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On Eccentricity Version of Zagreb Coindices

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Abstract

The eccentric connectivity coindex has recently been introduced (Hua and Miao, 2019) as the total eccentricity sum of all pairs of non-adjacent vertices in a graph. Considering the total eccentricity product of non-adjacent vertex pairs, we introduce here another invariant of connected graphs called the second Zagreb eccentricity coindex. We study some mathematical properties of the eccentric connectivity coindex and second Zagreb eccentricity coindex. We also determine the extremal values of the second Zagreb eccentricity coindex over some specific families of graphs such as trees, unicyclic graphs, connected graphs, and connected bipartite graphs and describe the extremal graphs. Moreover, we compare the second Zagreb eccentricity coindex with the eccentric connectivity coindex and give directions for further studies.

Keywords: distance in graph, vertex eccentricity, bound, extremal graphs.

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1. Introduction

A *graph invariant* or *topological index* is a real value directly derived from the structural graph of a molecule. It has been applied in theoretical chemistry for modelling different properties of molecules such as physico-chemical, biological, and pharmaceutical properties. Various graph invariants related to graph theoretical concept of eccentricity have already been suggested and used in QSAR/QSPR researches. Most of them have been recognized as efficient tools in predicting pharmaceutical properties. Here, we concentrate to two of these invariants known as

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the eccentric connectivity and second Zagreb eccentricity indices. These invariants are respectively expressed as the sum of eccentricity sum and the sum of eccentricity product of all pairs of adjacent vertices in a graph. Recently, Hua and Miao [21] introduced the eccentric connectivity coindex as the sum of eccentricity sum of all pairs of non-adjacent vertices. Considering the sum of eccentricity product of all pairs of non-adjacent vertices, we suggest here another graph invariant namely the second Zagreb eccentricity coindex. The idea of introducing the coindex related to a topological index was put forward by Došlić [10] in 2008 with the aim of improving the ability of quantifying the contributions of non-adjacent vertex pairs to different properties of molecules. The first and second Zagreb indices [17, 18] are the first topological indices for which the concept of coindex was applied. The motivation for introducing the eccentric connectivity coindex (second Zagreb eccentricity coindex, resp.) is that this invariant has a parallel form to the first (second, resp.) Zagreb coindex.

Hua and Miao [21] studied some extremal problems related to the eccentric connectivity coindex and gave several lower bounds on this invariant based on different parameters of graphs. The present author [6] investigated the behavior of the eccentric connectivity coindex for various product graphs. Several bounds on the eccentric connectivity coindex in terms of some existing invariants and the values of this coindex for some constructions on graphs were presented in [7].

The rest of the paper is as follows. In Section 2, we remind a number of preliminary definitions and lemmas. In Section 3, exact values of the eccentric connectivity and second Zagreb eccentricity coindices for some familiar graphs are derived and certain fundamental properties of these invariants are described. In Section 4, extremal graphs with respect to the second Zagreb eccentricity coindex among connected graphs, connected bipartite graphs, trees and unicyclic graphs with fixed number of vertices and among connected graphs with fixed number of vertices and edges are characterized and a Nordhaus-Gaddum-type result for this invariant is given. In Section 5, we compare the eccentric connectivity coindex and second Zagreb eccentricity coindex with each other and eventually in Section 6, we provide a conclusion and give directions for subsequent studies.

2. Definitions and Preliminaries

All over this section, Γ is considered to be a simple connected graph with order n and size m. The vertex and edge sets of Γ are respectively shown by $V(\Gamma)$ and $E(\Gamma)$. The complement $\overline{\Gamma}$ of Γ is a graph in which $V(\overline{\Gamma}) = V(\Gamma)$ and $u_\Gamma v_\Gamma \in E(\overline{\Gamma})$ if and only if $u_\Gamma v_\Gamma \notin E(\Gamma)$. The notation $\overline{m}$ represents the size of $\overline{\Gamma}$ which equals $\binom{n}{2} - m$. For vertices $u_\Gamma, v_\Gamma \in V(\Gamma)$, the degree of u_Γ and the distance between u_Γ, v_Γ in Γ are denoted by $d_\Gamma(u_\Gamma)$ and $d_\Gamma(u_\Gamma, u_\Gamma)$, respectively. The eccentricity $\varepsilon_\Gamma(u_\Gamma)$ of $u_\Gamma \in V(\Gamma)$ is defined as $\varepsilon_\Gamma(u_\Gamma) = \max_{v_\Gamma \in V(\Gamma)} d_\Gamma(u_\Gamma, v_\Gamma)$. The radius (diameter, resp.) $r(\Gamma)$ ($d(\Gamma)$, resp.) of Γ is the smallest (greatest, resp.) eccentricity of all vertices in Γ. If $d(\Gamma) = r(\Gamma)$, then Γ is self-centered. If Γ

