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Ordering graphs with large eccentricity-based topological indices

Yunfang Tang[1] and Xuli Qi[2,3*]

*Correspondence:
qixuli-1212@163.com
[2]School of Mathematics and Statistics, Central China Normal University, Wuhan, 430079, China
[3]Department of Mathematics and Statistics, Georgia State University, Atlanta, GA 30303, USA
Full list of author information is available at the end of the article

Abstract

For a connected graph, the first Zagreb eccentricity index ξ_1 is defined as the sum of the squares of the eccentricities of all vertices, and the second Zagreb eccentricity index ξ_2 is defined as the sum of the products of the eccentricities of pairs of adjacent vertices. In this paper, we mainly present a different and universal approach to determine the upper bounds respectively on the Zagreb eccentricity indices of trees, unicyclic graphs and bicyclic graphs, and characterize these corresponding extremal graphs, which extend the ordering results of trees, unicyclic graphs and bicyclic graphs in (Du et al. in Croat. Chem. Acta 85:359–362, 2012; Qi et al. in Discrete Appl. Math. 233:166–174, 2017; Li and Zhang in Appl. Math. Comput. 352:180–187, 2019). Specifically, we determine the n-vertex trees with the i-th largest indices ξ_1 and ξ_2 for i up to $\lfloor n/2+1 \rfloor$ compared with the first three largest results of ξ_1 and ξ_2 in (Du et al. in Croat. Chem. Acta 85:359–362, 2012), the n-vertex unicyclic graphs with respectively the i-th and the j-th largest indices ξ_1 and ξ_2 for i up to $\lfloor n/2-1 \rfloor$ and j up to $\lfloor 2n/5+1 \rfloor$ compared with respectively the first two and the first three largest results of ξ_1 and ξ_2 in (Qi et al. in Discrete Appl. Math. 233:166–174, 2017), and the n-vertex bicyclic graphs with respectively the i-th and the j-th largest indices ξ_1 and ξ_2 for i up to $\lfloor n/2-2 \rfloor$ and j up to $\lfloor 2n/15+1 \rfloor$ compared with the first two largest results of ξ_2 in (Li and Zhang in Appl. Math. Comput. 352:180–187, 2019), where $n \geq 6$. More importantly, we propose two kinds of index functions for the eccentricity-based topological indices, which can yield more general extremal results simultaneously for some classes of indices. As applications, we obtain and extend some ordering results about the average eccentricity of bicyclic graphs, and the eccentric connectivity index of trees, unicyclic graphs and bicyclic graphs.

Keywords: Zagreb eccentricity index; Tree; Unicyclic graph; Bicyclic graph; Eccentricity-based topological index; Index function

1 Introduction

Topological indices are numerical graph invariants that quantitatively characterize molecular structure, which are useful molecular descriptors that found considerable use in QSPR and QSAR studies [20, 21]. Several graph invariants based on vertex eccentricities have attracted much attention and have been subject to a large number of studies. We mainly study two kinds of eccentricity-based topological indices, that is, the first Zagreb eccentricity index and the second Zagreb eccentricity index, special cases of which have been studied due to their predictive capabilities for the physical and chemical properties of molecules.

All graphs considered in this paper are finite, simple, and connected. Let G be a graph with a vertex set $V(G)$ and an edge set $E(G)$. For $u \in V(G)$, $e_G(u)$ denotes the eccentricity of u in G, which is equal to the largest distance from u to other vertices of G.

The first Zagreb eccentricity index of G is defined as

$$\xi_1(G) = \sum_{u \in V(G)} e_G^2(u),$$

while the second Zagreb eccentricity index of G is defined as

$$\xi_2(G) = \sum_{uv \in E(G)} e_G(u)e_G(v).$$

These two types of Zagreb eccentricity indices were introduced by Vukičević and Graovac [22]. Some mathematical and computational properties of the Zagreb eccentricity indices have been obtained in [4, 6, 12, 13, 15, 16, 24]. Du et al. [6] determined the n-vertex trees with maximum, second-maximum, and third-maximum Zagreb eccentricity indices. Qi and Du [15] determined the trees with minimum Zagreb eccentricity indices when domination number, maximum degree, and bipartition size are respectively given, and they discussed the trees with maximum Zagreb eccentricity indices when domination number is given. Qi et al. [16] determined the n-vertex unicyclic graphs with maximum, second-maximum eccentricity index ξ_1, and maximum, second-maximum, and third-maximum eccentricity index ξ_2. Li and Zhang [12] determined the n-vertex bicyclic graphs with maximum and second-maximum eccentricity index ξ_2.

