CROATICA CHEMICA ACTA
CCACAA, ISSN 0011-1643, e-ISSN 1334-417X
Croat. Chem. Acta **85** (3) (2012) 359–362.
http://dx.doi.org/10.5562/cca2020

Original Scientific Article

Extremal Properties of the Zagreb Eccentricity Indices

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RECEIVED NOVEMBER 17, 2011; ACCEPTED SEPTEMBER 28, 2012

Abstract. We give sharp lower bounds for the Zagreb eccentricity indices of connected graphs with fixed numbers of vertices and edges, sharp lower and upper bounds for the Zagreb eccentricity indices of trees with fixed number of pendant vertices, sharp upper bounds for the Zagreb eccentricity indices of trees with fixed matching number (fixed maximum degree, respectively), and characterize the extremal graphs. (doi: 10.5562/cca2020)

Keywords: Zagreb eccentricity indices, trees, pendant vertices, matching number, maximum degree

INTRODUCTION

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, $d_G(u)$ or d_u denotes the degree of u in G.[1,2] The *first* Zagreb index of G is defined as:[3,4]

$$M_1(G) = \sum_{u \in V(G)} d_u^2,$$

while the *second* Zagreb index of G is defined as:[3,4]

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

The properties of these molecular indices and their derivatives are continuously studied, *e.g.*, in Reference 5. Let us also point to the timely paper that just appeared in this journal by Stevanović[6] reporting on the relationship between these two descriptors, a topic that is also in recent years considerably studied, *e.g.*, in References 7 and 8. It should be also pointed out that the Zagreb indices and their variants are useful molecular descriptors which found considerable use in QSPR and QSAR studies as summarized by Todeschini and Consonni.[9,10]

For a vertex $u \in V(G)$, $e_G(u)$ or e_u denotes the eccentricity of u in G, which is equal to the largest distance from u to other vertices.[1,2] The Zagreb eccentricity indices were introduced in an analogous way as the Zagreb indices by Vukičević and Graovac.[11] The *first* Zagreb eccentricity index of G is defined as:

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

while the *second* Zagreb eccentricity index of G is defined as:

$$\xi_2(G) = \sum_{uv \in E(G)} e_u e_v.$$

Vukičević and Graovac[11] studied the comparison of $\frac{\xi_1(G)}{n}$ and $\frac{\xi_2(G)}{m}$ for a graph G with n vertices and m edges. Some mathematical and computational properties of the Zagreb eccentricity indices have recently been established,[12] where the authors gave lower and upper bounds for the Zagreb eccentricity indices of connected graphs in terms of graph invariants such as the number of vertices, the number of edges, the radius, and the diameter, determined the n-vertex trees with the first a few smallest and largest Zagreb eccentricity indices for $n \geq 6$, and found lower and upper bounds for the Zagreb eccentricity indices of trees with fixed diameter, lower bounds for the Zagreb eccentricity indices of trees with fixed matching number.

In continuation to our study reported in Reference 12, in this paper, we give sharp lower bounds for the Zagreb eccentricity indices of connected graphs with fixed numbers of vertices and edges, sharp lower and upper bounds for the Zagreb eccentricity indices of trees with fixed number of pendant vertices, sharp upper bounds for the Zagreb eccentricity indices of trees with

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fixed matching number (fixed maximum degree, respectively), and characterize the extremal graphs.

PRELIMINARIES

Let K_n and P_n be, respectively, the complete graph and the path with n vertices.[1,2] By direct calculation, if $n \ge 2$ is *even*, then:[12]

$$\xi_1(P_n) = \frac{7n^3 - 9n^2 + 2n}{12},$$
$$\xi_2(P_n) = \frac{7n^3 - 21n^2 + 20n}{12},$$

and if $n \ge 3$ is *odd*, then:[12]

$$\xi_1(P_n) = \frac{7n^3 - 9n^2 - n + 3}{12},$$
$$\xi_2(P_n) = \frac{7n^3 - 21n^2 + 17n - 3}{12}.$$

Let G_1 and G_2 be the trees shown in Figure 1, where vertices u and v are adjacent, u has a unique neighbor in N. In G_1, u has at least one neighbor in M, and all of such neighbors are switched to be neighbors of v in G_2.

