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Original Scientific Article

On Zagreb Eccentricity Indices

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Abstract. Zagreb eccentricity indices were proposed analogously to Zagreb indices already known and used for almost forty years. For a connected graph, the first Zagreb eccentricity index is defined as the sum of the squares of the eccentricities of the vertices, and the second Zagreb eccentricity index is defined as the sum of the products of the eccentricities of pairs of adjacent vertices. We report mathematical properties, especially lower and upper bounds of trees and general graphs in terms of graph invariants and the corresponding extremal graphs, Nordhaus-Gaddum-type results, and the ordering of trees with small and large Zagreb eccentricity indices. (doi: 10.5562/cca1801)

Keywords: Zagreb indices, Zagreb eccentricity indices, lower and upper bounds, graph invariants, trees, general graphs

INTRODUCTION

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, $e_G(u)$ or e_u denotes the eccentricity of u in G, which is the length of a path from u to a vertex v that is farthest from u, *i.e.*, $e_u = \max\{d(u,v \mid G) : v \in V(G)\}$, where $d(u,v \mid G)$ denotes the distance between u and v in G.[1]

The Zagreb eccentricity indices are introduced in an analogy with the Zagreb indices[2–4] by replacing the vertex degrees with the vertex eccentricities. Thus, the *first* Zagreb eccentricity index of a graph G is defined as:

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

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

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

Note that degrees are "local properties", while eccentricities are "global properties" of the vertices.

These two indices are recently introduced by Vukičević and Graovac.[5] However, it should be pointed out that there were a number of eccentricity-based molecular descriptors already proposed in the literature,[6,7] such as the eccentric connectivity index[8,9] (see References 10–12 for recent results) and the eccentric adjacency index.[13] Vukičević and Graovac have shown in their paper[5] that $\frac{\xi_1(G)}{|V(G)|} \ge \frac{\xi_2(G)}{|E(G)|}$ if G is a tree or a unicyclic graph but is not true for bicyclic graphs.

In the present paper, we give lower and upper bounds for the first and the second Zagreb eccentricity indices of n-vertex trees with fixed diameter, and lower bounds for the first and the second Zagreb eccentricity indices of n-vertex trees with fixed matching number, and characterize the extremal cases, and determine the n-vertex trees with respectively the minimum, second-minimum and third-minimum, as well as the maximum, second-maximum and third-maximum indices ξ_1 and ξ_2 for $n \ge 6$. We also give lower and upper bounds for the first and the second 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, and give the Nordhaus-Gaddum-type results.[14]

PRELIMINARIES

For a connected graph G, the radius $r(G)$ and the diameter $D(G)$ are, respectively, the minimum and maximum eccentricities among the vertices of G.[1] A connected graph is called a self-centered graph if all of its vertices have the same eccentricity. Evidently, a connected graph G is self-centered if and only if $r(G) = D(G)$.

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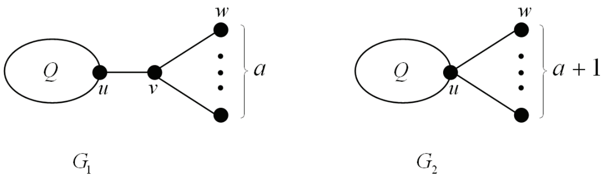

Figure 1. The trees G_1 and G_2 in Lemma 1.

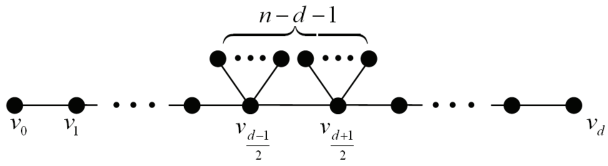

Figure 2. The structure of trees in $L_{n,d}$ with odd d.

