

On the extremal properties of the average eccentricity[☆]

Aleksandar Ilić

Faculty of Sciences and Mathematics, Višegradska 33, 18000 Niš, University of Niš, Serbia

ARTICLE INFO

Article history:

Received 25 February 2011

Received in revised form 22 April 2012

Accepted 29 April 2012

Keywords:

Distances

Average eccentricity

Vertex degree

AutoGraphiX

Extremal graph

ABSTRACT

The eccentricity of a vertex is the maximum distance from it to another vertex and the average eccentricity $ecc(G)$ of a graph G is the mean value of eccentricities of all vertices of G . The average eccentricity is deeply connected with a topological descriptor called the eccentric connectivity index, defined as a sum of products of vertex degrees and eccentricities. In this paper we analyze extremal properties of the average eccentricity, introducing two graph transformations that increase or decrease $ecc(G)$. Furthermore, we resolve four conjectures, obtained by the system AutoGraphiX, about the average eccentricity and other graph parameters (the clique number and the independence number), refute one AutoGraphiX conjecture about the average eccentricity and the minimum vertex degree and correct one AutoGraphiX conjecture about the domination number.

© 2012 Elsevier Ltd. All rights reserved.

1. Introduction

Let $G = (V, E)$ be a connected simple graph with $n = |V|$ vertices and $m = |E|$ edges. Let $deg(v)$ denote the degree of the vertex v . Let $\delta = \delta(G)$ be the minimum vertex degree, and $\Delta = \Delta(G)$ be the maximum vertex degree of a graph G .

For vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of a shortest path between u and v in G . The eccentricity of a vertex is the maximum distance from it to any other vertex,

$$\varepsilon(v) = \max_{u \in V} d(u, v).$$

The radius of a graph $r(G)$ is the minimum eccentricity of any vertex. The diameter of a graph $d(G)$ is the maximum eccentricity of any vertex in the graph, or the greatest distance between any pair of vertices. For an arbitrary vertex $v \in V$ it holds that $r(G) \leq \varepsilon(v) \leq d(G)$. A vertex c of G is called central if $\varepsilon(c) = r(G)$. The center $C(G)$ is the set of all central vertices in G . An eccentric vertex of a vertex v is a vertex farthest away from v . Every tree has exactly one or two central vertices [1].

The average eccentricity of a graph G is the mean value of eccentricities of vertices of G ,

$$ecc(G) = \frac{1}{n} \sum_{v \in V} \varepsilon(v).$$

For example, we have the following formulas for the average eccentricity of the complete graph K_n , complete bipartite graph $K_{n,m}$, hypercube H_n , path P_n , cycle C_n and star S_n ,

$$\begin{aligned} ecc(K_n) &= 1 & ecc(K_{n,m}) &= 2 & ecc(Q_n) &= n \\ ecc(P_n) &= \frac{1}{n} \left\lfloor \frac{3}{4}n^2 - \frac{1}{2}n \right\rfloor & ecc(C_n) &= \left\lfloor \frac{n}{2} \right\rfloor & ecc(S_n) &= 2 - \frac{1}{n}. \end{aligned}$$

[☆] The paper has been evaluated according to old Aims and Scope of the journal.

E-mail address: aleksandari@gmail.com.

Dankelmann et al. [2] presented some upper bounds and formulas for the average eccentricity regarding the diameter and the minimum vertex degree. Furthermore, they examine the change in the average eccentricity when a graph is replaced by a spanning subgraph, in particular the two extreme cases: taking a spanning tree and removing one edge. Dankelmann and Entringer [3] studied the average distance of G within various classes of graphs.

In theoretical chemistry molecular structure descriptors (also called topological indices) are used for modeling physico-chemical, pharmacological, toxicological, biological and other properties of chemical compounds [4]. There exist several types of such indices, especially those based on vertex and edge distances [5,6]. Arguably the best known of these indices is the Wiener index W , defined as the sum of distances between all pairs of vertices of the molecular graph [7]

$$W(G) = \sum_{u,v \in V} d(u, v).$$

Besides of use in chemistry, it was independently studied due to its relevance in social science, architecture, and graph theory.

Sharma et al. [8] introduced a distance-based molecular structure descriptor, the eccentric connectivity index, which is defined as

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

The eccentric connectivity index is deeply connected to the average eccentricity, but for each vertex v , $\xi^c(G)$ takes one local property (vertex degree) and one global property (vertex eccentricity) into account. For k -regular graph G , we have $\xi^c(G) = k \cdot n \cdot \text{ecc}(G)$.

The index ξ^c was successfully used for mathematical models of biological activities of diverse nature. The eccentric connectivity index has been shown to give a high degree of predictability of pharmaceutical properties, and provide leads for the development of safe and potent anti-HIV compounds [9–11]. The investigation of its mathematical properties started only recently, and has so far resulted in determining the extremal values and the extremal graphs [12,13], and also in a number of explicit formulas for the eccentric connectivity index of several classes of graphs [14] (for a recent survey see [15]).