Lemma 1. Let G_1 and G_2 be the trees shown in Figure 1.

(i) If there is a diametrical path of G_1 with all edges in $E(Q)$, then $\xi_1(G_1) > \xi_1(G_2)$ and $\xi_2(G_1) > \xi_2(G_2)$.

(ii) If there is a diametrical path of G_1 containing vertex u and some vertices in N and Q, and $e_{G_1}(u) \ge e_{G_1}(v)$, then $\xi_1(G_1) \ge \xi_1(G_2)$ and $\xi_2(G_1) \ge \xi_2(G_2)$ with either equality if and only if $e_{G_1}(u) = e_{G_1}(v)$.

Remark 1. In Lemma 1 (i) u is a vertex with degree at least three outside a diametrical path of G_1, while in Lemma 1 (ii) u is a vertex with degree at least three in a diametrical path of G_1.

Let $\mathscr{T}(n,p)$ be the set of trees with n vertices and p pendant vertices, where $2 \le p \le n-1$. The cases $p = 2, n-1$ are trivial.

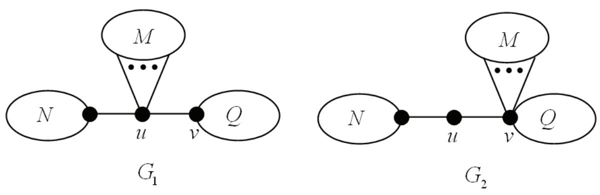

Figure 1. Trees G_1 and G_2 in Lemma 1.

Lemma 2. Let G be a tree in $\mathscr{T}(n,p)$ with minimum Zagreb eccentricity indices, where $3 \le p \le n-1$. Let $P = v_0 v_1 \ldots v_d$ be a diametrical path of G. Then the vertices with degree at least three in G can only be the central vertices of P.

For integers n and p with $3 \le p \le n-2$, let $k = \left\lfloor \frac{n-1}{p} \right\rfloor$ and $r = n-1-kp$, let $T_1^{(n,p)}$ be the tree obtained by attaching $p-r$ paths on k vertices and r paths on $k+1$ vertices to a common vertex, and if $n-2 \equiv 0 \pmod p$, then let $T_2^{(n,p)}(s)$ be the tree obtained by attaching s paths and $p-s$ paths on $\frac{n-2}{p}$ vertices, respectively, to the two end vertices of an edge, where $1 \le s \le \lfloor p/2 \rfloor$. Obviously, $T_2^{(n,p)}(1) \cong T_1^{(n,p)}$ if $n-2 \equiv 0 \pmod p$.

Lemma 3. Let $G \in \mathscr{T}(n,p)$, where $3 \le p \le n-2$. If G has exactly one vertex with degree at least three, then $\xi_1(G_1) \ge \xi_1(T_1^{(n,p)})$ and $\xi_2(G_1) \ge \xi_2(T_1^{(n,p)})$ with either equality if and only if $G \cong T_1^{(n,p)}$.

Let $T_a^{n,s}$ be the (n-vertex) tree obtained by attaching a and $s-a$ pendant vertices, respectively, to the two end vertices of the path P_{n-s}, where $1 \le a \le \lfloor s/2 \rfloor$. Let $\mathbf{T}^{n,s} = \left\{ T_a^{n,s} : 1 \le a \le \lfloor s/2 \rfloor \right\}$.

For integers d and n with $2 \le d \le n-1$, let

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

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

Lemma 4.[12] Let G be a tree with n vertices and diameter d. Then:

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

with either equality if and only if $G \in \mathbf{T}^{n,n-d+1}$. For $2 \le d \le n-2$, we have:

$$f_1(n,d) < f_1(n,d+1)$$
$$f_2(n,d) < f_2(n,d+1).$$

Recall that a pendant path at a vetex v of a tree T is a path in which no vetex other than v lies in any edges of T off the path, where the degree of v is at least three.