Let K_n be the n-vertex complete graph. Let S_n and P_n be the n-vertex star and path, respectively. By direct calculation, $\xi_1(K_n) = n$ and $\xi_2(K_n) = \frac{n(n-1)}{2}$ for $n \geq 2$, $\xi_1(S_n) = 4n-3$, and $\xi_2(S_n) = 2(n-1)$ for $n \geq 3$, and if $n \geq 2$ is *even*, then:

$$\begin{aligned}\xi_1(P_n) &= 2\sum_{i=n/2}^{n-1} i^2 = 2\left(\sum_{i=1}^{n-1} i^2 - \sum_{i=1}^{n/2-1} i^2\right) \\ &= \frac{1}{3}(n-1)n(2n-1) - \frac{1}{3}\left(\frac{n}{2}-1\right)\cdot\frac{n}{2}\cdot(n-1) \\ &= \frac{7n^3-9n^2+2n}{12},\end{aligned}$$

$$\begin{aligned}\xi_2(P_n) &= 2\sum_{i=n/2}^{n-2} i(i+1) + \left(\frac{n}{2}\right)^2 \\ &= 2\left(\sum_{i=1}^{n-2} i^2 - \sum_{i=1}^{n/2-1} i^2 + \sum_{i=n/2}^{n-2} i\right) + \frac{n^2}{4} \\ &= \frac{1}{3}(n-2)(n-1)(2n-3) - \frac{1}{3}\left(\frac{n}{2}-1\right)\cdot \\ &\quad \frac{n}{2}\cdot(n-1) + \left(\frac{n}{2}-1\right)\left(\frac{3n}{2}-2\right) + \frac{n^2}{4} \\ &= \frac{7n^3-21n^2+20n}{12},\end{aligned}$$

and if $n \geq 3$ is *odd*, then:

$$\begin{aligned}\xi_1(P_n) &= 2\sum_{i=(n+1)/2}^{n-1} i^2 + \left(\frac{n-1}{2}\right)^2 = 2\left(\sum_{i=1}^{n-1} i^2 - \sum_{i=1}^{(n-1)/2} i^2\right) + \left(\frac{n-1}{2}\right)^2 \\ &= \frac{1}{3}(n-1)n(2n-1) - \frac{1}{3}\cdot\frac{(n-1)}{2}\cdot\frac{(n+1)}{2}\cdot n + \left(\frac{n-1}{2}\right)^2 \\ &= \frac{7n^3-9n^2-n+3}{12},\end{aligned}$$

$$\begin{aligned}\xi_2(P_n) &= 2\sum_{i=(n-1)/2}^{n-2} i(i+1) = 2\left(\sum_{i=1}^{n-2} i^2 - \sum_{i=1}^{(n-3)/2} i^2 + \sum_{i=(n-1)/2}^{n-2} i\right) \\ &= \frac{1}{3}(n-2)(n-1)(2n-3) - \frac{1}{3}\cdot\frac{(n-3)}{2}\cdot\frac{(n-1)}{2}\cdot(n-2) + \\ &\quad \frac{(n-1)}{2}\cdot\frac{(3n-5)}{2} \\ &= \frac{7n^3-21n^2+17n-3}{12}.\end{aligned}$$

For a graph G and a subset E' of its edge set (E^* of the edge set of its complement, respectively), $G - E'$ ($G + E^*$, respectively) denotes the graph formed from G by deleting (adding, respectively) edges from E' (E^* respectively). For a graph G with $u \in V(G)$, $G - u$ denotes the graph formed from G by deleting the vertex u (and its incident edges).

RESULTS FOR TREES

In this section, we give lower and upper bounds for the first and the second Zagreb eccentricity indices of n-vertex trees with fixed diameter, and lower bounds for the first and the second Zagreb eccentricity indices of n-vertex trees with fixed matching number. We also determine the n-vertex trees with, respectively, the minimum, second-minimum and third-minimum, as well as the maximum, second-maximum and third-maximum indices ξ_1 and ξ_2 for $n \geq 6$.

Lemma 1. Let u be a vertex of a tree Q with at least two vertices. For integer $a \geq 1$, let G_1 be the tree obtained from Q by attaching a star S_{a+1} at its center v to u, G_2 the tree obtained from Q by attaching $a + 1$ pendant vertices to u, see Figure 1. Then $\xi_1(G_2) < \xi_1(G_1)$ and $\xi_2(G_2) < \xi_2(G_1)$.