The AutoGraphiX (AGX) computer system was developed by the GERAD group from Montréal [16–18]. AGX is an interactive software designed to help find conjectures in graph theory. It uses the Variable Neighborhood Search metaheuristic (Hansen and Mladenović [19,20]) and data analysis methods to find extremal graphs with respect to one or more invariants. Recently there has been vast research regarding AGX conjectures and a series of papers on various graph invariants have been written: average distance [21], independence number [22], proximity and remoteness [23], largest eigenvalue of adjacency and Laplacian matrix [24], Randić index [25,26], connectivity and distance measures [27], etc. In this paper we continue this work and resolve other conjectures from the thesis [16], available online at <http://www.gerad.ca/~agx/>.

Recall that the vertex connectivity ν of G is the smallest number of vertices whose removal disconnects G and the edge connectivity κ of G is the smallest number of edges whose removal disconnects G . Sedlar et al. [28] studied the lower and upper bounds of $\text{ecc} - \delta$, $\text{ecc} + \delta$ and ecc/δ , the lower bound for $\text{ecc} \cdot \delta$, and similar relations by replacing δ with ν and κ .

The paper is organized as follows. In Section 2 we introduce a simple graph transformation that increases the average eccentricity and characterize the extremal tree with maximum average eccentricity among trees on n vertices with given maximum vertex degree. In Section 3 we resolve a conjecture about the upper bound of the sum $\text{ecc} + \alpha$, where α is the independence number. In Section 4, we characterize the extremal graph having maximum value of average eccentricity in the class of n -vertex graphs with given clique number ω . In Section 5, we refute a conjecture about the maximum value of the product $\text{ecc} \cdot \delta$. We close the paper in Section 6 by restating some other AGX conjecture for the future research and correcting a conjecture about $\text{ecc} + \gamma$, where γ denotes the domination number.

2. The average eccentricity of trees with given maximum degree

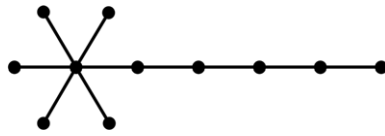
Theorem 2.1. *Let w be a vertex of a nontrivial connected graph G . For nonnegative integers p and q , let $G(p, q)$ denote the graph obtained from G by attaching to vertex w pendent paths $P = wv_1v_2 \dots v_p$ and $Q = wu_1u_2 \dots u_q$ of lengths p and q , respectively. If $p \geq q \geq 1$, then*

$$\text{ecc}(G(p, q)) < \text{ecc}(G(p+1, q-1)).$$

Proof. Since after this transformation the longer path has increased and the eccentricities of vertices of G are either the same or increased by one, we will consider three simple cases based on the longest path from the vertex w in the graph G . Denote by $\varepsilon'(v)$ the eccentricity of vertex v in $G(p+1, q-1)$.

Case 1. The length of the longest path from the vertex w in G is greater than p . This means that the vertex of G , most distant from w is the most distant vertex for all vertices of P and Q . It follows that $\varepsilon'(v) = \varepsilon(v)$ for all vertices $w, v_1, v_2, \dots, v_p, u_1, u_2, \dots, u_{q-1}$, while the eccentricity of u_q increased by $p+1-q$. Therefore,

$$\text{ecc}(G(p+1, q-1)) - \text{ecc}(G(p, q)) \geq \frac{p+1-q}{|V(G)|+p+q} > 0.$$

Fig. 1. The broom $B(11, 6)$.

Case 2. The length of the longest path from the vertex w in G is less than or equal to p and greater than q . This means that either the vertex of G that is most distant from w or the vertex v_p is the most distant vertex for all vertices of P , while for the vertices w, u_1, u_2, \dots, u_q the most distant vertex is v_p . It follows that $\varepsilon'(v) \geq \varepsilon(v)$ for vertices v_1, v_2, \dots, v_p , while $\varepsilon'(v) = \varepsilon(v) + 1$ for vertices $w, u_1, u_2, \dots, u_{q-1}$. Also the eccentricity of u_q increased by at least 1, and consecutively

$$\text{ecc}(G(p+1, q-1)) - \text{ecc}(G(p, q)) \geq \frac{q+1}{|V(G)| + p + q} > 0.$$

Case 3. The length of the longest path from the vertex w in G is less than or equal to q . This means that the pendent vertex most distant from the vertices of P and Q is either v_p or u_q , depending on the position. Therefore, for each vertex in G the eccentricity increased by 1. Using the average eccentricity of a path $P \cup Q$, we have

$$\text{ecc}(G(p+1, q-1)) - \text{ecc}(G(p, q)) \geq \frac{|V(G)|}{|V(G)| + p + q} > 0.$$

Since G is a nontrivial graph with at least one vertex, we have strict inequality.

This completes the proof. \square

Chemical trees (trees with maximum vertex degree at most four) provide the graph representations of alkanes [4]. It is therefore a natural problem to study trees with bounded maximum degree. The path P_n is the unique tree with $\Delta = 2$, while the star S_n is the unique tree with $\Delta = n - 1$. Therefore, we can assume that $3 \leq \Delta \leq n - 2$.

The broom $B(n, \Delta)$ is a tree consisting of a star $S_{\Delta+1}$ and a path of length $n - \Delta - 2$ attached to an arbitrary pendent vertex of the star (see Fig. 1). It is proven that among trees with maximum vertex degree equal to Δ , the broom $B(n, \Delta)$ uniquely minimizes the Estrada index [29], the largest eigenvalue of the adjacency matrix [30], distance spectral radius [31], etc.