BOUNDS AND EXTREMAL GRAPHS

Denote by $G \vee H$ the graph obtained from vertex-disjoint graphs G and H by adding edges between each vertex in G and each vertex in H. For positive integers n and m with $n-1 \le m < \binom{n}{2}$, let $a = a_{n,m} = \left\lfloor \frac{2n-1-\sqrt{(2n-1)^2-8m}}{2} \right\rfloor$, and $\mathbf{G}_{(n,m)}$ be the set of graphs $K_a \vee H$, where H is a graph with $n-a$ vertices and $m - \binom{a}{2} - a(n-a)$ edges. Note that a with $1 \le a < n$ is the largest integer satisfying $2m \ge a(n-1) + a(n-a)$, *i.e.*, $h(a) \ge 0$ with $h(a) = a^2 - 2na + a + 2m$, we have $\left[m - \binom{a}{2} - a(n-a)\right] - (n-a-1) = \frac{1}{2}h(a+1) < 0$. This implies that each vertex of H has eccentricity two in $K_a \vee H$.

Proposition 1. Let G be an n-vertex connected graph with m edges, where $n-1 \le m < \binom{n}{2}$. Let $a = a_{n,m} = \left\lfloor \frac{2n-1-\sqrt{(2n-1)^2-8m}}{2} \right\rfloor$. Then:

$$\xi_1(G) \ge 4n - 3a$$
$$\xi_2(G) \ge 4m - 3\binom{a}{2} - 2a(n-a)$$

with either equality if and only if $G \in \mathbf{G}_{(n,m)}$.

Clearly, $a_{n,n} = 1$ for $n \ge 4$, and $a_{n,n+1} = 1$ for $n \ge 5$.

Corollary 1. Let G be a unicyclic graph with $n \ge 4$ vertices. Then:

$$\xi_1(G) \ge 4n - 3$$

$$\xi_2(G) \ge 2n + 2$$

with either equality if and only if G is the graph obtained by adding an edge to the star S_n.

Corollary 2. Let G be a bicyclic graph with $n \ge 5$ vertices. Then:

$$\xi_1(G) \ge 4n - 3$$

$$\xi_2(G) \ge 2n + 6$$

with either equality if and only if G is a graph obtained by adding two edges to the star S_n.

Proposition 2. Let $G \in \mathcal{T}(n,p)$, where $3 \le p \le n-2$. Let $k = \left\lfloor \frac{n-1}{p} \right\rfloor$ and $r = n-1-kp$. Then:

$$\xi_1(G) \ge \begin{cases} \frac{pk}{6}(7k+1)(2k+1) + k^2 & \text{if } r = 0 \\ \frac{pk}{6}(14k+13)(k+1) + 2(k+1)^2 & \text{if } r = 1 \\ \frac{pk}{6}(14k+13)(k+1) + (4r+1)(k+1)^2 & \text{if } r \ge 2 \end{cases}$$

$$\xi_2(G) \ge \begin{cases} \frac{pk}{3}(7k^2-1) & \text{if } r = 0 \\ \frac{pk}{3}(7k+2)(k+1) + (k+1)^2 & \text{if } r = 1 \\ \frac{pk}{3}(7k+2)(k+1) + 2r(k+1)(2k+1) & \text{if } r \ge 2 \end{cases}$$

with either equality if and only if $G \cong T_1^{(n,p)}$ or $G \cong T_2^{(n,p)}(s)$ with $2 \le s \le \lfloor p/2 \rfloor$ if $n-2 \equiv 0 \pmod{p}$, and $G \cong T_1^{(n,p)}$ otherwise.