For a connected graph, the first Zagreb eccentricity index ξ_1 is defined as the sum of the squares of the eccentricities of all vertices, and the second Zagreb eccentricity index ξ_2 is defined as the sum of the products of the eccentricities of pairs of adjacent vertices. In this paper, we mainly present a different and universal approach to determine the upper bounds respectively on the Zagreb eccentricity indices of trees, unicyclic graphs and bicyclic graphs, and characterize these corresponding extremal graphs, which extend the ordering results of trees, unicyclic graphs, and bicyclic graphs in [6, 12, 16]. Specifically, we determine the n-vertex trees with the i-th largest indices ξ_1 and ξ_2 for i up to $\lfloor n/2+1 \rfloor$ compared with the first three largest results of ξ_1 and ξ_2 in [6], the n-vertex unicyclic graphs with respectively the i-th and the j-th largest indices ξ_1 and ξ_2 for i up to $\lfloor n/2-1 \rfloor$ and j up to $\lfloor 2n/5+1 \rfloor$ compared with respectively the first two and the first three largest results of ξ_1 and ξ_2 in [16], and the n-vertex bicyclic graphs with respectively the i-th and the j-th largest indices ξ_1 and ξ_2 for i up to $\lfloor n/2-2 \rfloor$ and j up to $\lfloor 2n/15+1 \rfloor$ compared with the first two largest results of ξ_2 in [12], where $n \geq 6$. More importantly, we propose two kinds of index functions for the eccentricity-based topological indices, which can yield more general extremal results simultaneously for some classes of indices. As applications, we obtain and extend some ordering results about the average eccentricity of bicyclic graphs and the eccentric connectivity index of trees, unicyclic graphs and bicyclic graphs.

2 Preliminaries

Let n_0 and d_0 be positive integers. Let $\mathbf{T}_{n_{\geq n_0}}$ (res. $\mathbf{U}_{n_{\geq n_0}}$, $\mathbf{B}_{n_{\geq n_0}}$) be the set of n-vertex trees (res. unicyclic graphs, bicyclic graphs), where $n \geq n_0$. Let $\mathbf{T}(n_{\geq n_0}, d_{\leq d_0})$ (res. $\mathbf{U}(n_{\geq n_0}, d_{\leq d_0})$,

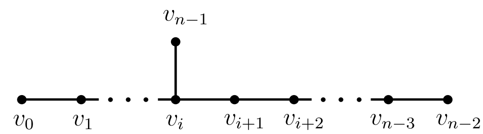

Figure 1 The graph T_n^i

$\mathbf{B}(n_{\geq n_0}, d_{\leq d_0})$) be the set of n-vertex trees (res. unicyclic graphs, bicyclic graphs) with the diameter d, where $n \geq n_0$ and $d \leq d_0$.

Let P_n be the path on n vertices. For $2 \leq d \leq n-1$, let $T^{(n,d)} = \{T_{n,d}^a : 1 \leq a \leq \lfloor (n+1-d)/2 \rfloor\}$, where $T_{n,d}^a$ is the n-vertex tree obtained by attaching a and $n+1-a-d$ pendent vertices respectively to the two end vertices of the path P_{d-1}. For $n \geq 4$, let T_n^i be the tree formed by attaching a pendent vertex v_{n-1} to a vertex v_i of the path $P_{n-1} = v_0 v_1 \cdots v_{n-2}$, where $1 \leq i \leq \lfloor \frac{n-2}{2} \rfloor$ (see Fig. 1). In particular, $T_n^0 = P_n$.

The following observation is obvious.

Observation 2.1 *If G is a connected graph such that $G-e$ is also connected for $e \in E(G)$, then $e_G(u) \leq e_{G-e}(u)$ for $u \in V(G)$, and thus $\xi_1(G) \leq \xi_1(G-e)$.*

Lemma 2.2 ([6]) *Let $G \in \mathbf{T}(n_{\geq 3}, d_{\leq n-1})$. Then*

$$\xi_1(G) \leq f_1(n,d), \qquad \xi_2(G) \leq f_2(n,d)$$

with equality if and only if $G \in T^{(n,d)}$, where

$$f_1(n,d) = \begin{cases} d^2 n - \frac{5d^3-2d}{12} & \text{if } d \text{ is even,} \\ d^2 n - \frac{5d^3-5d}{12} & \text{if } d \text{ is odd,} \end{cases}$$

$$f_2(n,d) = \begin{cases} d(d-1)n - \frac{5d^3-8d}{12} & \text{if } d \text{ is even,} \\ d(d-1)n - \frac{5d^3-11d-6}{12} & \text{if } d \text{ is odd,} \end{cases}$$

and $f_1(n,d)$ and $f_2(n,d)$ are increasing for $2 \leq d \leq n-1$.

For $n \geq 3$ and $0 \leq i \leq \lfloor \frac{n-3}{2} \rfloor$, let $P_{n,3}(i)$ be the n-vertex unicyclic graph formed by attaching two pendent paths with i and $n-3-i$ vertices respectively to the two vertices of a triangle (see Fig. 2). For $n \geq 4$ and $0 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$, let $P_{n,4}(i)$ be the n-vertex unicyclic graph formed by attaching two pendent paths with i and $n-4-i$ vertices respectively to the two non-adjacent vertices of a quadrangle (see Fig. 3). For $n \geq 4$ and $0 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$, let $B_n(i)$ be the n-vertex bicyclic graph formed by adding an edge between v_{n-1} and v_{i+1} in $P_{n,4}(i)$ (see Fig. 4).