is self-centered and $d(\Gamma) = 2$, then it is called 2-self-centered. A vertex $u_\Gamma \in V(\Gamma)$ with $d_\Gamma(u_\Gamma) = n - 1$ is known as a universal vertex. A spanning tree of Γ is a subgraph $\mathcal{T}$ of Γ with $V(\mathcal{T}) = V(\Gamma)$ which is a tree. For $e_\Gamma \in E(\Gamma)$, $\Gamma - e_\Gamma$ is a graph made from Γ by deleting the edge e_Γ and preserving the end-vertices of e_Γ.

The invariants $M_1(\Gamma)$ and $M_2(\Gamma)$ defined as

$$M_1(\Gamma) = \sum_{u_\Gamma \in V(\Gamma)} d_\Gamma(u_\Gamma)^2 = \sum_{u_\Gamma v_\Gamma \in E(\Gamma)} (d_\Gamma(u_\Gamma) + d_\Gamma(v_\Gamma)),$$
$$M_2(\Gamma) = \sum_{u_\Gamma v_\Gamma \in E(\Gamma)} d_\Gamma(u_\Gamma) d_\Gamma(v_\Gamma),$$

are called the *first and second Zagreb indices* of Γ (see [17]). The coindices of Zagreb indices were put forward by Doslić [10] as

$$\overline{M}_1(\Gamma) = \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \big(d_\Gamma(u_\Gamma) + d_\Gamma(v_\Gamma)\big),$$
$$\overline{M}_2(\Gamma) = \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} d_G(u_\Gamma) d_G(v_\Gamma).$$

More details on Zagreb indices and coindices can be searched in the survey [1], the papers [3, 16, 20, 24], and the references quoted therein.

In 1997, Sharma *et al.* [25] suggested the *eccentric connectivity index* of Γ as

$$\xi^c(\Gamma) = \sum_{u_\Gamma \in V(\Gamma)} d_\Gamma(u_\Gamma) \varepsilon_\Gamma(u_\Gamma) = \sum_{u_\Gamma v_\Gamma \in E(\Gamma)} \big(\varepsilon_\Gamma(u_\Gamma) + \varepsilon_\Gamma(v_\Gamma)\big).$$

The invariants $\zeta(\Gamma)$ and $\xi^{(2)}(\Gamma)$ defined as $\zeta(\Gamma) = \sum_{u_\Gamma \in V(\Gamma)} \varepsilon_\Gamma(u_\Gamma)$ and

$$\xi^{(2)}(\Gamma) = \sum_{u_\Gamma \in V(\Gamma)} d_\Gamma(u_\Gamma) \varepsilon_\Gamma(u_\Gamma)^2 = \sum_{u_\Gamma v_\Gamma \in E(\Gamma)} \big(\varepsilon_\Gamma(u_\Gamma)^2 + \varepsilon_\Gamma(v_\Gamma)^2\big),$$

are respectively called the *total eccentricity* and *second eccentric connectivity index* [5] of Γ. Some properties of the eccentric connectivity index have been investigated in [2, 4, 11, 26, 28].

The *first, second, and third Zagreb eccentricity indices* ([27, 29]) of Γ are respectively defined as

$$E_1(\Gamma) = \sum_{u_\Gamma \in V(\Gamma)} \varepsilon_\Gamma(u_\Gamma)^2,$$
$$E_2(\Gamma) = \sum_{u_\Gamma v_\Gamma \in E(\Gamma)} \varepsilon_\Gamma(u_\Gamma) \varepsilon_\Gamma(v_\Gamma),$$
$$E_3(\Gamma) = \sum_{u_\Gamma v_\Gamma \in E(\Gamma)} \left|\varepsilon_\Gamma(u_\Gamma) - \varepsilon_\Gamma(v_\Gamma)\right|.$$

Further information regarding the Zagreb eccentricity indices can be found in [5, 8, 19, 23].