Theorem 2.2. Let $T \not\cong B(n, \Delta)$ be an arbitrary tree on n vertices with maximum vertex degree Δ . Then

$$\text{ecc}(B(n, \Delta)) > \text{ecc}(T).$$

Proof. Fix a vertex v of degree Δ as a root and let $T_1, T_2, \dots, T_\Delta$ be the trees attached at v . We can repeatedly apply the transformation described in Theorem 2.1 at any vertex of degree at least three with largest eccentricity from the root in every tree T_i , as long as T_i does not become a path. When all trees $T_1, T_2, \dots, T_\Delta$ turn into paths, we can again apply transformation from Theorem 2.1 at the vertex v as long as there exist at least two paths of length greater than one, further increasing the average eccentricity. Finally, we arrive at the broom $B(n, \Delta)$ as the unique tree with maximum average eccentricity. \square

By direct verification, it holds

$$\text{ecc}(B(n, \Delta)) = \frac{1}{n} \left(\left\lfloor \frac{(n - \Delta + 2)(3(n - \Delta + 1) + 1)}{4} \right\rfloor + (n - \Delta + 1)(\Delta - 2) \right).$$

If $\Delta > 2$, we can apply the transformation from Theorem 2.1 at the vertex of degree Δ in $B(n, \Delta)$ and obtain $B(n, \Delta - 1)$. Thus, we have the following chain of inequalities

$$\text{ecc}(S_n) = \text{ecc}(B(n, n - 1)) < \text{ecc}(B(n, n - 2)) < \dots < \text{ecc}(B(n, 3)) < \text{ecc}(B(n, 2)) = \text{ecc}(P_n).$$

Also, it follows that $B(n, 3)$ has the second maximum average eccentricity among trees on n vertices. On the other hand, the addition of an arbitrary edge in G cannot increase the average eccentricity and clearly $\varepsilon(v) \geq 1$ with equality if and only if $\deg(v) = n - 1$.

Theorem 2.3. Among graphs on n vertices, the path P_n attains the maximum average eccentricity, while the complete graph K_n attains the minimum average eccentricity.

Note that Corollary 1 from [2] is a part of this theorem.

A starlike tree is a tree with exactly one vertex of degree at least 3. We denote by $S(n_1, n_2, \dots, n_k)$ the starlike tree of order n having a branching vertex v and

$$S(n_1, n_2, \dots, n_k) - v = P_{n_1} \cup P_{n_2} \cup \dots \cup P_{n_k},$$

where $n_1 \geq n_2 \geq \dots \geq n_k \geq 1$. Clearly, the numbers n_1, n_2, \dots, n_k determine the starlike tree up to isomorphism and $n = n_1 + n_2 + \dots + n_k + 1$. The starlike tree $BS(n, k) \cong S(n_1, n_2, \dots, n_k)$ is balanced if all paths have almost equal lengths, i.e., $|n_i - n_j| \leq 1$ for every $1 \leq i < j \leq k$.

Let $x = (x_1, x_2, \dots, x_n)$ and $y = (y_1, y_2, \dots, y_n)$ be two integer arrays of length n . We say that x majorizes y and write $x \succ y$ if the elements of these arrays satisfy following conditions:

- (i) $x_1 \geq x_2 \geq \dots \geq x_n$ and $y_1 \geq y_2 \geq \dots \geq y_n$,
- (ii) $x_1 + x_2 + \dots + x_k \geq y_1 + y_2 + \dots + y_k$, for every $1 \leq k < n$,
- (iii) $x_1 + x_2 + \dots + x_n = y_1 + y_2 + \dots + y_n$.

Theorem 2.4. Let $p = (p_1, p_2, \dots, p_k)$ and $q = (q_1, q_1, \dots, q_k)$ be two arrays of length $k \geq 2$, such that $p \succ q$ and $n - 1 = p_1 + p_2 + \dots + p_k = q_1 + q_2 + \dots + q_k$. Then

$$ecc(S(p_1, p_2, \dots, p_k)) \geq ecc(S(q_1, q_2, \dots, q_k)), \quad (1)$$

with equality if and only if $p_i = q_i$ for all $1 \leq i \leq k$.

Proof. We will proceed by induction on the size of the array k . For $k = 2$, we can directly apply transformation from Theorem 2.1 on tree $S(q_1, q_2)$ several times, in order to get $S(p_1, p_2)$. Assume that the inequality (1) holds for all lengths less than k . If there exists an index $1 \leq m < k$ such that $p_1 + p_2 + \dots + p_m = q_1 + q_2 + \dots + q_m$, we can apply the induction hypothesis on two parts $S(q_1, q_2, \dots, q_m) \cup S(q_{m+1}, q_{m+2}, \dots, q_k)$ and get $S(p_1, p_2, \dots, p_m) \cup S(p_{m+1}, p_{m+2}, \dots, p_k)$. Otherwise, we have strict inequalities $p_1 + p_2 + \dots + p_m > q_1 + q_2 + \dots + q_m$ for all indices $1 \leq m < k$ and note that $q_k > p_k \geq 1$. We can transform tree $S(q_1, q_2, \dots, q_k)$ into $S(q_1 + 1, q_2, \dots, q_{k-1}, q_k - 1)$. The condition $p \succ q$ is preserved, and we can continue until the array q transforms into p , while at every step we increase the average eccentricity. \square

Corollary 2.5. Let $T = S(n_1, n_2, \dots, n_k)$ be a starlike tree with n vertices and k pendent paths. Then

$$ecc(B(n, k)) \geq ecc(T) \geq ecc(BS(n, k)).$$

The left equality holds if and only if $T \cong B(n, k)$ and the right equality holds if and only if $T \cong BS(n, k)$.