Lemma 2.3 (1) *For $1 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$, $\xi_1(B_n(i-1)) = \xi_1(P_{n,4}(i-1)) = \xi_1(P_{n,3}(i)) = \xi_1(T_n^{i+1})$ and $\xi_1(P_{n,3}(0)) = \xi_1(T_n^1)$;*

(2) *For $1 \leq i \leq \lfloor \frac{n-6}{2} \rfloor$, $\xi_1(P_{n,3}(i-1)) > \xi_1(P_{n,3}(i)) > \xi_1(P_{n,3}(i+1))$, $\xi_1(P_{n,4}(i-1)) > \xi_1(P_{n,4}(i))$, and $\xi_1(B_n(i-1)) > \xi_1(B_n(i))$;*

(3) *For $1 \leq i \leq \lfloor \frac{n-6}{2} \rfloor$, $\xi_2(P_{n,3}(i-1)) > \xi_2(P_{n,4}(i-1)) > \xi_2(P_{n,3}(i)) > \xi_2(P_{n,4}(i)) > \xi_2(P_{n,3}(i+1))$ and $\xi_2(B_n(i-1)) > \xi_2(B_n(i))$.*

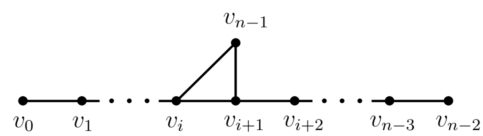

Figure 2 The graph $P_{n,3}(i)$

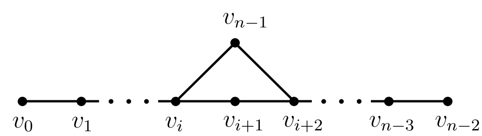

Figure 3 The graph $P_{n,4}(i)$

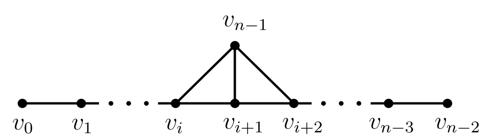

Figure 4 The graph $B_n(i)$

Proof Note that $P_{n,3}(i)$ (res. $P_{n,4}(i-1)$, $B_n(i-1)$) with $0 \le i \le \lfloor \frac{n-4}{2} \rfloor$ (res. $1 \le i \le \lfloor \frac{n-4}{2} \rfloor$) can be obtained from T_n^{i+1} by adding an edge $v_i v_{n-1}$ (res. $v_i v_{n-1}$, two edges $v_i v_{n-1}$ and $v_{i-1} v_{n-1}$). From the above fact we may easily find that vertices in $P_{n,3}(i)$, $P_{n,4}(i-1)$, $B_n(i-1)$, and T_n^{i+1} with the same label have equal eccentricity for $1 \le i \le \lfloor \frac{n-4}{2} \rfloor$, and so do the vertices in $P_{n,3}(0)$ and T_n^1. Thus result (1) follows.

Note that $e_{T_n^{i+1}}(v_j) = e_{T_n^i}(v_j)$ for $0 \le j \le n-2$ and $e_{T_n^i}(v_{n-1}) = n-1-i$ for $0 \le i \le \lfloor \frac{n-2}{2} \rfloor$. Then, for $0 \le i \le \lfloor \frac{n-4}{2} \rfloor$, we have $\xi_1(T_n^{i+1}) < \xi_1(T_n^i)$ and $\xi_2(T_n^{i+1}) < \xi_2(T_n^i)$. Thus, combining result (1), we have result (2) directly.

For $0 \le i \le \lfloor \frac{n-4}{2} \rfloor$,

$$\xi_2\bigl(P_{n,3}(i)\bigr) = \xi_2\bigl(T_n^{i+1}\bigr) + (n-i-2)^2.$$

For $1 \le i \le \lfloor \frac{n-4}{2} \rfloor$,

$$\xi_2\bigl(P_{n,4}(i-1)\bigr) = \xi_2\bigl(T_n^{i+1}\bigr) + (n-i-1)(n-i-2).$$

For $0 \le i \le \lfloor \frac{n-6}{2} \rfloor$,

$$\xi_2\bigl(B_n(i)\bigr) = \xi_2\bigl(T_n^{i+2}\bigr) + (n-3-i)(2n-5-2i).$$

Then, combining the fact that $\xi_2(T_n^{i+1}) < \xi_2(T_n^i)$, result (3) follows easily. □

3 Main results of Zagreb eccentricity indices

3.1 Ordering trees with large Zagreb eccentricity indices

Theorem 3.1 *Among the graphs in $\mathbf{T}_{n\ge 3}$, P_n for $n \ge 3$ is the unique graph with the largest eccentricity indices ξ_1 and ξ_2, and T_n^i for $n \ge 4$ and $1 \le i \le \lfloor n/2-1 \rfloor$ is the unique graph* *with the* $(i+1)$*th largest eccentricity indices* ξ_1 *and* ξ_2, *where*

$$\xi_1(P_n) = \begin{cases} \frac{7n^3-9n^2+2n}{12} & \text{if } n \text{ is even,} \\ \frac{7n^3-9n^2-n+3}{12} & \text{if } n \text{ is odd,} \end{cases}$$

$$\xi_2(P_n) = \begin{cases} \frac{7n^3-21n^2+20n}{12} & \text{if } n \text{ is even,} \\ \frac{7n^3-21n^2+17n-3}{12} & \text{if } n \text{ is odd,} \end{cases}$$

