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Some properties of the Zagreb eccentricity indices

Kinkar Ch. Das *

Department of Mathematics, Sungkyunkwan University
Suwon 440-746, Republic of Korea

Dae-Won Lee

Sungkyunkwan University, Suwon 440-746, Republic of Korea

Ante Graovac

Faculty of Science, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia

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Abstract

The concept of Zagreb eccentricity (E_1 and E_2) indices was introduced in the chemical graph theory very recently [5, 12]. The first Zagreb eccentricity (E_1) and the second Zagreb eccentricity (E_2) indices of a graph G are defined as

$$E_1 = E_1(G) = \sum_{v_i \in V(G)} e_i^2$$

and

$$E_2 = E_2(G) = \sum_{v_i v_j \in E(G)} e_i \cdot e_j \,,$$

where $E(G)$ is the edge set and e_i is the eccentricity of the vertex v_i in G. In this paper we give some lower and upper bounds on the first Zagreb eccentricity and the second Zagreb eccentricity indices of trees and graphs, and also characterize the extremal graphs.

Keywords: Graph, first Zagreb eccentricity index, second Zagreb eccentricity index, diameter, eccentricity.

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*Corresponding author.

E-mail addresses: kinkardas2003@googlemail.com (Kinkar Ch. Das), haverd2001@gmail.com (Dae-Won Lee), ante.graovac@irb.hr (Ante Graovac)

1 Introduction

Mathematical chemistry is a branch of theoretical chemistry using mathematical methods to discuss and predict molecular properties without necessarily referring to quantum mechanics [1, 8, 14]. Chemical graph theory is a branch of mathematical chemistry which applies graph theory in mathematical modeling of chemical phenomena [6]. This theory has an important effect on the development of the chemical sciences.

Topological indices are numbers associated with chemical structures derived from their hydrogen-depleted graphs as a tool for compact and effective description of structural formulas which are used to study and predict the structure-property correlations of organic compounds. Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [13]. One of the best known and widely used is the connectivity index, χ, introduced in 1975 by Milan Randić [11]. The Randić index is one of the most famous molecular descriptors and the paper in which it is defined is cited more than 1000 times. The first M_1, and the second M_2, Zagreb indices (see [2],[3],[4],[7],[9] and the references therein) are defined as:

$$M_1 = M_1(G) = \sum_{v_i \in V(G)} d_i^2$$

and

$$M_2 = M_2(G) = \sum_{v_i v_j \in E(G)} d_i \cdot d_j .$$

where d_i is the degree of the vertex $v_i \in V(G)$ in G.

Let $G = (V, E)$ be a connected simple graph with $|V(G)| = n$ vertices and $|E(G)| = m$ edges. Also let d_i be the degree of the vertex v_i, $i = 1, 2, \ldots, n$. For vertices v_i, $v_j \in V(G)$, the distance $d_G(v_i, v_j)$ is defined as the length of the shortest path between v_i and v_j in G. The eccentricity of a vertex is the maximum distance from it to any other vertex,

$$e_i = \max_{v_j \in V(G)} d_G(v_i, v_j) .$$

The maximum eccentricity over all vertices of G is called the diameter of G and denoted by d.

The invariants based on vertex eccentricities attracted some attention in Chmistry. In an analogy with the first and the second Zagreb indices, M. Ghorbani et al. and D. Vukičević et al. define the first E_1, and the second, E_2, Zagreb eccentricity indices by [5, 12]

$$E_1 = E_1(G) = \sum_{v_i \in V(G)} e_i^2 \tag{1.1}$$

and

$$E_2 = E_2(G) = \sum_{v_i v_j \in E(G)} e_i \cdot e_j . \tag{1.2}$$

where $E(G)$ is the edge set and e_i is the eccentricity of the vertex v_i in G.

