On augmented eccentric connectivity index of graphs and trees

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

June 19, 2013

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 $H_n = \sum_{i=1}^{n} \frac{i}{2}$. 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 $TB_n, \left\lceil \frac{n-1}{3} \right\rceil$ 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. $\xi_{ac}(P_n) = \begin{cases} 8(H_{n-1} - H_{n-2}) - \left(\frac{4}{n-1} + \frac{4}{n-2}\right), & \text{for } n \text{ even,} \\ 8(H_{n-1} - H_{n-2}) - \left(\frac{12}{n-1} + \frac{4}{n-2}\right), & \text{for } n \text{ odd,} \end{cases}$

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

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

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

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
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

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

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

\[
\Delta_1 = \frac{M(v_0)}{\varepsilon(v_0)} - \frac{M'(v_0)}{\varepsilon'(v_0)} + \frac{M(v_2)}{\varepsilon(v_2)} - \frac{M'(v_2)}{\varepsilon'(v_2)} \geq \frac{m_1}{D} - \frac{m_1 \cdot m_w}{D - 2} - \frac{m_1 \cdot c_2}{D - 2} = -\frac{m_1(m_w - 1)}{D} + \frac{m_1 \cdot c_2 \cdot (m_w - 1)}{D - 2} \geq 0.
\]

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

\[
\Delta_2 = \frac{M(v_1)}{\varepsilon(v_1)} - \frac{M'(v_1)}{\varepsilon'(v_1)} + \frac{M(v_3)}{\varepsilon(v_3)} - \frac{M'(v_3)}{\varepsilon'(v_3)} + \sum_{i=1}^{k} \left( \frac{M(w_i)}{\varepsilon(w_i)} - \frac{M'(w_i)}{\varepsilon'(w_i)} \right) \geq \frac{m_2}{D - 1} - \frac{(m_2 - k)(k + 1)}{D - 1} + \frac{m_2 \cdot c_3}{\varepsilon(v_3)} - \frac{(m_2 - k) \cdot c_3}{\varepsilon(v_3)} + \sum_{i=1}^{k} \left( \frac{m_2}{D - 1} - \frac{k + 1}{D - 1} \right) = -\frac{k \cdot (m_2 - k - 1)}{D - 1} + \frac{k \cdot c_3}{\varepsilon(v_3)} + \frac{k \cdot (m_2 - k - 1)}{D - 1} > 0.
\]
Therefore, 

\[ \xi^{ac}(T) - \xi^{ac}(T') \geq \Delta_1 + \Delta_2 > 0. \]

**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

\[
\Delta_1 = \frac{M(v_0)}{\varepsilon(v_0)} - \frac{M'(v_0)}{\varepsilon'(v_0)} + \frac{M(v_i)}{\varepsilon(v_i)} - \frac{M'(v_i)}{\varepsilon'(v_i)} \geq \frac{2 \cdot m_{w}}{D} - \frac{2 \cdot m_{w}}{D} + \frac{m_{i-1} \cdot m_w \cdot c_i}{\varepsilon(v_i)} - \frac{m_{i-1} \cdot c_i}{\varepsilon(v_i)} = \\
= -\frac{2(m_{w} - 1)}{D} + \frac{m_{i-1} \cdot c_i \cdot (m_{w} - 1)}{\varepsilon(v_i)} \geq 0.
\]

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

\[
\Delta_2 = \frac{M(v_1)}{\varepsilon(v_1)} - \frac{M'(v_1)}{\varepsilon'(v_1)} + \frac{M(v_{i-1})}{\varepsilon(v_{i-1})} - \frac{M'(v_{i-1})}{\varepsilon'(v_{i-1})} \geq \frac{2 \cdot m_{i}}{D - 1} - \frac{2(k + 1)}{D - 1} + \frac{2 \cdot m_i}{\varepsilon(v_{i-1})} - \frac{2 \cdot m_{i} - k}{\varepsilon(v_{i-1})} = \\
= -\frac{2k}{D - 1} + \frac{2k}{\varepsilon(v_{i-1})} > [\varepsilon(v_{i-1}) < D - 1] > 0.
\]

Therefore, we conclude

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

$$\xi^{ac}(S_{16}) = 1 + 15 \cdot \frac{15}{2} = 113.5,$$

$$\xi^{ac}(TM_{16,5}) = \frac{3^5}{2} + 5 \cdot \frac{5}{3} + 10 \cdot \frac{3}{4} = \frac{412}{3} = 137.33,$$