$$\xi_1(T_n^i) = \begin{cases} \frac{7n^3-30n^2+38n-12}{12} + (n-i-1)^2 & \text{if } n \text{ is even,} \\ \frac{7n^3-30n^2+41n-18}{12} + (n-i-1)^2 & \text{if } n \text{ is odd,} \end{cases}$$

$$\xi_2(T_n^i) = \begin{cases} \frac{7n^3-42n^2+80n-48}{12} + (n-i-1)(n-i-2) & \text{if } n \text{ is even,} \\ \frac{7n^3-42n^2+83n-48}{12} + (n-i-1)(n-i-2) & \text{if } n \text{ is odd.} \end{cases}$$

Proof Let $T \in \mathbf{T}(n_{\geq 3}, d_{\leq n-1})$. If $n = 3$ or $n = 4$, then the result follows easily. Suppose that $n \geq 5$. Note that $f_1(n,d)$ and $f_2(n,d)$ are increasing for $2 \leq d \leq n-1$ by Lemma 2.2. Then $\xi_k(T) \leq f_k(n,d) \leq f_k(n,n-3) < f_k(n,n-2) < f_k(n,n-1)$ for any $T \in \mathbf{T}(n_{\geq 5}, d_{\leq n-3})$, where $k = 1,2$. Note that $T^{(n,n-1)} = \{P_n\}$ and $T^{(n,n-2)} = \{T_n^1\}$. Then P_n and T_n^1 for $n \geq 5$ are respectively the unique n-vertex trees with the largest and the second largest eccentricity indices ξ_1 and ξ_2.

Suppose that $2 \leq i \leq \lfloor n/2 - 1 \rfloor$. Among the graphs in $\mathbf{T}_{n_{\geq 3}}$, the $(i+1)$th largest eccentricity indices ξ_1 and ξ_2 are achieved by the trees in $\mathbf{T}(n_{\geq 5}, d_{=n-2}) \setminus \{T_n^j : 1 \leq j \leq i-1\}$ or in $T^{(n,n-3)}$ with the largest eccentricity indices ξ_1 and ξ_2.

Let $T_1 \in \mathbf{T}(n_{\geq 5}, d_{=n-2}) \setminus \{T_n^j : 1 \leq j \leq i-1\}$. Since $\xi_1(T_n^i) < \xi_1(T_n^{i-1})$ and $\xi_2(T_n^i) < \xi_2(T_n^{i-1})$, we have $\xi_1(T_1) \leq \xi_1(T_n^i)$ and $\xi_2(T_1) \leq \xi_2(T_n^i)$, where the equalities hold if and only if $T_1 = T_n^i$. For $T_2 \in T^{(n,n-3)}$, by direct calculation, we have

$$\begin{aligned} \xi_1\big(T_n^{\lfloor n/2-1 \rfloor}\big) - \xi_1(T_2) &= \begin{cases} 5n-11 & \text{if } n \text{ is even,} \\ 6n-12 & \text{if } n \text{ is odd,} \end{cases} \\ &> 0, \\ \xi_2\big(T_n^{\lfloor n/2-1 \rfloor}\big) - \xi_2(T_2) &= \begin{cases} \frac{9n}{2} - 13 & \text{if } n \text{ is even,} \\ \frac{11n-27}{2} & \text{if } n \text{ is odd,} \end{cases} \\ &> 0. \end{aligned}$$

Thus T_n^i is the unique n-vertex tree with the $(i+1)$th largest eccentricity indices ξ_1 and ξ_2, where $1 \leq i \leq \lfloor n/2 - 1 \rfloor$. The result follows. □

In fact, from the proof of Theorem 3.1, we have the following corollary easily.

Corollary 3.2 *Among the graphs in* $\mathbf{T}_{n_{\geq 3}}$, $T^{(n,n-3)}$ *is the set of graphs with the* $\lfloor n/2 + 1 \rfloor$*th largest eccentricity indices* ξ_1 *and* ξ_2, *and* $f_k(n,n-3) < \xi_k(T_n^{\lfloor \frac{n-2}{2} \rfloor})$ *for* $k = 1,2$.

3.2 Ordering unicyclic graphs with large Zagreb eccentricity indices

Lemma 3.3 *Let* $G \in \mathbf{U}(n_{\geq 6}, d_{=n-2}) \setminus (\{P_{n,3}(i) : 0 \leq i \leq \lfloor \frac{n-4}{2} \rfloor\} \cup \{P_{n,4}(i) : 0 \leq i \leq \lfloor \frac{n-6}{2} \rfloor\})$. *Then* $\xi_k(G) < \xi_k(P_{n,3}(\lfloor \frac{n-4}{2} \rfloor))$ *for* $k = 1, 2$.

