\varepsilon'(v_2)} + \frac{M(v_3)}{\varepsilon(v_3)} - \frac{M'(v_3)}{\varepsilon'(v_3)} \leq$$
$$\leq \frac{2^{m_2-2} \cdot m_3}{\varepsilon'(v_2)} - \frac{m_3 + m_2 - 2}{\varepsilon'(v_2)} + \frac{m_2 \cdot 2^{m_3-3} \cdot m_4}{\varepsilon'(v_3)} - \frac{2 \cdot 2^{m_3-3} \cdot 2^{m_2-2} \cdot m_4}{\varepsilon'(v_3)}$$

Since $\varepsilon'(v_2) > \varepsilon'(v_3)$ and $m_4 \geq 2$, in order to prove that $\Delta_1 > 0$ it is sufficient to prove that

$$m_3 \cdot (2^{m_2-2} - 1) - m_2 + 2 \leq 2^{m_3-3} \cdot 2 \cdot \left(2 \cdot 2^{m_2-2} - m_2\right).$$

If $m_3 = 3$, then this inequality becomes $2^{m_2-2} - m_2 + 1 \geq 0$ which is actually inequality (2) for $m_2 \geq 2$ and therefore holds. If $m_3 \geq 4$, then since $m_2 - 2 \geq 0$, it is sufficient to prove

$$m_3 \cdot (2^{m_2-2} - 1) \leq 2^{m_3-3} \cdot 2 \cdot \left(2 \cdot 2^{m_2-2} - m_2\right)$$

which follows from (3) for $m_3 \geq 4$ and (2) for $m_2 \geq 2$. Also, from $\varepsilon'(u_2) > \varepsilon'(u_3)$ follows that

$$\Delta_2 = \frac{M(u_2)}{\varepsilon(u_2)} - \frac{M'(u_2)}{\varepsilon'(u_2)} + \frac{M(u_3)}{\varepsilon(u_3)} - \frac{M'(u_3)}{\varepsilon'(u_3)} \leq \frac{m_2}{\varepsilon'(u_2)} - \frac{2}{\varepsilon'(u_2)} + \frac{m_3}{\varepsilon'(u_3)} - \frac{m_3 + m_2 - 2}{\varepsilon'(u_3)} < 0.$$

Now

$$\xi^{ac}(T) - \xi^{ac}(T') \leq \Delta_1 + \Delta_2 < 0.$$

Case 2. v_2 has one pendent vertex and v_3 has no pendant vertices.

Let us denote with u_2 pendant vertex of v_2. In this case $k = m_2 - 2$. We have

$$\xi^{ac}(T) - \xi^{ac}(T') \leq \frac{M(v_2)}{\varepsilon(v_2)} - \frac{M'(v_2)}{\varepsilon'(v_2)} + \frac{M(v_3)}{\varepsilon(v_3)} - \frac{M'(v_3)}{\varepsilon'(v_3)} + \frac{M(u_2)}{\varepsilon(u_2)} - \frac{M'(u_2)}{\varepsilon'(u_2)} \leq$$
$$\leq \frac{m_3 \cdot \left(2^{m_2-2} - 1\right)}{\varepsilon'(v_2)} - \frac{m_2 - 2}{\varepsilon'(v_2)} - \frac{2^{m_3-2} \cdot m_4 \cdot \left(2 \cdot 2^{m_2-2} - m_2\right)}{\varepsilon'(v_3)} + \frac{m_2 - 2}{\varepsilon'(u_2)}$$

Since $\varepsilon'(u_2) > \varepsilon'(v_2) > \varepsilon'(v_3)$ and $m_4 \geq 2$, it is sufficient to prove that

$$m_3 \cdot \left(2^{m_2-2} - 1\right) \leq 2^{m_3-2} \cdot 2 \cdot \left(2 \cdot 2^{m_2-2} - m_2\right).$$

But this follows from inequality (1) for $m_3 \geq 2$ and (2) for $m_2 \geq 2$.

Case 3. v_2 has no pendent vertices.

Note that in this case edge v_2v_3 must be included in a perfect matching, therefore v_3 cannot have pendent vertices. In this case $k = m_2 - 1$. Note that $\varepsilon'(w_i) = \varepsilon'(v_2)$. We have

$$\xi^{ac}(T) - \xi^{ac}(T') \leq \frac{M(v_2)}{\varepsilon(v_2)} - \frac{M'(v_2)}{\varepsilon'(v_2)} + \frac{M(v_3)}{\varepsilon(v_3)} - \frac{M'(v_3)}{\varepsilon'(v_3)} + \sum_{i=1}^{k} \left(\frac{M(w_i)}{\varepsilon(w_i)} - \frac{M'(w_i)}{\varepsilon'(w_i)} \right) \leq$$
$$\leq \frac{m_3 \cdot \left(2^{m_2-1} - 1\right) - m_2 + 1}{\varepsilon'(v_2)} - \frac{2^{m_3-2} \cdot m_4 \cdot \left(2 \cdot 2^{m_2-1} - m_2\right)}{\varepsilon'(v_3)} +$$
$$+ \frac{(m_2 - 1)(1 - m_3)}{\varepsilon'(v_2)}$$