Proposition 3. Let $G \in \mathcal{T}(n,p)$, where $2 \le p \le n-1$. Then:

$$\xi_1(G) \le \begin{cases} (n-p+1)^2 n - \frac{5(n-p+1)^3 - 2(n-p+1)}{12} & \text{if } n-p \text{ is odd} \\ (n-p+1)^2 n - \frac{5(n-p+1)^3 - 5(n-p+1)}{12} & \text{if } n-p \text{ is even} \end{cases}$$

$$\xi_2(G) \le \begin{cases} (n-p+1)(n-p)n - \frac{5(n-p+1)^3 - 8(n-p+1)}{12} & \text{if } n-p \text{ is odd} \\ (n-p+1)(n-p)n - \frac{5(n-p+1)^3 - 11(n-p+1) - 6}{12} & \text{if } n-p \text{ is even} \end{cases}$$

with either equality if and only if $G \in \mathbf{T}^{n,p}$.

Recall that the matching number of a graph G is the maximum number of edges of matchings in G.[2] For $2 \le \beta \le \lfloor n/2 \rfloor$, the tree with minimum Zagreb eccentricity indices among trees with n vertices and matching number β has been determined.[12]

Proposition 4. Let G be an *n*-vertex tree with matching number β, where $2 \le \beta \le \lfloor n/2 \rfloor$. Then:

$$\xi_1(G) \le 4\beta^2 n - \frac{10\beta^3 - \beta}{3}$$

$$\xi_2(G) \le (4\beta - 2)\beta n - \frac{10\beta^3 - 4\beta}{3}$$

with either equality if and only if $G \in \mathbf{T}^{n,n-2\beta+1}$.

Proposition 5. Let G be an n-vertex tree with maximum degree Δ, where $2 \le \Delta \le n-1$. Then:

$$\xi_1(G) \le \begin{cases} (n-\Delta+1)^2 n - \dfrac{5(n-\Delta+1)^3 - 2(n-\Delta+1)}{12} & \text{if } n-\Delta \text{ is odd} \\ (n-\Delta+1)^2 n - \dfrac{5(n-\Delta+1)^3 - 5(n-\Delta+1)}{12} & \text{if } n-\Delta \text{ is even} \end{cases}$$

$$\xi_2(G) \le \begin{cases} (n-\Delta+1)(n-\Delta)n - \dfrac{5(n-\Delta+1)^3 - 8(n-\Delta+1)}{12} & \text{if } n-\Delta \text{ is odd} \\ (n-\Delta+1)(n-\Delta)n - \dfrac{5(n-\Delta+1)^3 - 11(n-\Delta+1) - 6}{12} & \text{if } n-\Delta \text{ is even} \end{cases}$$

with either equality if and only if $G \cong T_1^{n,\Delta}$.

Supplementary Materials. – Supporting informations to the paper are enclosed to the electronic version of the article. These data can be found on the website of *Croatica Chemica Acta* (http://hrcak.srce.hr/cca)

Acknowledgements. This work was supported by the Guangdong Provincial Natural Science Foundation of China (Grant No. S2011010005539) and the Ministry of Science, Education and Sports of Croatia (Grant No. 098-1770945-2919).

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SUPPLEMENTARY MATERIALS

Proof of Lemma 1

Note that for a diametrical path P of G_1 and $x \in V(G_1)$, there is a pendant vertex, say y, in P such that the distance from x to y in G_1 is equal to $e_{G_1}(x)$. Note that $e_{G_1}(x) = e_{G_2}(x)$ for $x \in V(G_1) \setminus V(M)$ and $e_{G_1}(x) - e_{G_2}(x) = e_{G_1}(u) - e_{G_2}(v) = e_{G_1}(u) - e_{G_1}(v)$ for $x \in V(M)$ in (i) and (ii), while $e_{G_1}(u) > e_{G_1}(v)$ in (i) and $e_{G_1}(u) \ge e_{G_1}(v)$ in (ii). Then the result follows easily.

Proof of Lemma 2

The cases $d = 2, 3$ are obvious. Suppose that $d \ge 4$. By Lemma 1 (i) and Remark 1, there is no vertex in G outside P with degree at least three. Now we show that the vertices with degree at least three on P can only be the central vertices of P.