Proof If n is even, then $G = P_{n,4}(\frac{n-4}{2})$. If n is odd, then $G \in \{P_{n,3}(\frac{n-3}{2}), P_{n,4}(\frac{n-5}{2})\}$. By direct computation, we have

$$\xi_1\left(P_{n,4}\left(\left\lfloor \frac{n-4}{2} \right\rfloor\right)\right) - \xi_1\left(P_{n,3}\left(\left\lfloor \frac{n-4}{2} \right\rfloor\right)\right) = \left\lceil \frac{n-2}{2} \right\rceil^2 - \left\lceil \frac{n}{2} \right\rceil^2 < 0,$$

$$\xi_2\left(P_{n,4}\left(\left\lfloor \frac{n-4}{2} \right\rfloor\right)\right) - \xi_2\left(P_{n,3}\left(\left\lfloor \frac{n-4}{2} \right\rfloor\right)\right) = \begin{cases} -\frac{n}{2} & \text{if } n \text{ is even,} \\ -n & \text{if } n \text{ is odd,} \end{cases}$$
$$< 0,$$

and for odd n,

$$\xi_1\left(P_{n,3}\left(\frac{n-3}{2}\right)\right) - \xi_1\left(P_{n,3}\left(\frac{n-5}{2}\right)\right) = \left(\frac{n-1}{2}\right)^2 - \left(\frac{n+1}{2}\right)^2 < 0,$$

$$\xi_2\left(P_{n,3}\left(\frac{n-3}{2}\right)\right) - \xi_2\left(P_{n,3}\left(\frac{n-5}{2}\right)\right) = \frac{-3n+1}{2} < 0.$$

Thus the result follows. □

Theorem 3.4 *Among the graphs in* $\mathbf{U}_{n_{\geq 6}}$, $P_{n,3}(0)$ *is the unique graph with the largest eccentricity index* ξ_1, *and* $P_{n,3}(i)$ *and* $P_{n,4}(i-1)$ *with* $1 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$ *are the graphs with the* $(i+1)$*th largest eccentricity index* ξ_1, *where*

$$\xi_1(P_{n,3}(0)) = \begin{cases} \frac{7n^3-30n^2+38n-12}{12} + (n-2)^2 & \text{if } n \text{ is even,} \\ \frac{7n^3-30n^2+41n-18}{12} + (n-2)^2 & \text{if } n \text{ is odd,} \end{cases}$$

$$\xi_1(P_{n,3}(i)) = \xi_1(P_{n,4}(i-1)) = \begin{cases} \frac{7n^3-30n^2+38n-12}{12} + (n-i-2)^2 & \text{if } n \text{ is even,} \\ \frac{7n^3-30n^2+41n-18}{12} + (n-i-2)^2 & \text{if } n \text{ is odd.} \end{cases}$$

Proof Let $G \in \mathbf{U}(n_{\geq 6}, d_{\leq n-2})$. From Lemmas 2.3(2) and 3.3, we only need to show that $\xi_1(G) < \xi_1(P_{n,3}(\lfloor \frac{n-4}{2} \rfloor))$ for $G \in \mathbf{U}(n_{\geq 6}, d_{\leq n-3})$.

It is easy to find that there exists an edge e on the cycle of G such that the diameter of $G - e$ is at most $n-3$. Note that $f_1(n, n-3) < \xi_1(T_n^{\lfloor \frac{n-2}{2} \rfloor})$ by Corollary 3.2. Then, by Observation 2.1 and Lemmas 2.2 and 2.3(1), we have

$$\xi_1(G) \leq \xi_1(G-e) \leq f_1(n, n-3) < \xi_1\left(T_n^{\lfloor \frac{n-2}{2} \rfloor}\right) = \xi_1\left(P_{n,3}\left(\left\lfloor \frac{n-4}{2} \right\rfloor\right)\right).$$

Thus we have the result. □

Combining Lemmas 2.3(3) and 3.3, we have the following proposition.

Proposition 3.5 *Among the graphs in* $\mathbf{U}(n_{\geq 6}, d_{=n-2})$, $P_{n,3}(i)$ *with* $0 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$ *is the unique graph with the* $(2i+1)$*th largest eccentricity index* ξ_2, *and* $P_{n,4}(i-1)$ *with* $1 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$ *is the unique graph with the* $(2i)$*th largest eccentricity index* ξ_2.

Theorem 3.6 *Among the graphs in* $\mathbf{U}_{n_{\geq 6}}$, $P_{n,3}(i)$ *with* $0 \leq i \leq \lfloor \frac{n}{5} \rfloor$ *is the unique graph with the* $(2i+1)$*th largest eccentricity index* ξ_2, *and* $P_{n,4}(i-1)$ *with* $1 \leq i \leq \lfloor \frac{n}{5} \rfloor$ *is the unique graph with the* $(2i)$*th largest eccentricity index* ξ_2, *where*

$$\xi_2\big(P_{n,3}(i)\big) = \begin{cases} \frac{7n^3-42n^2+80n-48}{12} + (2n-2i-5)(n-i-2) & \text{if } n \text{ is even}, \\ \frac{7n^3-42n^2+83n-48}{12} + (2n-2i-5)(n-i-2) & \text{if } n \text{ is odd}, \end{cases}$$

$$\xi_2\big(P_{n,4}(i-1)\big) = \begin{cases} \frac{7n^3-42n^2+80n-48}{12} + (2n-2i-4)(n-i-2) & \text{if } n \text{ is even}, \\ \frac{7n^3-42n^2+83n-48}{12} + (2n-2i-4)(n-i-2) & \text{if } n \text{ is odd}. \end{cases}$$

Proof Suppose that $G \in \mathbf{U}(n_{\geq 6}, d_{\leq n-2})$. By Proposition 3.5, we only need to show that $\xi_2(G) < \xi_2(P_{n,3}(\lfloor \frac{n}{5} \rfloor))$ for $G \in \mathbf{U}(n_{\geq 6}, d_{\leq n-3})$.