Let $\mathbf{T}(n,d)$ be the set of n-vertex trees with diameter d, where $2 \leq d \leq n-1$. For $2 \leq d \leq n-2$, let $L_{n,d}$ be the set of n-vertex trees obtained from $P_{d+1} = v_0 v_1 \cdots v_d$ by attaching $n-d-1$ pendant vertices to $v_{\lfloor d/2 \rfloor}$ and/or $v_{\lceil d/2 \rceil}$. Let $L_{n,n-1} = \{P_n\}$. Note that in $L_{n,d}$, there is only one tree for even d, and $\left\lfloor \frac{n-d+1}{2} \right\rfloor$ trees for odd d. Let $U_{n,d}^a$ be the n-vertex tree obtained by attaching a and $n+1-a-d$ pendant vertices, respectively, to the two end vertices of the path P_{d-1} for $1 \leq a \leq \left\lfloor \frac{n+1-d}{2} \right\rfloor$, and let $U_{n,d} = \left\{U_{n,d}^a : 1 \leq a \leq \left\lfloor \frac{n+1-d}{2} \right\rfloor\right.$. See Figures 2–4 for the trees in $L_{n,d}$ and the tree $U_{n,d}^a$.

Proposition 1. Let $T \in \mathbf{T}(n,d)$, where $2 \leq d \leq n-1$. Then:

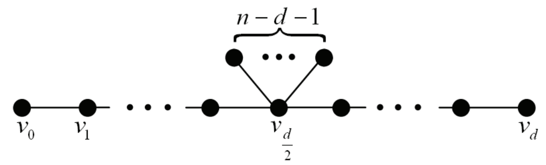

Figure 3. The tree in $L_{n,d}$ with even d.

$$\xi_1(T) \geq \begin{cases} \dfrac{3(d+2)^2 n + 4d^3 - 3d^2 - 22d - 12}{12} & \text{if } d \text{ is even} \\ \dfrac{3(d+3)^2 n + 4d^3 - 9d^2 - 40d - 27}{12} & \text{if } d \text{ is odd,} \end{cases}$$

$$\xi_2(T) \geq \begin{cases} \dfrac{3d(d+2)n + 4d^3 - 9d^2 - 10d}{12} & \text{if } d \text{ is even} \\ \dfrac{3(d+1)(d+3)n + 4d^3 - 15d^2 - 22d - 3}{12} & \text{if } d \text{ is odd} \end{cases}$$

with either equality if and only if $T \in L_{n,d}$.

Proposition 2. Let $T \in \mathbf{T}(n,d)$, where $2 \leq d \leq n-1$. Then:

$$\xi_1(T) \leq \begin{cases} d^2 n - \dfrac{5d^3 - 2d}{12} & \text{if } d \text{ } is \text{ even} \\ d^2 n - \dfrac{5d^3 - 5d}{12} & \text{if } d \text{ is odd,} \end{cases}$$

$$\xi_2(T) \leq \begin{cases} (d^2 - d)n - \dfrac{5d^3 - 8d}{12} & \text{if } d \text{ is even} \\ (d^2 - d)n - \dfrac{5d^3 - 11d - 6}{12} & \text{if } d \text{ is odd} \end{cases}$$

with either equality if and only if $T \in U_{n,d}$.

Now we consider the *n*-vertex trees with fixed matching number. A matching M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. A matching M of G is said to be maximum, if for any other matching M_1 of G, $|M_1| \leq |M|$. The matching number of G is the number of edges of a maximum matching in G. If M is a matching of a graph G and vertex $v \in V(G)$ is incident with an edge of M, then v is said to be *M*-saturated, and if every vertex of G is *M*-saturated, then M is a perfect matching. For integers n and $1 \leq m \leq \lfloor n/2 \rfloor$, let $\mathbf{T}_{(n,m)}$ be the set of *n*-vertex trees

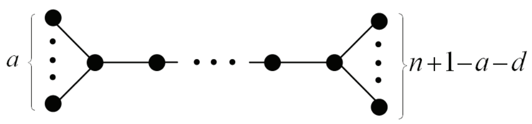

Figure 4. The tree $U^a_{n.d}$.

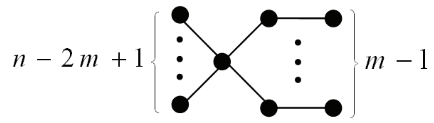

Figure 5. The tree $T_{n,m}$.

with matching number *m*. Obviously, $\mathbf{T}_{(n,1)} = \{S_n\}$. For $3 \leq m \leq \lfloor n/2 \rfloor$, let $T_{n,m}$ be the tree obtained by attaching $m-1$ paths on two vertices to the center of the star S_{n-2m+2}, see Figure 5.