Let v_i with $1 \le i \le d-1$ be a vertex on P with degree at least three. If $e_G(v_i) > e_G(v_{i+1})$ ($e_G(v_i) > e_G(v_{i-1})$, respectively), then making use of Lemma 1 (ii) to $G_1 = G$ by setting $u = v_i$ and $v = v_{i+1}$ ($v = v_{i-1}$, respectively), we may get another tree in $\mathcal{T}(n,p)$ with smaller Zagreb eccentricity indices, a contradiction. Thus $e_G(v_i) \le e_G(v_{i+1})$ and $e_G(v_i) \le e_G(v_{i-1})$. Obviously, $e_G(v_i) = d-i$ or i. In the former case, $i \le d-i$, $d-i \le i+1$ since $e_G(v_i) \le e_G(v_{i+1})$, and thus $2i = d-1$ or d. In the latter case, $i \ge d-i$, $i \le d-i+1$ since $e_G(v_i) \le e_G(v_{i-1})$, and thus $2i = d$ or $d+1$. Thus $2i = d-1$, d or $d+1$, *i.e.*, v_i is a central vertex of P.

Proof of Lemma 3

Let G be a tree with minimum Zagreb eccentricity indices satisfying the given condition. Then there are p pendant paths at a common vertex, say v. Among these pendant paths, let Q_1 be a path with maximum length a, Q_2 a path with maximum length b except the path Q_1, and Q_3 a path with minimum length c, where $a \ge b \ge c$. Let v_1 be the neighbor of v in Q_1. If $a > b+1$, then $e_G(v_1) < e_G(v)$, and thus making use of Lemma 1 (ii) to $G_1 = G$ by setting $u = v$ and $v = v_1$, we may get another tree (also satisfying the given condition) with smaller Zagreb eccentricity indices, a contradiction. Thus $a = b$ or $b+1$. Suppose that $a \ge c+2$. Let v_2 (v_3, respectively) be the pendant vertex in Q_1 (Q_3, respectively), and v_4 the neighbor of v_2. Let G_1 be the tree obtained from G by deleting the edge v_2v_4 and adding the edge v_2v_3. Obviously, $G_1 \in \mathcal{T}(n,p)$, and G_1 has exactly one vertex with degree at least three. Then $e_{G_1}(x) \le e_G(x)$ for $x \in V(G)$, $e_{G_1}(v_2) = b+c+1 < a+b = e_G(v_2)$, and $e_{G_1}(v_3) = b+c < a+b-1 = e_G(v_4)$. Thus $\xi_1(G) > \xi_1(G_1)$ and $\xi_2(G) > \xi_2(G_1)$, a contradiction. It follows that $a = c$ or $c+1$, *i.e.*, $G \cong T_1^{(n,p)}$.

Proof of Proposition 1

Note that $1 \le a < n$. Let k be the number of vertices with degree $n-1$ in G, where $0 \le k \le n-2$. If $k = 0$, then $\xi_1(G) \ge 4n > 4n - 3a$ and $\xi_2(G) \ge 4m > 4m - 3\binom{a}{2} - 2a(n-a)$. Suppose that $k \ge 1$. Then all the $n-k$ vertices of degree less than $n-1$ have eccentricity two, and thus:

$$\xi_1(G) = 1^2 \cdot k + 2^2 \cdot (n-k) = 4n - 3k,$$

$$\xi_2(G) = 1 \cdot 1 \cdot \binom{k}{2} + 1 \cdot 2 \cdot k(n-k) + 2 \cdot 2 \cdot \left(m - \binom{k}{2} - k(n-k) \right) = 4m - 3\binom{k}{2} - 2k(n-k).$$

Note that $2m \ge k(n-1) + k(n-k)$ and recall that a is the largest integer satisfying $2m \ge a(n-1) + a(n-a)$, implying that $k \le a$. Note that both $4n - 3k$ and $4m - 3\binom{k}{2} - 2k(n-k)$ are decreasing on k, and thus $\xi_1(G) \ge 4n - 3a$ and $\xi_2(G) \ge 4m - 3\binom{a}{2} - 2a(n-a)$ with either equality if and only if G has exactly a vertices of degree $n-1$ and all other vertices have eccentricity two, *i.e.*, $G \in \mathbf{G}_{(n,m)}$.