Note that there exists an edge e such that $G-e$ is a spanning tree with the diameter at most $n-3$ and the maximum eccentricities of the two vertices on the edge e are $n-3$ and $n-3$. Then, by Observation 2.1 and Lemma 2.2, we have

$$\xi_2(G) \leq \xi_2(G-e) + (n-3)(n-3) \leq f_2(n, n-3) + (n-3)(n-3).$$

Thus, by direct calculation, for $0 \leq i \leq \frac{n}{5}$, we have

$$\begin{aligned} \xi_2\big(P_{n,3}(i)\big) - \xi_2(G) &\geq \begin{cases} \frac{3n^2}{4} - (4i-2)n + 2i^2 + 9i - 12 & \text{if } n \text{ is even}, \\ \frac{3n^2}{4} - (4i-\frac{5}{2})n + 2i^2 + 9i - \frac{49}{4} & \text{if } n \text{ is odd}, \end{cases} \\ &\geq \begin{cases} \frac{3n^2}{100} + \frac{19n}{5} - 12 & \text{if } n \text{ is even}, \\ \frac{3n^2}{100} + \frac{43n}{10} - \frac{49}{4} & \text{if } n \text{ is odd}, \end{cases} \\ &> 0, \end{aligned}$$

and the result follows. □

3.3 Ordering bicyclic graphs with large Zagreb eccentricity indices

Lemma 3.7 *Let* $G \in \mathbf{B}(n_{\geq 6}, d_{=n-2}) \setminus \{B_n(i) : 0 \leq i \leq \lfloor \frac{n-6}{2} \rfloor\}$. *Then* $\xi_k(G) < \xi_k(B_n(\lfloor \frac{n-6}{2} \rfloor))$ *for* $k = 1, 2$.

Proof If n is even, then $G = B_n(\frac{n-4}{2})$. If n is odd, then $G = B_n(\frac{n-5}{2})$. By direct computation, we have

$$\xi_1\left(B_n\left(\left\lfloor \frac{n-4}{2} \right\rfloor\right)\right) - \xi_1\left(B_n\left(\left\lfloor \frac{n-6}{2} \right\rfloor\right)\right) = \left\lceil \frac{n-2}{2} \right\rceil^2 - \left\lceil \frac{n}{2} \right\rceil^2 < 0,$$

$$\xi_2\left(B_n\left(\left\lfloor \frac{n-4}{2} \right\rfloor\right)\right) - \xi_2\left(B_n\left(\left\lfloor \frac{n-6}{2} \right\rfloor\right)\right) = \begin{cases} -2n+1 & \text{if } n \text{ is even,} \\ -\frac{5n+1}{2} & \text{if } n \text{ is odd,} \end{cases}$$

$$< 0.$$

Thus the result follows. □

Theorem 3.8 *Among the graphs in* $\mathbf{B}_{n_{\geq 6}}$, $B_n(i)$ *with* $0 \leq i \leq \lfloor \frac{n-6}{2} \rfloor$ *is the unique graph with the* $(i+1)$*th largest eccentricity index* ξ_1, *where*

$$\xi_1\left(B_n(i)\right) = \begin{cases} \frac{7n^3-30n^2+38n-12}{12} + (n-i-3)^2 & \textit{if } n \textit{ is even,} \\ \frac{7n^3-30n^2+41n-18}{12} + (n-i-3)^2 & \textit{if } n \textit{ is odd.} \end{cases}$$

Proof Suppose that $G \in \mathbf{B}(n_{\geq 6}, d_{\leq n-2})$. From Lemmas 2.3(2) and 3.7, we only need to show that $\xi_1(G) < \xi_1(B_n(\lfloor \frac{n-6}{2} \rfloor))$ and $G \in \mathbf{B}(n_{\geq 6}, d_{\leq n-3})$.

It is easy to find that there exist two edges e_1 and e_2 on the cycle of G such that the diameter of $G - e_1 - e_2$ is at most $n-3$. Note that $f_1(n, n-3) < \xi_1(T_n^{\lfloor \frac{n-2}{2} \rfloor})$ by Corollary 3.2. Then, by Observation 2.1 and Lemmas 2.2 and 2.3(1), we have

$$\xi_1(G) \leq \xi_1(G - e_1 - e_2) \leq f_1(n, n-3) < \xi_1\left(T_n^{\lfloor \frac{n-2}{2} \rfloor}\right) = \xi_1\left(B_{n,2}\left(\left\lfloor \frac{n-6}{2} \right\rfloor\right)\right).$$

Thus the result follows. □

Combining Lemmas 2.3(3) and 3.3, we have the following proposition.