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 $P = v_0v_1 \ldots v_D$ be a diametric path such that $M(v_2)/\deg(v_1) \leq M(v_{D-2})/\deg(v_{D-1})$. Let $w_1, \ldots, w_k$ be all pendant 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

$$\xi^{ac}(T) - \xi^{ac}(T') \leq \frac{M(v_2)}{\varepsilon(v_2)} - \frac{M'(v_2)}{\varepsilon'(v_2)} + \frac{M(v_{D-2})}{\varepsilon(v_{D-2})} - \frac{M'(v_{D-2})}{\varepsilon'(v_{D-2})} \leq$$

$$\leq \frac{(m_1 - 1) \cdot M(v_2)/m_1}{\varepsilon'(v_2)} + \frac{(m_{D-1} - m_{D-1} - m_1 + 1) \cdot M(v_{D-1})/m_{D-1}}{\varepsilon'(v_{D-2})} =$$

$$= \frac{(m_1 - 1) \cdot M(v_2)/m_1}{\varepsilon'(v_2)} - \frac{(m_{D-1} - 1) \cdot M(v_{D-1})/m_{D-1}}{\varepsilon'(v_{D-2})}$$

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 $\xi^{ac}(T) - \xi^{ac}(T') < 0$. ■
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 $c = M(u)/\langle m_1 \cdot m_k \rangle$. 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

\[
\xi(T) - \xi(T') = \frac{m_1 \cdot c \cdot m_k}{2} - \frac{(m_1 + 1) \cdot c \cdot (m_k - 1)}{2} + (m_1 - 1) \left( \frac{m_1}{4} - \frac{m_1 + 1}{4} \right) + \\
+ (m_k - 2) \left( \frac{m_k}{4} - \frac{m_k - 1}{4} \right) + \left( \frac{m_k}{4} - \frac{m_1 + 1}{4} \right) \\
= \frac{1}{2} (c - 1) (m_1 - m_k + 1) \leq \frac{1}{2} (c - 1) (-2 + 1) < 0.
\]

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 \( \xi^{ac} \). Now, we can obtain the increase in \( \xi^{ac} \) 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 \( \deg(v_k) \geq 4 \) then 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

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

which concludes the proof.

By combining Lemmas 6 and 7 we can conclude that we have restricted our search for trees with extremal \( \xi^{ac} \) 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
\[
\xi^{ac}(T) \leq \xi^{ac}(TB_{n,\left\lceil \frac{n-1}{k} \right\rceil})
\]
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 $p \neq \left\lceil \frac{n-1}{k} \right\rceil$. That means there are at least three 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 $\text{deg}(v_i)$. Let $w_1$ be a pendant vertex of $v_1$. Now, let $T'$ be a tree obtained from $T$ by deleting edges $w_1v_1, v_1v_2$ and adding edges $v_2v_1, v_3w_1$. We will show that $\xi^{ac}$ 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
\[
\xi^{ac}(T') = \left( \frac{c \cdot 8}{2} - \frac{c \cdot 9}{2} \right) + (k-1) \left( \frac{k}{3} - \frac{k-1}{3} \right) + \left( \frac{k}{3} - \frac{3}{4} \right) + 3 \left( \frac{2}{4} - \frac{3}{4} \right)
\]
\[
= \frac{2}{3}k\frac{c}{2} - \frac{11}{6} \leq [c \geq 2k-3] \leq \frac{2}{3}k - 2k - \frac{11}{6} \leq \frac{3}{3} - 2k - \frac{11}{6} = \frac{1}{3} < 0.
\]

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

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
\[
\xi^{ac}(T) < \xi^{ac}(S_n) \quad \text{or} \quad \xi^{ac}(T) < \xi^{ac}(TB_{n,\left\lceil \frac{n-1}{k} \right\rceil})
\]

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
\[
n = 1 + 2t + (k-t) = 1 + t + k,
\[
k = n - t - 1.
\]

Now we have
\[
\xi^{ac}(TB_{n,k}) = \frac{2t}{2} + k \cdot \frac{k}{3} + t \cdot \frac{2}{4} = 2^t - 1 + \frac{(n-t-1)^2}{3} + \frac{t}{2} = f(t).
\]

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
\[
f'(2) = 2^{2-1} \cdot \ln 2 + \frac{2}{3} \cdot 2 + \frac{7}{6} - \frac{2}{3}n < 0 \quad \text{for} \quad n \geq 7,
\]
\[
f'(\frac{n-1}{2}) = 2^{\frac{n-1}{2}-1} \cdot \ln 2 + \frac{2}{3} \cdot \frac{n-1}{2} + \frac{7}{6} - \frac{2}{3}n > 0 \quad \text{for} \quad n \geq 7,
\]