Let $G = (V(G), E(G))$. If $V(G)$ is the disjoint union of two nonempty sets $V_1(G)$ and $V_2(G)$ such that every vertex in $V_1(G)$ has degree r and every vertex in $V_2(G)$ has degree

s, then G is (r, s)-semiregular graph. When $r = s$, is called a regular graph. As usual, $K_{a,b}$ $(a + b = n)$, P_n and $K_{1,n-1}$ denote respectively the complete bipartite graph, the path and the star on n vertices. A vertex of a graph is said to be pendent if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendent if one of its vertices is a pendent vertex. Now we calculate

$$E_1(P_n) = \begin{cases} \frac{1}{12}\,(n-1)(7n^2 - 2n) & \text{if } n \text{ is even} \\ \frac{1}{12}\,(n-1)(7n^2 - 2n - 3) & \text{if } n \text{ is odd.} \end{cases} \tag{1.3}$$

and

$$E_2(P_n) = \begin{cases} \frac{1}{12}\,n(7n^2 - 21n + 20) & \text{if } n \text{ is even} \\ \frac{1}{12}\,(n-1)(7n^2 - 14n + 3) & \text{if } n \text{ is odd.} \end{cases} \tag{1.4}$$

Also we have

$$E_1(K_{1,n-1}) = 4n - 3 \text{ and } E_2(K_{1,n-1}) = 2n - 2.$$

Denote by $\tilde{T}_n$, is a tree of order n with maximum degree $n - 2$. We have $E_1(\tilde{T}_n) = 9n - 10$, $E_2(\tilde{T}_n) = 6n - 8$.

In this paper we give some lower and upper bounds on the first Zagreb eccentricity and the second Zagreb eccentricity indices of trees and graphs, and also characterize the extremal graphs.

2 Lower and upper bounds on Zagreb eccentricity indices

We now give lower and upper bounds on the Zagreb eccentricity indices of trees.

Theorem 2.1. Let T be a tree with n vertices. Then

$$\text{(i)} \qquad E_1(K_{1,n-1}) \le E_1(T) \le E_1(P_n) \tag{2.1}$$

$$\text{and (ii)} \qquad E_2(K_{1,n-1}) \le E_2(T) \le E_2(P_n). \tag{2.2}$$

Moreover, the left hand side (right hand side, respectively) equality holds in (2.1) and (2.2) if and only if $G \cong K_{1,n-1}$ ($G \cong P_n$, respectively).

Proof. Upper bound: If T is isomorphic to path P_n, then the right hand side equality holds in (2.1) and (2.2). Otherwise, $T \ncong P_n$. Let d be the diameter of tree T. Then there exists a path $P_{d+1} : v_1 v_2 \ldots v_{d+1}$ of length d in T. Thus we have the eccentricity of a vertex v_i in tree T,

$$e_i = \max\{d_G(v_i, v_1),\ d_G(v_i, v_{d+1})\}\,.$$

Since T is a tree, both vertices v_1 and v_{d+1} are pendent vertices. Thus we have $e_i \le d$ for each $v_i \in V(G)$. Since $T \ncong P_n$, let v_k $(k \neq 1,\ d+1)$ be a vertex of degree one, adjacent to vertex v_j in T. We transform T into another tree T^* by deleting the edge $v_k v_j$ and join the vertices v_{d+1} and v_k by an edge. Then the longest path $P_{d+2} : v_1 v_2 \ldots v_{d+1} v_k$ of length $d + 1$ in T^*. Let the vertex eccentricities be $e_1^*,\ e_2^*, \ldots, e_n^*$ in T^*. Therefore we have $e_t^* = \max\{d_G^*(v_t, v_1),\ d_G^*(v_t, v_k)\} = \max\{d_G(v_t, v_1),\ d_G(v_t, v_{d+1}) + 1\} \ge \max\{d_G(v_t, v_1),\ d_G(v_t, v_{d+1})\} = e_t$ (as $d_G^*(v_t, v_k) = d_G(v_t, v_{d+1}) + 1$) for $t \neq k$ whereas $e_k^* = d+1 > d \ge e_k$ ($d_G^*(v_i, v_j)$ is the length of the shortest path between vertices