In 2019, Hua and Miao [21] proposed the *eccentric connectivity coindex* (or ECC for short) of Γ as

$$\overline{\xi}^c(\Gamma) = \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \big(\varepsilon_\Gamma(u_\Gamma) + \varepsilon_\Gamma(v_\Gamma)\big).$$

An alternative formula for ECC was given in [21] as

$$\overline{\xi}^c(\Gamma) = \sum_{u_\Gamma \in V(\Gamma)} \big(n - 1 - d_\Gamma(u_\Gamma)\big)\varepsilon_\Gamma(u_\Gamma). \tag{1}$$

By considering the sum of eccentricity product of non-adjacent pairs of vertices in Γ, we introduce here another invariant of Γ which we call the *second Zagreb eccentricity coindex* (or SZEC for short). More formally, the SZEC of Γ is defined as

$$\overline{E}_2(\Gamma) = \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma).$$

We close this section with expressing two previously-proved lemmas.

Lemma 2.1. [30] If $d(\Gamma) > 3$ and $\overline{\Gamma}$ is connected, then $d(\overline{\Gamma}) = 2$.

Lemma 2.2. [5] For any connected graph Γ,

$$\xi^{(2)}(\Gamma) = E_3(\Gamma) + 2E_2(\Gamma). \tag{2}$$

3. Some Properties of Coindices

Here, we explore some fundamental properties of the ECC and SZEC. The following results on the values of these invariants for r-vertex path, r-vertex cycle, r-vertex star, r-vertex complete graph, and complete bipartite graph on $r + s$ vertices are deduced by an easy computation.

Lemma 3.1. *The following relations hold:*

(i) $\overline{\xi}^c(P_r) = \begin{cases} \frac{1}{4}(r-2)(3r^2 - 5r + 4) & 2 \mid r, \\ \frac{1}{4}(r-1)^2(3r-5) & 2 \nmid r, \end{cases}$

$\overline{E}_2(P_r) = \begin{cases} \frac{1}{32}r(r-2)(9r^2 - 22r + 28) & 2 \mid r, \\ \frac{1}{32}(r-1)(9r^3 - 31r^2 + 35r - 5) & 2 \nmid r, \end{cases}$

(ii) $\overline{\xi}^c(C_r) = r(r-3)\lfloor \frac{r}{2} \rfloor$, $\overline{E}_2(C_r) = \frac{1}{2}r(r-3)\lfloor \frac{r}{2} \rfloor^2$,

(iii) $\overline{\xi}^c(S_r) = \overline{E}_2(S_r) = 2(r-1)(r-2)$,

(iv) $\overline{\xi}^c(K_r) = \overline{E}_2(K_r) = 0$,

(v) $\overline{\xi}^c(K_{r,s}) = \overline{E}_2(K_{r,s}) = 2r(r-1) + 2s(s-1)$.

Theorem 3.2. *For n-vertex connected graph Γ,*

$$\overline{\xi}^c(\Gamma) = (n-1)\zeta(\Gamma) - \xi^c(\Gamma), \tag{3}$$

$$\overline{E}_2(\Gamma) = \frac{1}{2}\big(\zeta(\Gamma)^2 - E_1(\Gamma)\big) - E_2(\Gamma). \tag{4}$$

Proof. Equation (3) follows from Equation (1), straightforwardly. To prove Equation (4), we start with the identity

$$\sum_{u_\Gamma \in V(\Gamma)} \sum_{v_\Gamma \in V(\Gamma)} \varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma) = \zeta(\Gamma)^2.$$

The left-hand side summation in the above relation can be partitioned as follows.

$$\begin{aligned}\sum_{u_\Gamma \in V(\Gamma)} \sum_{v_\Gamma \in V(\Gamma)} \varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma) =& 2 \sum_{u_\Gamma v_\Gamma \in E(\Gamma)} \varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma) \\ &+ 2 \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma) + \sum_{u_\Gamma \in V(\Gamma)} \varepsilon_\Gamma(u_\Gamma)^2 \\ =& 2E_2(\Gamma) + 2\overline{E}_2(\Gamma) + E_1(\Gamma).\end{aligned}$$

Combining the above relations, we arrive at $\zeta(\Gamma)^2 = 2E_2(\Gamma) + 2\overline{E}_2(\Gamma) + E_1(\Gamma)$, from which Equation (4) is deduced. □

Theorem 3.3. *Let both Γ and $\overline{\Gamma}$ be connected, Γ be of size m and $d(\Gamma) > 3$. Then*

$$\xi^c(\overline{\Gamma}) = E_2(\overline{\Gamma}) = 4\overline{m}, \qquad \overline{\xi}^c(\overline{\Gamma}) = \overline{E}_2(\overline{\Gamma}) = 4m.$$