Proof of Proposition 2

Let G be a tree in $\mathcal{T}(n,p)$ with minimum Zagreb eccentricity indices. Let $V_1(G)$ be the set of vertices in G with degree at least three. By Lemma 2, $|V_1(G)| = 1$ or 2. If $|V_1(G)| = 1$, then by Lemma 3, we have $G \cong T_1^{(n,p)}$. Suppose that $|V_1(G)|=2$. Let $V_1(G)=\{u,v\}$, and P be a diametrical path of G. By Lemma 2, u,v are adjacent in P, and $e_G(u)=e_G(v)$. Among the pendant paths at u, let k_1 and k_2 be, respectively, the maximum and minimum length of them. Suppose that $k_1>k_2$. Obviously, the pendant path at u with all vertices on P is of length k_1. Let G_1 be the tree obtained from G by switching all neighbors of u in G outside P to be neighbors of v in G_1. By Lemma 1 (ii), we have $\xi_1(G)=\xi_1(G_1)$ and $\xi_2(G)=\xi_2(G_1)$. Note that $|V_1(G_1)|=1$, and there are two pendant paths with lengths k_1+1 and k_2 at v in G_1. Since $k_1+1-k_2>1$, by Lemma 3, $\xi_1(G)=\xi_1(G_1)>\xi_1(T_1^{(n,p)})$ and $\xi_2(G)=\xi_2(G_1)>\xi_2(T_1^{(n,p)})$, a contradiction. Thus, all pendant paths at u in G have the same length. Similarly, all pendant paths at v in G have the same length. It follows that $G\cong T_2^{(n,p)}(s)$ with $2\le s\le\lfloor p/2\rfloor$.

Proof of Proposition 3

Let d be the diameter of G. Note that there are $d-1$ non-pendant vertices on a diametrical path of G, and thus $p\le n-(d-1)$, *i.e.*, $d\le n-p+1$. By Lemma 4, $\xi_1(G)\le f_1(n,d)\le f_1(n,n-p+1)$ and $\xi_2(G)\le f_2(n,d)\le f_2(n,n-p+1)$. Obviously, $\xi_1(G)=f_1(n,n-p+1)$ and $\xi_2(G)=f_2(n,n-p+1)$ if and only if $G\in\mathbf{T}^{n,p}$.

Proof of Proposition 4

Let d be the diameter of G. If $d\ge 2\beta+1$, then we may construct a matching with $\beta+1$ edges by choosing pair-wise disjoint edges on a diametrial path of G, a contradiction. Thus $d\le 2\beta$. By Lemma 4, $\xi_1(G)\le f_1(n,d)\le f_1(n,2\beta)$ and $\xi_2(G)\le f_2(n,d)\le f_2(n,2\beta)$. Obviously, $\xi_1(G)=f_1(n,2\beta)$ and $\xi_2(G)=f_2(n,2\beta)$ if and only if $G\in\mathbf{T}^{n,n-2\beta+1}$.

Proof of Proposition 5

Let d be the diameter of G, and p be the number of pendant vertices of G. Recall that $d\le n-p+1$ and note that $\Delta\le p$, and thus $d\le n-\Delta+1$. By Lemma 4, $\xi_1(G)\le f_1(n,d)\le f_1(n,n-\Delta+1)$ and $\xi_2(G)\le f_2(n,d)\le f_2(n,n-\Delta+1)$. Obviously, $\xi_1(G)=f_1(n,n-\Delta+1)$ and $\xi_2(G)=f_2(n,n-\Delta+1)$ if and only if $G\cong T_1^{n,\Delta}$.