v_i and v_j in T^*). So we have $e_r^* \, e_s^* \geq e_r \, e_s$ for $v_r v_s \neq v_k v_j, \; v_k v_{d+1}$ and $e_k^* \, e_{d+1}^* = d(d+1) > d^2 \geq e_k \, e_j$. Using above result we get

$$E_1(T^*) - E_1(T) = \sum_{v_i \in V(T^*)} e_i^{*2} - \sum_{v_i \in V(T)} e_i^2 \geq e_k^{*2} - e_k^2 > 0$$

and

$$E_2(T^*) - E_2(T) = \sum_{v_r \, v_s \in E(T^*)} e_r^* \, e_s^* - \sum_{v_r \, v_s \in E(T)} e_r \, e_s \geq e_k^* \, e_{d+1}^* - e_k \, e_j > 0.$$

Therefore we have

$$E_i(T^*) > E_i(T), \;\; i = 1, 2.$$

By the above described construction we have increased the value of $E_i(T)$, $i = 1, 2$. If T^* is the path, we are done. If not, then we continue the construction as follows. Next we choose one pendent vertex ($\neq \; v_1, \; v_k$) from T^*, etc. Repeating the procedure sufficient number of times, we arrive at a tree in which the maximum degree 2, that is, we arrive at path P_n.

Lower bound: If T is isomorphic to star $K_{1,n-1}$, then the left hand side equality holds in (2.1) and (2.2). If T is isomorphic to $\tilde{T}_n$, then the left hand side inequality is strict in (2.1) and (2.2). Otherwise, $T \ncong K_{1,n-1} \, , \tilde{T}_n$. Suppose that a path $P_{d+1} \, : \; v_1 v_2 \ldots v_{d+1}$ of length d in T, where d is the diameter of T. Without loss of generality, we can assume that $d_2 \geq d_d$ (the degree of vertex v_2 is greater than or equal to the degree of vertex v_d). Now choose v_i to be an arbitrary maximum degree vertex, unless v_d has maximum degree, in which case v_i is chosen to be v_2. We transform T into another tree $\hat{T}$ by deleting the edge $v_d \, v_{d+1}$ and join the vertices v_i and v_{d+1} by an edge. Let the vertex eccentricities be $\hat{e}_1, \; \hat{e}_2, \ldots, \hat{e}_n$ in tree $\hat{T}$. Similarly, as before we obtain $\hat{e}_t \leq e_t$ for all $t = 1, 2, \ldots, n$. Using above we get

$$E_1(\hat{T}) - E_1(T) = \sum_{v_i \in V(\hat{T})} \hat{e}_i^2 - \sum_{v_i \in V(T)} e_i^2 \leq 0$$

and

$$E_2(\hat{T}) - E_2(T) = \sum_{v_r \, v_s \in E(\hat{T})} \hat{e}_r \, \hat{e}_s - \sum_{v_r \, v_s \in E(T)} e_r \, e_s \leq 0.$$

Therefore we have

$$E_i(\hat{T}) \leq E_i(T), \;\; i = 1, 2.$$

By the above described construction we have non-increased the value of $E_i(T)$, $i = 1, 2$. If $\hat{T}$ is to the tree $\tilde{T}_n$, we are done. If not, then we continue the construction as follows. Next we choose one pendent vertex from longest path in $\hat{T}$ such that its adjacent vertex is not maximum degree vertex. Now we delete that pendent edge and join the pendent vertex to the maximum degree vertex, etc. Repeating the procedure sufficient number of times, we arrive at a tree in which the maximum degree $n-2$, that is, we arrive at tree $\tilde{T}_n$. This completes the proof. □

We now give lower and upper bounds on the Zagreb eccentricity indices of bipartite graph.

Theorem 2.2. Let G be a connected bipartite graph of order n with bipartition $V(G) = U \cup W$, $U \cap W = \emptyset$, $|U| = p$ and $|W| = q$. Then

$$\text{(i)} \qquad E_1(K_{p,q}) \leq E_1(G) \leq E_1(P_n) \tag{2.3}$$

$$\text{and (ii)} \qquad E_2(K_{p,q}) \leq E_2(G) \leq E_2(P_n). \tag{2.4}$$

Moreover, the left hand side (right hand side, respectively) equality holds in (2.3) and (2.4) if and only if $G \cong K_{p,q}$ ($G \cong P_n$, respectively).