Proof. The graph $\overline{\Gamma}$ has no universal vertices as Γ is connected. Now by Lemma 2.1, one can deduce that $\overline{\Gamma}$ is 2-self-centered. So

$$\begin{aligned}\xi^c(\overline{\Gamma}) &= \sum_{u_\Gamma v_\Gamma \in E(\overline{\Gamma})} \big(\varepsilon_{\overline{\Gamma}}(u_\Gamma) + \varepsilon_{\overline{\Gamma}}(v_\Gamma)\big) = \sum_{u_\Gamma v_\Gamma \in E(\overline{\Gamma})} (2+2) = 4\overline{m}, \\ \overline{\xi}^c(\overline{\Gamma}) &= \sum_{u_\Gamma v_\Gamma \notin E(\overline{\Gamma})} \big(\varepsilon_{\overline{\Gamma}}(u_\Gamma) + \varepsilon_{\overline{\Gamma}}(v_\Gamma)\big) = \sum_{u_\Gamma v_\Gamma \in E(\Gamma)} (2+2) = 4m.\end{aligned}$$

Similarly, we can prove that $E_2(\overline{\Gamma}) = 4\overline{m}$ and $\overline{E}_2(\overline{\Gamma}) = 4m$. □

4. Extremal Results

In this section, some extremal problems related to the SZEC are studied.

Theorem 4.1. *For any connected graph* Γ *of order* n *and size* m*,*

$$\overline{E}_2(\Gamma) \geq \ 4\overline{m}, \tag{5}$$

and the equality case occurs if and only if $d(\Gamma) \leq 2$*.*

Proof. Evidently, for any $u_\Gamma v_\Gamma \notin E(\Gamma)$, $\varepsilon_\Gamma(u_\Gamma), \varepsilon_\Gamma(v_\Gamma) \geq 2$. Now from the definition of the SZEC,

$$\overline{E}_2(\Gamma) = \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma) \geq \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} (2 \times 2) = 4\overline{m},$$

and Equation (5) holds. The equality case occurs in Equation (5) if and only if for any $u_\Gamma v_\Gamma \notin E(\Gamma)$, $\varepsilon_\Gamma(u_\Gamma) = \varepsilon_\Gamma(v_\Gamma) = 2$, which is equivalent to $d(\Gamma) \leq 2$. □

As a consequence of Theorem 4.1, we arrive at:

Corollary 4.2. *For any connected unicyclic graph* Γ *with* $n \geq 6$ *vertices,*

$$\overline{E}_2(\Gamma) \geq 2n(n-3),$$

and the equality case occurs if and only if Γ *is made from* S_n *by joining two of its pendent vertices with an edge.*

Now we use Theorem 4.1 to give a Nordhaus-Gaddum-type result for the SZEC.

Corollary 4.3. *For any connected graph* Γ *of order* n *with a connected complement* $\overline{\Gamma}$*,*

$$\overline{E}_2(\Gamma) + \overline{E}_2(\overline{\Gamma}) \geq 2n(n-1), \tag{6}$$

and the equality case occurs if and only if Γ *and* $\overline{\Gamma}$ *are* 2*-self centered.*

Proof. Let $|E(\Gamma)| = m$. From Theorem 4.1, we get

$$\overline{E}_2(\Gamma) + \overline{E}_2(\overline{\Gamma}) \geq 4\overline{m} + 4m = 2n(n-1),$$

and the inequality in Equation (6) holds. Based on Theorem 4.1, the equality case occurs in Equation (6) if and only if $d(\Gamma), d(\overline{\Gamma}) \leq 2$. Since both Γ and $\overline{\Gamma}$ are connected, they contain no universal vertices. Hence the equality case occurs in Equation (6) if and only if Γ and $\overline{\Gamma}$ are 2-self centered. □

Theorem 4.4. *For any tree* $\mathcal{T}$ *of order* n*,*

$$\overline{E}_2(S_n) \leq \overline{E}_2(\mathcal{T}) \leq \overline{E}_2(P_n). \tag{7}$$

Moreover, the equality in left-hand side (right-hand side, resp.) of Equation (7) *happens if and only if* $\mathcal{T} \cong S_n$ ($\mathcal{T} \cong P_n$*, resp.).*

Proof. Based on Theorem 4.1,

$$\overline{E}_2(\mathcal{T}) \geq \ 4\left(\binom{n}{2} - (n-1)\right) = 2(n-1)(n-2) = \overline{E}_2(S_n),$$

and the equality case occurs if and only if $\mathcal{T}$ has diameter at most 2. Since the only tree of order n with diameter at most 2 is S_n, so the equality in left-hand side of Equation (7) happens if and only if $\mathcal{T} \cong S_n$.