Proposition 3.9 *Among the graphs in* $\mathbf{B}(n_{\geq 6}, d_{=n-2})$, $B_n(i)$ *with* $0 \leq i \leq \lfloor \frac{n-6}{2} \rfloor$ *is the unique graph with the* $(i+1)$*th largest eccentricity index* ξ_2.

Theorem 3.10 *Among all the graphs in* $\mathbf{B}_{n_{\geq 6}}$, $B_n(i)$ *is the* $(i+1)$*th largest eccentricity index* ξ_2 *with* $0 \leq i \leq \lfloor \frac{2n}{15} \rfloor$, *where*

$$\xi_2\left(B_n(i)\right) = \begin{cases} \frac{7n^3-42n^2+80n-48}{12} + 3(n-i-3)^2 & \textit{if } n \textit{ is even,} \\ \frac{7n^3-42n^2+83n-48}{12} + 3(n-i-3)^2 & \textit{if } n \textit{ is odd.} \end{cases}$$

Proof Suppose that $G \in \mathbf{B}(n_{\geq 6}, d_{\leq n-2})$. Then, by Proposition 3.9, we only need to show that $\xi_2(G) < \xi_2(B_n(\lfloor \frac{2n}{15} \rfloor))$ for $G \in \mathbf{B}(n_{\geq 6}, d_{\leq n-3})$.

Note that there exist two edges e_1, e_2 on the cycle(s) such that $G - e_1 - e_2$ is a spanning tree with the diameter at most $n-3$, and all the vertices incident to the edges e_1, e_2 have eccentricities at most $n-3$. Then, by Observation 2.1 and Lemma 2.2, we have

$$\xi_2(G) \leq \xi_2(G - e_1 - e_2) + 2(n-3)^2 \leq f_2(n, n-3) + 2(n-3)^2.$$

Thus, for $0 \leq i \leq \frac{2n}{15}$, we have

$$\xi_2\left(B_n(i)\right) - \xi_2(G) \geq \begin{cases} \frac{3n^2}{4} - (6i+1)n + 3i^2 + 18i - 4 & \text{if } n \text{ is even,} \\ \frac{3n^2}{4} - (6i+\frac{1}{2})n + 3i^2 + 18i - \frac{17}{4} & \text{if } n \text{ is odd,} \end{cases}$$

$$\geq \begin{cases} \frac{n^2}{300} + \frac{7n}{5} - 4 & \text{if } n \text{ is even,} \\ \frac{n^2}{300} + \frac{19n}{10} - \frac{17}{4} & \text{if } n \text{ is odd,} \end{cases}$$

$$> 0,$$

and the result follows. □

4 Ordering graphs with large eccentricity-based topological indices

Most papers on this topic study just one topological index and find its extremal values (or perhaps several near-extreme values) over n-vertex trees or other simple classes. We propose studying such problems in terms of general properties of some index functions for the eccentricity-based topological indices. Requiring only the properties needed for the argument yields a more general extremal result simultaneously for a class of indices. In the following, we consider two kinds of index functions, that is, a vertex-weight index function and an edge-weight index function.

Definition 4.1 The *weight* $\omega(u)$ of a vertex u in a graph G is $e_G(u)$. Given a positive real-valued function t_v, the *vertex-weight index function* for a graph G is defined by $f(G; v) = \sum_{u\in V(G)} t_v(\omega(u))$.

The total eccentricity index of G, introduced by Farooq et al. [8], is defined as $\tau(G) = \sum_{u\in V(G)} e_G(u)$ using $t_v(\omega(u)) = \omega(u)$; the average eccentricity of G, introduced by Bukley et al. [1], is defined as $avec(G) = \frac{1}{n}\tau(G)$ using $t_v(\omega(u)) = \frac{1}{n}\omega(u)$. For more recent results on average eccentricity, see [2, 3, 5, 11].

The first Zagreb eccentricity index of G is defined as $\xi_1(G) = \sum_{u\in V(G)} e_G^2(u)$ using $t_v(\omega(u)) = \omega^2(u)$.

Note that those above indices have similar extremal values (or perhaps several near-extremal values) over n-vertex trees, unicyclic graphs, and bicyclic graphs. Tang and Zhou have determined similar extremal values of the average eccentricity over n-vertex trees [18] and unicyclic graphs [19]. Like the discussion of the first Zagreb eccentricity index, we also obtain a similar result about the average eccentricity of bicyclic graphs in the following Theorem 4.2, whose proof is omitted since we use a similar method.

Theorem 4.2 *Among the graphs in* $\mathbf{B}_{n_{\geq 6}}$, $B_n(i)$ *is the unique graph with the* $(i+1)$*th largest average eccentricity, equal to* $\frac{3(n-1)^2+2n-4i-11}{4n}$ *for even* n *and* $\frac{3(n-1)^2+2n-4i-10}{4n}$ *for odd* n*, where* $0 \leq i \leq \lfloor\frac{n}{2}\rfloor - 3$.