Proposition 3. Let $T \in \mathbf{T}_{(2m,m)}$ with $m \geq 3$. Then $\xi_1(T) \geq 25m - 12$, $\xi_2(T) \geq 18m - 12$ with either equality if and only if $T = T_{2m,m}$.

Proposition 4. Let $T \in \mathbf{T}_{(n,m)}$ with $2 \leq m \leq |n/2|$.
If $m = 2$, then $\xi_1(T) \geq 9n - 10$ and $\xi_2(T) \geq 6n - 8$ with either equality if and only if $T \in \mathbf{T}(n,3)$;
If $m \geq 3$, then $\xi_1(T) \geq 9n + 7m - 12$ and $\xi_2(T) \geq 6n + 6m - 12$ with either equality if and only if $T = T_{n,m}$.

Now we use the result for the first and the second Zagreb eccentricity indices of the *n*-vertex trees with fixed diameter to determine the *n*-vertex trees with small and large indices ξ_1 and ξ_2.

Proposition 5. Among the *n*-vertex trees, S_n for $n \geq 3$, the trees in $L_{n,3}$ for $n \geq 4$, and the trees in $L_{n,4}$ for $n \geq 5$ are, respectively, the unique trees with the minimum, second-minimum and third-minimum indices ξ_1 and ξ_2, the first Zagreb eccentricity indices of which are equal to $4n-3$, $9n-10$ and $9n+9$, respectively, while the second Zagreb eccentricity indices of which are equal to $2n-2$, $6n-8$ and $6n+6$, respectively.

For $n \geq 4$, let P'_n be the tree formed by attaching a pendant vertex to the neighbor of an end-vertex of the path P_{n-1}. For $n \geq 6$, let P''_n be the tree formed by attaching a pendant vertex to the second neighbor of an end-vertex of the path P_{n-1}.

Proposition 6. Among the *n*-vertex trees, P_n for $n \geq 3$, P'_n for $n \geq 4$, and P''_n for $n \geq 5$ are, respectively, the unique trees with the maximum, second-maximum and third-maximum indices ξ_1 and ξ_2, where:

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

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

$$\xi_1(P_n')=\begin{cases}\dfrac{7n^3-18n^2-10n+36}{12} & \text{if } n \text{ is even}\\ \dfrac{7n^3-18n^2-7n+30}{12} & \text{if } n \text{ is odd,}\end{cases}$$

$$\xi_2(P_n')=\begin{cases}\dfrac{7n^3-30n^2+20n+24}{12} & \text{if } n \text{ is even}\\ \dfrac{7n^3-30n^2+23n+24}{12} & \text{if } n \text{ is odd,}\end{cases}$$

$$\xi_1(P_n'')=\begin{cases}\dfrac{7n^3-18n^2-34n+96}{12} & \text{if } n \text{ is even}\\ \dfrac{7n^3-18n^2-31n+90}{12} & \text{if } n \text{ is odd,}\end{cases}$$

$$\xi_2(P_n'')=\begin{cases}\dfrac{7n^3-30n^2-4n+96}{12} & \text{if } n \text{ is even}\\ \dfrac{7n^3-30n^2-n+96}{12} & \text{if } n \text{ is odd.}\end{cases}$$

RESULTS FOR GENERAL CONNECTED GRAPHS

In this section, we give lower and upper bounds for the first and the second 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, and we also come up with the Nordhaus-Gaddum-type results.[14] Moreover, among the n-vertex connected graphs, we establish lower and upper bounds for the first Zagreb eccentricity index, and lower bound for the second Zagreb eccentricity index, respectively, and characterize the extremal cases.

Proposition 7. Let G be a connected graph with n vertices and m edges. Then:

$$nr(G)^2 \le \xi_1(G) \le nD(G)^2,$$
$$mr(G)^2 \le \xi_2(G) \le mD(G)^2$$

with any equality if and only if G is a self-centered graph.