Proof. If G is isomorphic to a complete bipartite graph $K_{p,q}$, then the left hand side equality holds in (2.3) and (2.4). Otherwise, $G \ncong K_{p,q}$. If we add an edge in G, then each vertex eccentricity will non-increase. Thus we have $e_i(G+e) \leq e_i(G)$. Using this property, one can see easily that $E_1(G) \geq E_1(K_{p,q} \backslash \{e\}) > E_1(K_{p,q})$ and $E_2(G) \geq E_2(K_{p,q} \backslash \{e\}) > E_2(K_{p,q})$, where e is any edge in $K_{p,q}$.

Let T be a spanning tree of connected bipartite graph G. Then by the above property, $E_1(G) \leq E_1(T)$ and $E_2(G) \leq E_2(T)$. Using this result with Theorem 2.1, we get the right hand side inequality in (2.3) and (2.4). Moreover, the right hand side equality holds in (2.3) and (2.4) if and only if $G \cong P_n$. This completes the proof. □

In [10], Hua et al. proved the following result in Theorem 3.1.

Lemma 2.3. Let G be a connected graph with $e_i = n - d_i$ for any vertex $v_i \in V(G)$. If $G \ncong P_4$, then $e_i \leq 2$ for any vertex $v_i \in V(G)$.

We now give some relation between first Zagreb index and the first Zagreb eccentricity index of graphs.

Theorem 2.4. Let G be a connected graph of order n with m edges. Then

$$E_1(G) \leq M_1(G) - 4mn + n^3, \tag{2.5}$$

where $M_1(G)$ is the first Zagreb index in G. Moreover, the equality holds in (2.5) if and only if $G \cong P_4$ or $G \cong K_n$ or G is isomorphic to a $(n-1, n-2)$-semiregular graph.

Proof. If $G \cong P_4$, then the equality holds in (2.5). Otherwise, $G \ncong P_4$. Now,

$$\begin{aligned} E_1(G) = \sum_{v_i \in V(G)} e_i^2 \leq \sum_{v_i \in V(G)} (n-d_i)^2 \ \text{ as } e_i \leq n - d_i \\ = M_1(G) - 4mn + n^3 \ \text{ as } M_1(G) = \sum_{v_i \in V(G)} d_i^2, \sum_{v_i \in V(G)} d_i = 2m. \end{aligned}$$

First part of the proof is over.

Now suppose that equality holds in (2.5). Then $e_i = n - d_i$ for all $v_i \in V(G)$. By Lemma 2.3, we conclude that $e_i \leq 2$ for any vertex $v_i \in V(G)$ as $G \ncong P_4$. Since $e_i = n - d_i$ for any vertex $v_i \in V(G)$, we must have $d_i = n-1$ or $n-2$ for any vertex $v_i \in V(G)$, that is, $G \cong K_n$ or G is isomorphic to a $(n-1, n-2)$-semiregular graph.

Conversely, one can see easily that (2.5) holds for P_4 or K_n or $(n-1, n-2)$-semiregular graph. □

Remark 2.5. $(n-1, n-2)$-semiregular graph is obtained by deleting i independent edges from K_n, $1 \leq i \leq \lfloor \frac{n}{2} \rfloor$.

We now give some relation between first Zagreb index, second Zagreb index and the second Zagreb eccentricity index of graphs.

Theorem 2.6. Let G be a connected graph of order n with m edges. Then

$$E_2(G) \leq M_2(G) - nM_1(G) + mn^2, \tag{2.6}$$

where $M_1(G)$ is the first Zagreb index, $M_2(G)$ is the second Zagreb index in G. Moreover, the equality holds in (2.6) if and only if $G \cong P_4$ or $G \cong K_n$ or G is isomorphic to a $(n-1, n-2)$-semiregular graph.