Definition 2.6. Let uv be a bridge of the graph G and let H and H' be the nontrivial components of G , such that $u \in H$ and $v \in H'$. Construct the graph G' by identifying the vertices u and v (and call this vertex also u') with additional pendent edge $u'v'$. We say that $G' = \sigma(G, uv)$ is a σ -transform of G .

Theorem 2.7. Let $G' = \sigma(G, uv)$ be a σ -transform of G . Then,

$$ecc(G') < ecc(G).$$

Proof. Let x be a vertex on the maximum distance from u in the graph H and let y be a vertex on the maximum distance from v in the graph H' . Without loss of generality assume that $d(u, x) \geq d(v, y)$. It can be easily seen that for arbitrary vertex $w \in G$ different from v and y , it holds that $\varepsilon_G(w) \geq \varepsilon_{G'}(w)$. For the vertex y we have $\varepsilon_G(y) = d(y, v) + 1 + d(u, x) > d(y, u') + d(u', x) = \varepsilon_{G'}(y)$. For the vertex v we have $\varepsilon_G(v) = 1 + d(u, x) = 1 + d(u', x) = \varepsilon_{G'}(v')$. Finally, we have strict inequality $\sum_{w \in G} \varepsilon(w) > \sum_{w \in G'} \varepsilon(w')$ and the result follows. \square

Using the previous theorem, one can easily prove that the star S_n is the unique tree with minimal value of the average eccentricity $ecc(S_n) = 2 - \frac{1}{n}$ among trees with n vertices. Furthermore, by repeated use of σ transformation, the graph S'_n (obtained from a star S_n with additional edge connecting two pendent vertices) has minimal value of the average eccentricity $ecc(S'_n) = 2 - \frac{1}{n}$ among unicyclic graphs with n vertices. This can be alternatively proven in the following way: let G be the extremal unicyclic graph with minimal value of the average eccentricity. If G contains the vertex of degree $n - 1$, then $G \cong S'_n$, otherwise there are no vertices of degree $n - 1$ and the eccentricity of all vertices is larger than 2, i.e. $ecc(G) > 2$.

3. Conjecture regarding the independence number

A set of vertices S in a graph G is independent if no neighbor of a vertex of S belongs to S . The independence number $\alpha = \alpha(G)$ is the maximum cardinality of any independent set of G .

Conjecture 3.1 (A.478-U). For every $n \geq 4$ it holds

$$\alpha(G) + ecc(G) \leq \begin{cases} \frac{3n^2 - 2n - 1}{4n} + \frac{n + 1}{2} & \text{if } n \text{ is odd} \\ \frac{3n^2 - 4n - 4}{4n} + \frac{n + 2}{2} & \text{if } n \text{ is even} \end{cases},$$

with equality if and only if $G \cong P_n$ for odd n and $G \cong B(n, 3)$ for even n .

Clearly, the sum $\alpha(G) + ecc(G)$ is maximized for some tree. Let T^* be an extremal tree and let $P = v_0 v_1 \dots v_d$ be a diametrical path of T^* . The maximum possible independence number of this tree is $\lceil \frac{d+1}{2} \rceil + n - d - 1$.

Lemma 3.2. *Let T be an arbitrary tree on n vertices, not isomorphic to a path P_n . Then there is a pendent vertex v such that for each $u \in T$ it holds*

$$\varepsilon_T(u) = \varepsilon_{T-v}(u).$$

Proof. Let d be a diameter of T , and let $P = v_0 v_1 \dots v_d$ be a diametrical path of the tree T . Since each tree has exactly one or two center vertices, these vertices belong to P . Therefore, for each vertex $u \in T$, the eccentricity of u is equal to $d(u, v_0)$ or $d(u, v_d)$. There exist a pendent vertex v different than v_0 and v_d , whose removal does not change the eccentricities of other vertices of T . This completes the proof. \square

By finding a pendent vertex from Lemma 3.2 and reattaching it to v_1 or v_{d-1} , we do not increase the value of $\alpha(G) + ecc(G)$, while keeping the diameter the same. It follows that the broom tree $B(n, n - d + 1)$ has the same value $\alpha(G) + ecc(G)$ as the extremal tree T^* . By direct calculation we have

$$\begin{aligned} ecc(B(n, \Delta)) + \alpha(B(n, \Delta)) &= \frac{1}{n} \left(\left\lfloor \frac{(n - \Delta + 2)(3(n - \Delta + 2) - 2)}{4} \right\rfloor + (n - \Delta + 1)(\Delta - 2) \right) \\ &\quad + \left\lfloor \frac{n - \Delta + 2}{2} \right\rfloor + (\Delta - 2) \\ &= \begin{cases} \frac{5n}{4} - \frac{\Delta(\Delta - 2)}{4n} - \frac{1}{2} & \text{if } n - \Delta \text{ is even} \\ \frac{5n}{4} - \frac{\Delta(\Delta - 2)}{4n} - \frac{1}{4n} & \text{if } n - \Delta \text{ is odd} \end{cases}. \end{aligned}$$