Since $\varepsilon'(v_2) > \varepsilon'(v_3)$ and $m_4 \geq 2$ it is sufficient to prove that

$$m_3 \cdot \left(2^{m_2-1} - 1\right) - m_2 + 1 + (m_2 - 1)(1 - m_3) \leq 2^{m_3-2} \cdot 2 \cdot \left(2 \cdot 2^{m_2-1} - m_2\right),$$

which is equivalent to

$$m_3 \cdot \left(2^{m_2-1} - m_2\right) \leq 2^{m_3-1} \left(2 \cdot 2^{m_2-1} - m_2\right)$$

and follows from (1) for $m_3 \geq 2$. ■

Now, as a corollary to this theorem we obtain the only extremal tree with respect to augmented ECI among trees with perfect matching.

Corollary 13 *Let $T \neq TB_{n,\frac{n}{2}}$ be a tree on n vertices with perfect matching. Then*

$$\xi^{ac}(T) < \xi^{ac}(TB_{n,\frac{n}{2}}).$$

Proof. We apply the transformation from Theorem 12 on T. Note that each transformation decreases diameter by 1 until finally we obtain the tree of diameter 4. The only tree of diameter 4 which has perfect matching is $TB_{n,\frac{n}{2}}$. ■

5 Extremal graphs

Let us now establish extremal graphs among all simple connected graphs. Those results will follow easily from results for threes. First, the following proposition obviously holds, since contribution of every vertex to ξ^{ac} in complete graph K_n is maximum possible.

Proposition 14 *For a graph $G \neq K_n$ on n vertices holds*

$$\xi^{ac}(G) < \xi^{ac}(K_n).$$

Therefore, we have established only maximal graphs with respect to the value of augmented ECI. In the following proposition we establish minimal graphs.

Proposition 15 *For a graph $G \neq P_n$ on n vertices holds*

$$\xi^{ac}(G) > \xi^{ac}(P_n).$$

Proof. Let T be spanning tree of G. From definition of spanning tree follows that T is obtained from G by deleting some edges. Note that deleting edges does not decrease eccentricities of vertices. If G is already a tree, then the result follows from Corollary 3. If G is not a tree, then we have to delete at least one edge. Note that by deleting edges degrees of vertices (and therefore values $M(v)$) do not increase. Since we deleted at least one edge, that means that the degree of at least one vertex decreased and we have

$$\xi^{ac}(G) > \xi^{ac}(T) \geq \xi^{ac}(P_n)$$

which concludes the proof. ■

6 Conclusion

In this paper we studied augmented eccentric connectivity index on graphs and trees. We established that minimal trees with respect to augmented ECI are paths P_n (Corollary 3), while maximal trees are either stars S_n for $n \leq 15$ either degree balanced trees $TB_{n,\lceil \frac{n-1}{3} \rceil}$ for $n \geq 16$ (Theorem 11). Using similar techniques we proved that in the class of trees with perfect matching minimal trees are again paths P_n, while maximal trees are $TB_{n,\frac{n}{2}}$ (Corollary 13). In the class of general simple connected graphs on n vertices, maximal graphs with respect to augmented ECI are complete graphs K_n (Proposition 14), while minimal graphs are paths P_n (Proposition 15). The explicit formulas for the values of augmented ECI of all these graphs which turned out to be extremal are derived and presented in Proposition 1.

There are many open questions for further study. In this paper we only initiated studying extremal trees with given parameter (trees with perfect matching). One could try to establish extremal trees with given diameter, radius, number of pendant vertices, maximum degree (chemical trees), etc. Also, one could try to establish extremal unicyclic graphs with respect to augmented ECI. Deriving exact formulas for the value of augmented ECI on some special kinds of graphs would also be interesting, just as studying of how augmented ECI behaves with respect to graph operations.

Finally, there is also super augmented ECI, which is similar to augmented ECI, and is defined with

$$\xi^{ac}(G) = \sum_{u \in V} \frac{M(u)}{\varepsilon^2(u)}.$$

It would be interesting to derive all those results for that index too. As for the results from this paper, we mostly relied on order of $\varepsilon(v)$ between pairs of vertices. Since the same order holds for $\varepsilon^2(v)$ then the results for $\xi^{sac}(G)$ should be perfectly analogous.

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