Proof. Now,

$$\begin{aligned} E_2(G) &= \sum_{v_i v_j \in E(G)} e_i \cdot e_j \\ &\leq \sum_{v_i v_j \in E(G)} (n-d_i)(n-d_j) \ \text{ as } e_i \leq n - d_i \text{ and } e_j \leq n - d_j \\ &= \sum_{v_i v_j \in E(G)} \Big(n^2 + d_i d_j - (d_i + d_j)n\Big) \\ &= M_2(G) - nM_1(G) + mn^2. \end{aligned}$$

First part of the proof is over. Moreover, one can see easily that the equality holds in (2.6) if and only if $G \cong P_4$ or $G \cong K_n$ or G is isomorphic to a $(n-1, n-2)$-semiregular graph, by the proof of Theorem 2.4. □

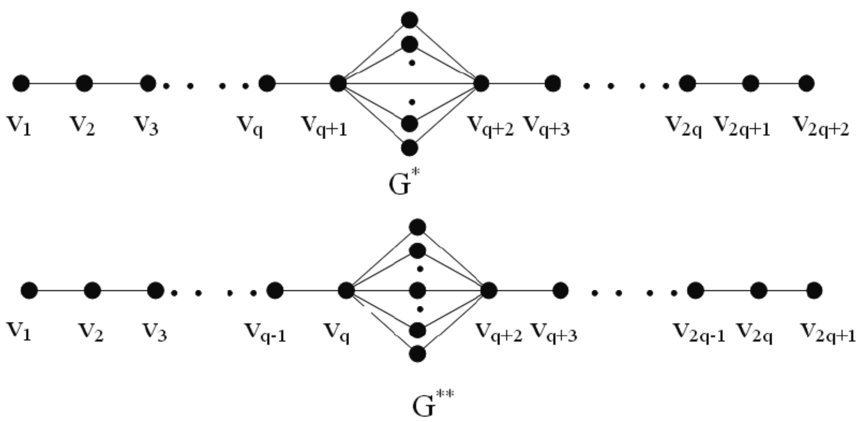

Figure 1: Graphs G^* and G^{**}.

Let $K^1_{2,a-2}$ be a connected graph of order a obtained from the complete bipartite graph $K_{2,a-2}$ with the vertices of degree $a-2$ are adjacent. Denote by G^*, is a connected graph of order n, obtained from $K^1_{2,n-2q-2}$ by attaching two paths P_{q+1} to two of its vertices of degree $n-2q-1$. Let Γ_1 be the class of graphs $H_1 = (V, E)$ such that H_1 is connected graph of diameter d ($d = 2q+1$) with $V(G^*) = V(H_1)$ and $E(G^*) \subseteq E(H_1)$.

Let $K^2_{3,a-2}$ be a connected graph of order $a+1$ obtained from the complete bipartite graph $K_{2,a-2}$ with the vertices of degree $a-2$ are adjacent to a new vertex. Denote by G^{**}, is a connected graph of order n, obtained from $K^2_{3,n-2q-1}$ by attaching two paths P_q to two of its vertices of degree $n-2q$. Let Γ_2 be the class of graphs $H_2 = (V, E)$ such that H_2 is connected graph of diameter d ($d = 2q+2$) with $V(G^*) = V(H_2)$ and $E(G^*) \subseteq E(H_2)$.

We now give another lower bound on $E_1(G)$ in terms of n, d and also characterize the extremal graphs.

Theorem 2.7. Let G be a connected graph of order n with diameter d. Then

$$E_1(G) \geq \begin{cases} \frac{1}{12}\,(3nd^2 + 6nd + 3n + 4d^3 + 3d^2 - 4d - 3) & \text{if } d+1 \text{ is even} \\ \frac{d}{12}\,(3nd + 4d^2 + 9d + 2) & \text{if } d+1 \text{ is odd} \end{cases} \tag{2.7}$$

with equality holding if and only if $G \cong P_n$ or $G \in \Gamma_1$ or $G \in \Gamma_2$.