For $\Delta = 2$ and $\Delta = 3$, we have

$$\begin{aligned} ecc(B(n, 2)) + \alpha(B(n, 2)) &= \begin{cases} \frac{5n}{4} - \frac{1}{2} & \text{if } n \text{ is even} \\ \frac{5n}{4} - \frac{1}{4n} & \text{if } n \text{ is odd} \end{cases} \\ ecc(B(n, 3)) + \alpha(B(n, 3)) &= \begin{cases} \frac{5n}{4} - \frac{3}{4n} - \frac{1}{2} & \text{if } n \text{ is odd} \\ \frac{5n}{4} - \frac{3}{4n} - \frac{1}{4n} & \text{if } n \text{ is even} \end{cases} \end{aligned}$$

It follows that for $n \geq 3$ the maximum value of $ecc(G) + \alpha(G)$ is achieved uniquely for $B(n, 2) \cong P_n$ if n is odd, and for $B(n, 3)$ if n is even. This completes the proof of Conjecture 3.1.

Remark 3.3. Actually the extremal trees are double brooms $D(d, a, b)$, obtained from the path P_{d-1} by attaching a endvertices to one end and b endvertices to the other end of the path P_{d-1} . The double broom has diameter d , order $n = d + a + b + 1$ and the same average eccentricity as the broom $B(n, n - d + 1)$. The authors in [2] showed that the extremal graph with the maximum average eccentricity for given order n and radius r is any double broom of diameter $2r$.

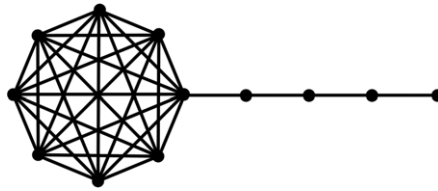
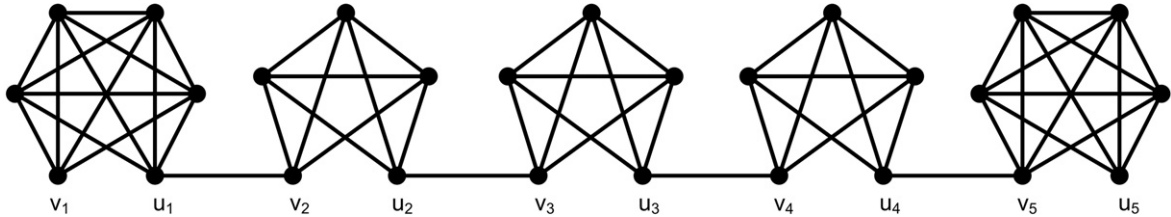
4. Conjecture regarding the clique number

The clique number of a graph G is the size of a maximal complete subgraph of G and it is denoted as $\omega(G)$.

The lollipop graph $LP(n, k)$ is obtained from a complete graph K_k and a path P_{n-k+1} , by joining one of the end vertices of P_{n-k+1} to one vertex of K_k (see Fig. 2). An asymptotically sharp upper bound for the eccentric connectivity index is derived independently in [32,33], with the extremal graph $LP(n, \lfloor n/3 \rfloor)$. Furthermore, it is shown that the eccentric connectivity index grows no faster than a cubic polynomial in the number of vertices.

Conjecture 4.1 (A.488-U). *For every $n \geq 4$ the maximum value of $ecc(G) \cdot \omega(G)$ is achieved for some lollipop graph.*

Let C be an arbitrary clique of size k . Since the removal of the edges potentially increases $ecc(G)$, we can assume that trees are attached to the vertices of C . Then by applying Theorem 2.1, we get the graph composed of the clique C and pendent paths attached to the vertices of C . Using the transformation similar to $G(p, q) \mapsto G(p + 1, q - 1)$ where we increase the length of the longest path attached to C , it follows that the extremal graph is exactly $LP(n, k)$. Since $ecc(LP(n, k)) = ecc(B(n, k))$, we have

Fig. 2. The lollipop graph $LP(12, 8)$.Fig. 3. The graph $PC(5, 4)$ with 27 vertices.

$$\begin{aligned} \text{ecc}(LP(n, k)) \cdot \omega(LP(n, k)) &= \frac{1}{n} \cdot \left((n - k - 2) \text{ecc}(P_{n-k-2}) + (n - k + 1)(k - 2) \right) \cdot k \\ &= \frac{k}{n} \cdot \left\lfloor \frac{-k^2 - 2k(-1 + n) + n(2 + 3n)}{4} \right\rfloor. \end{aligned}$$

Let $f(x) = x(-x^2 + 2x - 2xn + 2n + 3n^2)$ and $f'(x) = -3x^2 - 4x(n - 1) + n(3n + 2)$. By simple analysis for $x \in [1, n]$, it follows that the function $f(x)$ achieves the maximum value exactly for the larger root of the equation $f'(x) = 0$. Therefore, the maximum value of $\text{ecc}(G) \cdot \omega(G)$ is achieved for integers closest to

$$k^* = \frac{1}{3} \left(2 - 2n + \sqrt{4 - 2n + 13n^2} \right).$$

5. Conjecture regarding the minimum vertex degree

A matching in a graph G is a set of edges in which no two edges are adjacent. A vertex is matched (or saturated) if it is incident to an edge in the matching; otherwise the vertex is unmatched. A perfect matching (or 1-factor) is a matching which matches all vertices of the graph.