9
we conclude that maximum of \( f(t) = \xi^{ac}(TB_{n,k}) \) 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 \( \xi^{ac}(T) < \xi^{ac}(S_n) \). If \( t = \left\lfloor \frac{n-1}{2} \right\rfloor \) and \( n \) is odd then by Lemma 5 we conclude that \( \xi^{ac}(T) < \xi^{ac}(TM_{n,3}) \). 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 \( \xi^{ac} \) 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

\[
\xi^{ac}(T) - \xi^{ac}(T') = \left( \frac{2t^2}{2} + \frac{(t+1)^2}{3} + \frac{t}{2} \right) - \left( \frac{3 \cdot 2^{t-1}}{2} + \frac{t^2}{3} + \frac{t-1}{2} + 2 \cdot \frac{3}{4} \right) = \frac{2t - \frac{1}{4} 2^t - \frac{2}{3} \leq -\frac{1}{3} < 0
\]

which completes the proof. \( \blacksquare \)

Therefore, a tree with extremal value of augmented ECI must be either \( S_n \) or \( TB_{n,\left\lfloor \frac{n-1}{2} \right\rfloor} \). To decide which is it, we need following lemma.

**Lemma 10** Holds

\[ \xi^{ac}(TB_{n,\left\lfloor \frac{n-1}{2} \right\rfloor}) > \xi^{ac}(S_n) \]

if and only if \( n \geq 16 \).

**Proof.** Let \( T = TB_{n,\left\lfloor \frac{n-1}{2} \right\rfloor} \) and let \( k = \left\lfloor \frac{n-1}{3} \right\rfloor \) 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 4 we have

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

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 of \( n = 3k \),
- for \( k \geq 6 \) (\( n \geq 17 \)) in the case of \( n = 3k - 1 \).

Otherwise, the difference is strictly negative. That concludes the proof. \( \blacksquare \)

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

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

\[
\xi^{ac}(T) \leq \begin{cases} 
\xi^{ac}(S_n) & \text{if } n \leq 15, \\
\xi^{ac}(TB_{n,\left\lfloor \frac{n-1}{2} \right\rfloor}) & \text{if } n \geq 16,
\end{cases}
\]

with equality holding if and only if \( T = S_n \) for \( n \leq 15 \) and \( T = \xi^{ac}(TB_{n,\left\lfloor \frac{n-1}{2} \right\rfloor}) \) 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 \( P = v_0v_1 \ldots v_D \) 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 pendant 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 \( \xi^{ac} \) is trivial - it is \( P_n \). But star \( S_n \) and degree balanced tree \( TB_n[\frac{n-1}{2}] \) do not have a perfect matching. Therefore finding a tree with perfect matching and maximum \( \xi^{ac} \) 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 \( \xi^{ac} \). 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 \( P = v_0v_1 \ldots v_D \) 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 \( v_3 \) is included among \( w_1, \ldots, w_k \). Let \( m_2 \) denote a degree of \( v_3 \) \( \in P \). Note that \( m_2 - 1 \leq k \leq m_2 - 1 \) 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 pendant vertex of \( v_2 \) (if such exists). We distinguish three cases.

Case 1. \( v_2 \) has one pendant vertex and \( v_3 \) has one pendant 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

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

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

\[
m_3 \cdot (2^{m_2 - 2} - 1) - m_2 + 2 \leq 2^{m_3 - 3} \cdot 2 \cdot (2 \cdot 2^{m_2 - 2} - m_2).
\]

If \( m_3 = 3 \), then this inequality becomes \( 2^{m_2 - 2} - m_2 + 1 \geq 0 \) which is actually inequality 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

\[
m_3 \cdot (2^{m_2 - 2} - 1) \leq 2^{m_3 - 3} \cdot 2 \cdot (2 \cdot 2^{m_2 - 2} - m_2)
\]
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

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

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 pendent vertices.

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

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

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

\[
m_3 \cdot (2^{m_2-2} - 1) \leq 2^{m_3-2} \cdot 2 \cdot (2 \cdot 2^{m_2-2} - m_2).
\]

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

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

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

\[
m_3 \cdot (2^{m_2-1} - 1) - m_2 + 1 + (m_2 - 1) (1 - m_3) \leq 2^{m_3-2} \cdot 2 \cdot (2 \cdot 2^{m_2-1} - m_2),
\]

which is equivalent to

\[
m_3 \cdot (2^{m_2-1} - m_2) \leq 2^{m_3-1} (2 \cdot 2^{m_2-1} - m_2)
\]

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 trees. First, the following proposition obviously holds, since contribution of every vertex to $\xi^{ac}$ 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. $\blacksquare$

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 $TB_{\frac{n-1}{3}}$ 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 $TB_{\frac{n-1}{2}}$ (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 \( \xi^{ac}(G) \) should be perfectly analogous.