Proof. Since G has diameter d, G contains a path P_{d+1}: $v_1\, v_2\, \ldots, v_{d+1}$. Moreover, $n \geq d+1$ and $e_i \geq \lceil \frac{d}{2} \rceil$, $i = 1, 2, \ldots, n$. If $n = d+1$, then $G \cong P_n$ and the equality holds in (2.7). Otherwise, $n > d+1$. By (1.3), we get

$$\sum_{i=1}^{d+1} e_i^2 = \begin{cases} \frac{d}{12}\,(7d^2 + 12d + 5) & \text{if } d+1 \text{ is even} \\ \frac{d}{12}\,(7d^2 + 12d + 2) & \text{if } d+1 \text{ is odd.} \end{cases} \tag{2.8}$$

Since $e_i \geq \left\lceil \frac{d}{2} \right\rceil$, $i = 1, 2, \ldots, n$, using above result, we get

$$\begin{aligned} E_1(G) &= \sum_{i=1}^{d+1} e_i^2 + \sum_{i=d+2}^{n} e_i^2 \\ &\geq \begin{cases} \frac{d}{12}\,(7d^2 + 12d + 5) + (n-d-1)\lceil \frac{d}{2} \rceil^2 & \text{if } d+1 \text{ is even} \\ \frac{d}{12}\,(7d^2 + 12d + 2) + \frac{1}{4}\,(n-d-1)d^2 & \text{if } d+1 \text{ is odd,} \end{cases} \end{aligned} \tag{2.9}$$

from which we get the required result (2.7). First part of the proof is over.

Now suppose that equality holds in (2.7) with $n > d+1$. From equality in (2.9), we get

$$e_i = \left\lceil \frac{d}{2} \right\rceil \quad \text{for } i = d+2, d+3, \ldots, n.$$

Using above result we conclude that all the vertices $v_{d+2}, v_{d+3}, \ldots, v_{n-1}$ and v_n are adjacent to vertices v_q and v_{q+2} (when $d = 2q$), or v_{q+1} and v_{q+2} (when $d = 2q+1$). Hence $G \in \Gamma_1$ or $G \in \Gamma_2$.

Conversely, one can see easily that (2.7) holds for path P_n or graph G, where $G \in \Gamma_1$ or $G \in \Gamma_2$. $\square$

We now give another lower bound on $E_2(G)$ in terms of m, d and also characterize the extremal graphs.

Theorem 2.8. Let G be a connected graph of order n with diameter d. Then

$$E_2(G) \geq \begin{cases} \frac{1}{12}\,(3md^2+6md+4d^3-6d^2-4d+3m+6) & \text{if } d+1 \text{ is even} \\ \frac{d}{12}\,(3md+4d^2-4) & \text{if } d+1 \text{ is odd} \end{cases} \tag{2.10}$$

with equality holding if and only if $G \cong P_n$ or $G \in \Gamma_1$ or $G \in \Gamma_2$.

Proof. By (1.3), we get

$$\sum_{v_iv_j \in E(P_{d+1})} e_i\, e_j = \begin{cases} \frac{d+1}{12}\,(7d^2-7d+6) & \text{if } d+1 \text{ is even} \\ \frac{d}{12}\,(7d^2-4) & \text{if } d+1 \text{ is odd.} \end{cases} \tag{2.11}$$

Since $e_i \geq \left\lceil \frac{d}{2} \right\rceil$, $i = 1\,, 2\,, \ldots\,, n$, we have

$$\begin{aligned} E_2(G) &= \sum_{v_iv_j \in E(P_{d+1})} e_i\, e_j + \sum_{v_iv_j \in E(G \setminus P_{d+1})} e_i\, e_j \\ &\geq \begin{cases} \frac{d+1}{12}\,(7d^2-7d+6) + (m-d)\lceil \frac{d}{2} \rceil^2 & \text{if } d+1 \text{ is even} \\ \frac{d}{12}\,(7d^2-4) + \frac{1}{4}\,(m-d)d^2 & \text{if } d+1 \text{ is odd,} \end{cases} \end{aligned}$$

from which we get the required result (2.10). Rest of the proof is similar as Theorem 2.7. □

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