Conjecture 5.1 (A.100-U). For every $n \geq 4$ it holds

$$\delta(G) \cdot \text{ecc}(G) \leq \begin{cases} 2n - 2 & \text{if } n \text{ is even} \\ (n - 2) \left(2 - \frac{1}{2} \right) & \text{if } n \text{ is odd} \end{cases},$$

with equality if and only if $G \cong K_n \setminus M$, where M is a perfect matching if n is even, or a perfect matching on $n - 1$ vertices with an additional edge between the non-saturated vertex and another vertex if n is odd.

Let $K_n \setminus \{uv\}$ be the graph obtained from a complete graph K_n by deleting the edge uv . Define the almost-path-clique graph $PC(k, \delta)$ from a path P_k by replacing each vertex of degree 2 by the graph $K_{\delta+1} \setminus \{u_i v_i\}$, $i = 2, 3, \dots, k - 1$ and replacing pendent vertices by the graphs $K_{\delta+2} \setminus \{u_1 v_1\}$ and $K_{\delta+2} \setminus \{u_k v_k\}$. Furthermore, for each $i = 1, 2, \dots, k - 1$ the vertices u_i and v_{i+1} are adjacent (see Fig. 3).

The graph $PC(k, \delta)$ has $n = k(\delta + 1) + 2$ vertices and minimum vertex degree δ . Assume that k is an even number. For each $i = 1, 2, \dots, \frac{k}{2}$, we have the following contributions of the vertices in $K_{\delta+1} \setminus \{u_i v_i\}$:

- the vertex u_i has eccentricity $\frac{3k}{2} + 3 \left(\frac{k}{2} - i \right) = 3k - 3i$,
- the vertex v_i has eccentricity $\frac{3k}{2} + 2 + 3 \left(\frac{k}{2} - i \right) = 3k - 3i + 2$,
- the remaining $\delta - 1$ or δ vertices have eccentricity $\frac{3k}{2} + 1 + 3 \left(\frac{k}{2} - i \right) = 3k - 3i + 1$.

Finally, the average eccentricity of the graph $PC(k, \delta)$ is equal to

$$\begin{aligned} ecc(PC(k, \delta)) &= \frac{2}{n} \cdot \left(3k - 2 + \sum_{i=1}^{k/2} (3k - 3i) + (3k - 3i + 2) + (\delta - 1)(3k - 3i + 1) \right) \\ &= \frac{1}{k(\delta + 1) + 2} \cdot \left(\frac{9\delta k^2}{4} + \frac{9k^2}{4} + \frac{11k}{2} - \frac{\delta k}{2} - 4 \right) \\ &= \frac{9k}{4} - \frac{1}{2} + \frac{3(k - 2)}{2(k\delta + k + 2)}. \end{aligned}$$

The product of the average eccentricity and the minimum vertex degree is equal to

$$ecc(PC(k, \delta)) \cdot \delta(PC(k, \delta)) = \frac{9k\delta}{4} - \frac{\delta}{2} + \frac{3\delta(k - 2)}{2(k\delta + k + 2)}.$$

For each $k \geq \delta \geq 10$ we have the following inequality

$$\frac{9k\delta}{4} - \frac{\delta}{2} > 2(k\delta + k + 2) - 4,$$

which is equivalent with

$$k\delta - 8k - 2\delta = k(\delta - 8) - 2\delta > 0.$$

This refutes [Conjecture 5.1](#), and one can easily construct similar counterexamples for odd k or n not of the form $k(\delta + 1) + 2$. Note that this construction is very similar to the one described in [2], but is derived independently.

6. Concluding remarks

In this paper we studied the mathematical properties of the average eccentricity $ecc(G)$ of a connected graph G , which is deeply connected with the eccentric connectivity index. We resolved or refuted five conjectures on the average eccentricity and other graph invariants — clique number, independence number and minimum vertex degree.

We conclude the paper by restating some other conjectures dealing with the average eccentricity. All conjectures were generated by AGX system [16] and we also verified them on the set of all graphs with ≤ 10 vertices and trees with ≤ 20 vertices (with the help of Nauty [34] for the generation of non-isomorphic graphs).

The Randić index of a graph G is defined as

$$Ra(G) = \sum_{uv \in E} \frac{1}{\sqrt{\deg(v) \cdot \deg(u)}}.$$

Conjecture 6.1 (A.462-L). For every $n \geq 4$ it holds

$$Ra(G) + ecc(G) \geq \sqrt{n - 1} + 2 - \frac{1}{n},$$

with equality if and only if $G \cong S_n$.

Conjecture 6.2 (A.464-L). For every $n \geq 4$ it holds

$$Ra(G) \cdot ecc(G) \geq \begin{cases} \frac{n}{2} & \text{if } n \leq 13 \\ \sqrt{n - 1} \cdot \left(2 - \frac{1}{n} \right) & \text{if } n > 13 \end{cases},$$

with equality if and only if $G \cong K_n$ for $n \leq 13$ or $G \cong S_n$ for $n > 13$.