Proposition 8. Let G be a connected graph with $n \ge 2$ vertices. Then:

$$\xi_1(K_n) \le \xi_1(G) \le \xi_1(P_n)$$

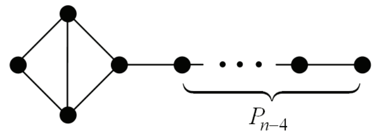

Figure 6. The graph B_n.

with left equality if and only if $G = K_n$ and right equality if and only if $G = P_n$.

Corollary 1. Let G be a connected bipartite graph with $n \ge 3$ vertices. Then $\xi_1(G) \ge 4n-3$ with equality if and only if $G = S_n$.

Proposition 9. Let G be a connected graph with $n \ge 2$ vertices. Then:

$$\xi_2(G) \ge \begin{cases}1 & \text{if } n=2\\ 3 & \text{if } n=3\\ 2(n-1) & \text{if } n\ge 4\end{cases}$$

with equality if and only if $G = K_n$ for $n = 2,3$, $G = K_4$ or S_4 for $n = 4$, and $G = S_n$ for $n \ge 5$.

Remark. By Proposition 8, among the n-vertex connected graphs, P_n is the unique graph with the maximum first Zagreb eccentricity index. However, P_n is not the graph with the maximum second Zagreb eccentricity index for $n \ge 9$. For $n \ge 5$, let B_n be the bicyclic graph obtained by attaching a path P_{n-4} (at one end vertex) to a vertex of degree two in the bicyclic graph obtained by adding an edge to the quadrangle, see Figure 6. Then:

$$\xi_2(B_n) = \xi_2(P_{n-1}) + (n-2)(n-3) + (n-3)^2 + (n-3)(n-4)$$
$$=\begin{cases}\dfrac{7n^3-6n^2-136n+276}{12} & \text{if } n \text{ is even}\\ \dfrac{7n^3-6n^2-133n+276}{12} & \text{if } n \text{ is odd.}\end{cases}$$

For $n \ge 9$:

$$\xi_2(B_n)-\xi_2(P_n)=$$
$$=\begin{cases}\dfrac{7n^3-6n^2-136n+276}{12}-\dfrac{7n^3-21n^2+20n}{12} & \text{if } n \text{ is even}\\ \dfrac{7n^3-6n^2-133n+276}{12}-\dfrac{7n^3-21n^2+17n-3}{12} & \text{if } n \text{ is odd}\end{cases}$$
$$=\begin{cases}\dfrac{15n^2-156n+276}{12} & \text{if } n \text{ is even}\\ \dfrac{15n^2-150n+279}{12} & \text{if } n \text{ is odd}\end{cases}$$
$$>0,$$

and then $\xi_2(B_n) > \xi_2(P_n)$.

Denote by $\overline{G}$ the complement of a graph G. There is only one connected graph P_4 on four vertices with the connected complement $\overline{P_4} = P_4$. Obviously, we have $\xi_1(P_4) + \xi_1(\overline{P_4}) = 2\xi_1(P_4) = 52$. For $n \geq 5$, the diameter of $\overline{P_n}$ is two.

Now we give the Nordhaus-Gaddum-type results.

Proposition 10. Let G be a connected graph with $n \geq 4$ vertices for which $\overline{G}$ is also connected. Then:

$$8n \leq \xi_1(G) + \xi_1(\overline{G}) \leq \xi_1(P_n) + \xi_1(\overline{P_n})$$

with left equality if and only if G and $\overline{G}$ are self-centered graphs with radius two and right equality if and only if $G = P_n$ or $\overline{P_n}$, and $\xi_2(G) + \xi_2(\overline{G}) \geq 2n(n-1)$ with equality if and only if G and $\overline{G}$ are self-centered graphs with radius two.

CONCLUSION

In this paper, we study the novel molecular descriptors, called Zagreb eccentricity indices, which were proposed analogously to Zagreb indices already known and used for almost forty years. We give lower and upper bounds for Zagreb eccentricity indices of trees and general graphs in terms of graph invariants, and characterize the extremal graphs, and determine the *n*-vertex trees with small and large Zagreb eccentricity indices. We also give Nordhaus-Gaddum-type results for Zagreb eccentricity indices. The lower and upper bounds for a molecular descriptor in terms of some graph invariants (*e.g.*, the number of vertices) are important information for a molecule in the sense that they establish the range of the descriptor.

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://public.carnet.hr/ccacaa).

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