Definition 4.3 The *weight* $\omega(e)$ of an edge $e = uv$ in a graph G is $e_G(u)e_G(v)$, and the *weight* $\omega^*(e)$ of an edge $e = uv$ in a graph G is $e_G(u) + e_G(v)$. Given a positive real-valued function t_e, the *edge-weight index functions* for a graph G are defined by $f_1(G; e) = \sum_{e\in E(G)} t_e(\omega(e))$, $f_2(G; e) = \sum_{e\in E(G)} t_e(\omega^*(e))$, and $f_3(G; e) = \sum_{e\in E(G)} t_e(\omega(e), \omega^*(e))$, respectively.

The second Zagreb eccentricity index of G is defined as $\xi_2(G) = \sum_{uv\in E(G)} e_G(u)e_G(v)$ using $t_e(\omega(e)) = \omega(e)$. The eccentric connectivity index of G, introduced by Sharma et al. in [17], is defined as $\xi^c(G) = \sum_{v\in V(G)} e_G(v)d_G(v) = \sum_{uv\in E(G)}(e_G(u) + e_G(v))$ using $t_e(\omega^*(e)) = \omega^*(e)$, which is also called the third Zagreb eccentricity index by Ghorbani et al. [10]. For some recent results of the eccentric connectivity index, see [14, 23].

Like the discussion of the second Zagreb eccentricity index, we also obtain similar results about the eccentric connectivity index of trees, unicyclic graphs, and bicyclic graphs in the following propositions and theorems (omitting their proofs).

Theorem 4.4 *Among the graphs in $\mathbf{T}_{n\geq 3}$, P_n for $n \geq 3$ is the unique graph with the largest eccentricity connectivity index ξ^c, equal to $\frac{1}{2}(3n^2-6n+4)$ for even n and $\frac{1}{2}(3n^2-6n+3)$ for odd n, and T_n^i is the unique graph with the $(i+1)$th largest eccentricity connectivity index ξ^c, equal to $\frac{1}{2}(3n^2-8n-4i+6)$ for even n and $\frac{1}{2}(3n^2-8n-4i+7)$ for odd n, where $1 \leq i \leq \lfloor n/2-1 \rfloor$.*

Proposition 4.5 *Among the graphs in $\mathbf{U}(n_{\geq 6}, d_{=n-2})$, $P_{n,3}(i)$ with $0 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$ is the unique graph with the $(2i+1)$th largest eccentricity connectivity index ξ^c, and $P_{n,4}(i-1)$ with $1 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$ is the unique graph with the $(2i)$th largest eccentricity index ξ^c.*

Theorem 4.6 *Among the graphs in $\mathbf{U}_{n\geq 6}$, $P_{n,3}(i)$ with $0 \leq i \leq \lfloor (n+3)/4 \rfloor$ is the unique graph with the $(2i+1)$th largest eccentricity connectivity index ξ^c, equal to $\frac{1}{2}(3n^2-4n-8i-6)$ for even n and $\frac{1}{2}(3n^2-4n-8i-5)$ for odd n, and $P_{n,4}(i-1)$ with $1 \leq i \leq \lfloor (n+3)/4 \rfloor$ is the unique graph with the $(2i)$th largest eccentricity connectivity index ξ^c, equal to $\frac{1}{2}(3n^2-4n-8i-4)$ for even n and $\frac{1}{2}(3n^2-4n-8i-3)$ for odd n.*

Proposition 4.7 *Among the graphs in $\mathbf{B}(n_{\geq 6}, d_{=n-2})$, $B_n(i)$ with $0 \leq i \leq \lfloor \frac{n-6}{2} \rfloor$ is the unique graph with the $(i+1)$th largest eccentricity connectivity index ξ^c.*

Theorem 4.8 *Among all the graphs in $\mathbf{B}_{n\geq 6}$, $B_n(i)$ is the $(i+1)$ th largest eccentricity connectivity index ξ^c, equal to $\frac{1}{2}(3n^2-12i-24)$ for even n and $\frac{1}{2}(3n^2-12i-23)$ for odd n, where $0 \leq i \leq \lfloor \frac{n}{6} \rfloor$.*

In addition, the eccentricity based geometric-arithmetic (GA) index of G, introduced by Ghorbani and Khaki [9], is defined as $GA_4(G) = \sum_{uv\in E(G)} \frac{2\sqrt{e_G(u)e_G(v)}}{e_G(u)+e_G(v)}$ using $t_e(\omega(e), \omega^*(e)) = \frac{2\sqrt{\omega(e)}}{\omega^*(e)}$. The ABC eccentric index of G (a new version of the ABC index), introduced by Farahani [7], is defined as $ABC_5(G) = \sum_{uv\in E(G)} \sqrt{\frac{e_G(u)+e_G(v)-2}{e_G(u)e_G(v)}}$ using $t_e(\omega(e), \omega^*(e)) = \sqrt{\frac{\omega^*(e)-2}{\omega(e)}}$. We speculate that the extremal problems for $GA_4(G)$ and $ABC_5(G)$ can be solved by using some similar methods.

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Author details
[1]Department of Mathematics, China Jiliang University, Hangzhou, 310018, China. [2]School of Mathematics and Statistics, Central China Normal University, Wuhan, 430079, China. [3]Department of Mathematics and Statistics, Georgia State University, Atlanta, GA 30303, USA.

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