Conjecture 6.3 (A.458-L). For every $n \geq 4$ it holds

$$\lambda(G) + ecc(G) \geq \sqrt{n - 1} + \left(2 - \frac{1}{n} \right),$$

with equality if and only if $G \cong S_n$, where $\lambda(G)$ is the largest eigenvalue of the adjacency matrix of G .

Conjecture 6.4 (A.460-L). For every $n \geq 4$ it holds

$$\lambda(G) \cdot ecc(G) \geq \sqrt{n - 1} \cdot \left(2 - \frac{1}{n} \right),$$

with equality if and only if $G \cong S_n$.

Conjecture 6.5 (A.479-U). For every $n \geq 4$ the maximum value of $\text{ecc}(G)/\alpha(G)$ is achieved for some graph G composed of two cliques linked by a path.

Conjecture 6.6 (A.492-U). For every $n \geq 4$ the maximum value of $\text{ecc}(G) \cdot \chi(G)$ is achieved for some lollipop graph, where $\chi(G)$ denotes the chromatic number of G .

A dominating set of a graph G is a subset D of V such that every vertex not in D is joined to at least one member of D by some edge. The domination number $\gamma(G)$ is the number of vertices in a smallest dominating set for G [35].

Conjecture 6.7 (A.464-L). For every $n \geq 4$ it holds

$$\gamma(G) + \text{ecc}(G) \leq \begin{cases} \left\lfloor \frac{n+1}{3} \right\rfloor + \frac{(3n+1)n}{4(n-1)} & \text{if } n \text{ is odd and } n \not\equiv 1 \pmod{3} \\ \left\lfloor \frac{n+1}{3} \right\rfloor + \frac{3n-2}{4} & \text{if } n \text{ is even and } n \not\equiv 1 \pmod{3} \\ \frac{13n-16}{12} - \frac{3}{4n} & \text{if } n \text{ is odd and } n \equiv 1 \pmod{3} \\ \frac{13n-16}{12} - \frac{1}{n} & \text{if } n \text{ is even and } n \equiv 1 \pmod{3} \end{cases},$$

with equality if and only if $G \cong P_n$ for $n \not\equiv 1 \pmod{3}$ or G is a tree with $D = n-2$ and $\gamma = \left\lfloor \frac{n+1}{3} \right\rfloor$ for $n \equiv 1 \pmod{3}$.

We tested this conjecture and derived the following corrected version

Conjecture 6.8 (A.464-L). For every $n \geq 4$ it holds

$$\gamma(G) + \text{ecc}(G) \leq \begin{cases} \left\lceil \frac{n}{3} \right\rceil + \frac{1}{n} \left[\frac{3}{4}n^2 - \frac{1}{2}n \right] & \text{if } n \not\equiv 0 \pmod{3} \\ \frac{n}{3} + 2 - \frac{3}{n} + \frac{1}{n} \left[\frac{3}{4}(n-1)^2 - \frac{1}{2}(n-1) \right] & \text{if } n \equiv 0 \pmod{3} \end{cases},$$

with equality if and only if $G \cong P_n$ for $n \not\equiv 0 \pmod{3}$ or $G \cong D_n$ for $n \equiv 0 \pmod{3}$, where $D_n \cong S(n-4, 2, 1)$ is a tree obtained from a path $P_{n-1} = v_1 v_2 \dots v_{n-1}$ by attaching a pendent vertex to v_3 .

Similarly as for the independence number, the extremal graphs are trees. The domination number of a path P_n is $\left\lceil \frac{n}{3} \right\rceil$, and since the path has maximum average eccentricity in order to prove the conjecture one has to consider trees with $\left\lceil \frac{n}{3} \right\rceil < \gamma \leq \left\lfloor \frac{n}{2} \right\rfloor$.

It would be also interesting to determine extremal regular (cubic) graphs with respect to the average eccentricity, or to study some other derivative indices (such as eccentric distance sum [36], or augmented and super augmented eccentric connectivity indices [37]).

Acknowledgments

This work was supported by Research Grant 144007 of Serbian Ministry of Science and Technological Development. I am grateful to the anonymous referees for their remarks that helped to improve the article and I am indebted to Zhibin Du for several useful suggestions while preparing the article.

References

- [1] F. Buckley, F. Harary, Distance in Graphs, Addison-Wesley, Redwood City, California, 1990.
- [2] P. Dankelmann, W. Goddard, C.S. Swart, The average eccentricity of a graph and its subgraphs, Util. Math. 65 (2004) 41–51.
- [3] P. Dankelmann, R. Entringer, Average distance, minimum distance, and spanning trees, J. Graph Theory 33 (2000) 1–13.
- [4] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin, 1986.
- [5] A. Ilić, S. Klavžar, M. Milanović, On distance balanced graphs, Electron. J. Combin. 31 (2010) 733–737.
- [6] M.K. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, S.G. Wagner, Some new results on distance-based graph invariants, Electron. J. Combin. 30 (2009) 1149–1163.
- [7] A.A. Dobrynin, R.C. Entringer, I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math. 66 (2001) 211–249.
- [8] 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.
- [9] S. Gupta, M. Singh, A.K. Madan, Application of graph theory: relationship of eccentric connectivity index and Wiener's index with anti-inflammatory activity, J. Math. Anal. Appl. 266 (2002) 259–268.
- [10] V. Kumar, S. Sardana, A.K. Madan, Predicting anti-HIV activity of 2, 3-diaryl-1, 3 thiazolidin-4-ones: computational approach using reformed eccentric connectivity index, J. Mol. Model. 10 (2004) 399–407.
- [11] S. Sardana, A.K. Madan, Predicting anti-HIV activity of TIBO derivatives: a computational approach using a novel topological descriptor, J. Mol. Model. 8 (2002) 258–265.