7 Acknowledgements

Partial support of the Ministry of Science, Education and Sport of the Republic of Croatia (grant. no. 083-0831510-1511) and of project Gregas is gratefully acknowledged.

References

[1] A.R. Ashrafi, T. Došlić, M. Saheli, The eccentric connectivity index of TUC4C8(R) nanotubes, MATCH Commun. Math. Comput. Chem. 65 (2011) 221–230.

[2] S. Bajaj, S. S. Sambi, S. Gupta, A. K. Madan, Model for prediction of anti-HIV activity of 2-pyridinone derivatives using novel topological descriptor, QSAR Comb. Sci. 25 (2006) 813–823.

[3] S. Bajaj, S. S. Sambi, A. K. Madan, Topological models for prediction of anti-HIV activity of acylthiocarbamates, Bioorg. Med. Chem. 13 (2005) 3263–3268.

[4] T. Došlić, A. Graovac, O. Ori, Eccentric connectivity indices of hexagonal belts and chains, MATCH Commun. Math. Comput. Chem. 65 (2011) 745–752.

[5] T. Došlić, M. Saheli, Augmented eccentric connectivity index, to appear in Miskolc Mathematical Notes.

[6] T. Došlić, M. Saheli, D. Vukičević, Eccentric connectivity index: extremal graphs and values, Iranian J. Math. Chem. 1 (2010) 45–56.

[7] H. Dureja, S. Gupta, A. K. Madan, Predicting anti-HIV-1 activity of 6-arylbenzonitriles: Computational approach using superaugmented eccentric connectivity topochemical in-dices, J. Mol. Graph. Model. 26 (2008) 1020–1029.

[8] H. Dureja, A. K. Madan, Predicting anti-HIV activity of dimethylaminopyridin-2-ones: Computational approach using topochemical descriptors, Chem. Biol. Drug Des. 73 (2009) 258–270.

[9] S. Gupta, M. Singh, A. K. Madan, Eccentric distance sum: A novel graph invariant for predicting biological and physical properties, J. Math. Anal. Appl. 275 (2002) 386–401.

[10] A. Ilić, Eccentric connectivity index, in I. Gutman, B. Furtula (Eds.), Novel Molecular Structure Descriptors – Theory and Applications II, Univ. Kragujevac, Kragujevac, 2010, pp. 139–168.
[11] A. Ilić, I. Gutman, Eccentric connectivity index of chemical trees, MATCH Commun. Math. Comput. Chem. 65 (2011) 731–744.

[12] A. Ilić, G. Yu, L. Feng, On the eccentric distance sum of graphs, J. Math. Anal. Appl. 381 (2011) 590–600.

[13] V. Kumar, S. Sardana, A.K. Madan, Predicting anti-HIV activity of 2,3-diaryl-1,3-thiazolidin-4-ones: computational approaches using reformed eccentric connectivity index, J. Mol. Model. 10 (2004) 399–407.

[14] V. Lather, A.K. Madan, Predicting Dopamine Receptors Binding Affinity of N-[4-(4-Arylpiperazin-1-yl)butyl]Aryl Carboxamides: Computational Approach Using Topological Descriptors, Curr. Drug Discov. Tech. 2 (2005) 115–121.

[15] S. Sardana, A. K. Madan, Relationship of Wiener’s index and adjacent eccentric distance sum index with nitroxide free radicals and their precursors as modifiers against oxidative damage, J. Mol. Struct. (Theochem) 624 (2003) 53–59.

[16] V. Sharma, R. Goswami, A.K. Madan, Eccentric connectivity index: A Novel Highly Discriminating Topological Descriptor for Structure-Property and Structure-Activity Studies. J. Chem. Inf. Comput. Sci. 37 (1997) 273–282.

[17] G. Yu, L. Feng, A. Ilić, On the eccentric distance sum of trees and unicyclic graphs, J. Math. Anal. Appl. 375 (2011) 934–944.

[18] B. Zhou, Z. Du, On eccentric connectivity index, MATCH Commun. Math. Comput. Chem. 63 (2010) 181–198.