- [12] A. Ilić, I. Gutman, Eccentric connectivity index of chemical trees, *MATCH Commun. Math. Comput. Chem.* 65 (2011) 731–744.
- [13] B. Zhou, Z. Du, On eccentric connectivity index, *MATCH Commun. Math. Comput. Chem.* 63 (2010) 181–198.
- [14] T. Došlić, M. Saheli, Eccentric connectivity index of composite graphs, 2009, manuscript.
- [15] A. Ilić, Eccentric connectivity index, in: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications II*, in: *Mathematical Chemistry Monographs*, vol. 9, University of Kragujevac, 2010.
- [16] M. Aouchiche, Comparaison automatisée d'invariants en théorie des graphes, Ph.D. Thesis, École Polytechnique de Montréal, February 2006.
- [17] M. Aouchiche, J.M. Bonnefoy, A. Fidahoussen, G. Caporossi, P. Hansen, L. Hiesse, J. Lacheré, A. Monhait, Variable neighborhood search for extremal graphs, 14. The AutoGraphiX 2 System, in: L. Liberti, N. Maculan (Eds.), *Global Optimization: From Theory to Implementation*, Springer, 2006, pp. 281–310.
- [18] G. Caporossi, P. Hansen, Variable neighborhood search for extremal graphs. I. the AutoGraphiX system, *Discrete Math.* 212 (2000) 29–44.
- [19] P. Hansen, N. Mladenović, Variable neighborhood search: principles and applications, *Eur. J. Oper. Res.* 130 (2001) 449–467.
- [20] P. Hansen, N. Mladenović, J.A. Moreno Pérez, Variable neighborhood search: algorithms and applications, *Annals Oper. Res.* 175 (2010) 367–407.
- [21] M. Aouchiche, P. Hansen, Automated results and conjectures on average distance in graphs, in: *Graph Theory in Paris*, in: *Trends Math.*, vol. VI, 2007, pp. 21–36.
- [22] M. Aouchiche, G. Brinkmann, P. Hansen, Variable neighborhood search for extremal graphs. 21. Conjectures and results about the independence number, *Discrete Appl. Math.* 156 (2008) 2530–2542.
- [23] M. Aouchiche, P. Hansen, Nordhaus–Gaddum relations for proximity and remoteness in graphs, *Comput. Math. Appl.* 59 (2010) 2827–2835.
- [24] M. Aouchiche, P. Hansen, A survey of automated conjectures in spectral graph theory, *Linear Algebra Appl.* 432 (2010) 2293–2322.
- [25] G. Caporossi, I. Gutman, P. Hansen, L. Pavlović, Graphs with maximum connectivity index, *Comput. Biol. Chem.* 27 (2003) 85–90.
- [26] P. Hansen, D. Vukičević, Variable neighborhood search for extremal graphs. 23. on the Randić index and the chromatic number, *Discrete Math.* 309 (2009) 4228–4234.
- [27] J. Sedlar, D. Vukičević, M. Aouchiche, P. Hansen, Variable Neighborhood Search for extremal graphs. 25. Products of connectivity and distance measures, G-2007-47, 2007, manuscript.
- [28] J. Sedlar, D. Vukičević, P. Hansen, Using size for bounding expressions of graph invariants, G-2007-100, 2007, manuscript.
- [29] A. Ilić, D. Stevanović, The Estrada index of chemical trees, *J. Math. Chem.* 47 (2010) 305–314.
- [30] W. Lin, X. Guo, Ordering trees by their largest eigenvalues, *Linear Algebra Appl.* 418 (2006) 450–456.
- [31] D. Stevanović, A. Ilić, Distance spectral radius of trees with fixed maximum degree, *Electron. J. Linear Algebra* 20 (2010) 168–179.
- [32] T. Došlić, M. Saheli, D. Vukičević, Eccentric connectivity index: Extremal graphs and values, *Iranian J. Math. Chem.* 1 (2010) 45–56.
- [33] M.J. Morgan, S. Mukwambi, H.C. Swart, On the eccentric connectivity index of a graph, *Discrete Math.* 311 (2011) 1229–1234.
- [34] B. McKay, Nauty, <http://cs.anu.edu.au/~bdkm/nauty/>.
- [35] T.W. Haynes, S. Hedetniemi, P. Slater, *Fundamentals of Domination in Graphs*, Marcel Dekker, New York, 1998.
- [36] G. Yu, L. Feng, A. Ilić, On the eccentric distance sum of trees and unicyclic graphs, *J. Math. Anal. Appl.* 375 (2011) 99–107.
- [37] H. Dureja, S. Gupta, A.K. Madan, Predicting anti-HIV-1 activity of 6-arylbenzonitriles: computational approach using supraugmented eccentric connectivity topochemical indices, *J. Mol. Graph. Model.* 26 (2008) 1020–1029.