We proceed with the proof of the right-hand side inequality. Let $d(\mathcal{T}) = d$. If $\mathcal{T} \cong P_n$, then the equality in right-hand side of Equation (7) occurs. Now let $\mathcal{T} \ncong P_n$. This implies that, $n \geq 4$, $d \leq n-2$, and $\mathcal{T}$ contains at least three pendent vertices. Let $V(\mathcal{T}) = \{v_1, v_2, \ldots, v_n\}$ and $v_1v_2 \ldots v_{d+1}$ be a diametral path in $\mathcal{T}$. We denote by ε_i the eccentricity of v_i in $\mathcal{T}$, $1 \leq i \leq n$. Hence $\varepsilon_i = \max\{d_{\mathcal{T}}(v_i, v_1), d_{\mathcal{T}}(v_i, v_{d+1})\}$. Since $\mathcal{T}$ is a tree, both v_1 and v_{d+1} are pendent vertices. Thus for every vertex v_i of $\mathcal{T}$, $\varepsilon_i \leq d$. Suppose v_k $(k \neq 1, d+1)$ is a vertex of degree one adjacent to v_j in $\mathcal{T}$. We convert the tree $\mathcal{T}$ into the tree $\mathcal{T}^*$ by removing v_kv_j from $E(\mathcal{T})$ and adding $v_{d+1}v_k$ to $E(\mathcal{T})$. Then $v_1v_2 \ldots v_{d+1}v_k$ is the longest path in $\mathcal{T}^*$ with length $d+1$. Denote the vertex eccentricities in $\mathcal{T}^*$ by $\varepsilon_1^*, \varepsilon_2^*, \ldots, \varepsilon_n^*$. Therefore for every $t \neq k$, $1 \leq t \leq n$, we have

$$\begin{aligned}\varepsilon_t^* = \max\{d_{\mathcal{T}^*}(v_t, v_1), d_{\mathcal{T}^*}(v_t, v_k)\} =& \max\{d_{\mathcal{T}}(v_t, v_1), d_{\mathcal{T}}(v_t, v_{d+1}) + 1\} \\ \geq& \max\{d_{\mathcal{T}}(v_t, v_1), d_{\mathcal{T}}(v_t, v_{d+1})\} = \varepsilon_t,\end{aligned}$$

whereas $\varepsilon_k^* = d + 1 > d \geq \varepsilon_k$. We define

$$\begin{aligned}A =& \{v_rv_s \notin E(\mathcal{T}),\ r, s \neq k\} = \{v_rv_s \notin E(\mathcal{T}^*),\ r, s \neq k\}, \\ B =& \{v_rv_k \notin E(\mathcal{T}),\ r \neq d+1\} = \{v_rv_k \notin E(\mathcal{T}^*),\ r \neq j\}.\end{aligned}$$

Then $E(\overline{\mathcal{T}}) = A \cup B \cup \{v_kv_{d+1}\}$ and $E(\overline{\mathcal{T}^*}) = A \cup B \cup \{v_kv_j\}$. For each $v_rv_s \in A$, $\varepsilon_r^*\varepsilon_s^* \geq \varepsilon_r\varepsilon_s$ and for each $v_rv_k \in B$, $\varepsilon_r^*\varepsilon_k^* = \varepsilon_r^*(d+1) > \varepsilon_r^*d \geq \varepsilon_rd \geq \varepsilon_r\varepsilon_k$. Also,

$$\begin{aligned}\varepsilon_k^*\varepsilon_j^* - \varepsilon_k\varepsilon_{d+1} =& (d+1)\varepsilon_j^* - (\varepsilon_j + 1)d = (\varepsilon_j^* - \varepsilon_j)d + (\varepsilon_j^* - d) \\ \geq& \varepsilon_j^* - d \geq 2 - (n-2) = 4 - n.\end{aligned}$$

Thus

$$\begin{aligned}\overline{E}_2(\mathcal{T}^*) - \overline{E}_2(\mathcal{T}) =& \sum_{v_rv_s \in A} (\varepsilon_r^*\varepsilon_s^* - \varepsilon_r\varepsilon_s) + \sum_{v_rv_k \in B} (\varepsilon_r^*\varepsilon_k^* - \varepsilon_r\varepsilon_k) + (\varepsilon_k^*\varepsilon_j^* - \varepsilon_k\varepsilon_{d+1}) \\ \geq& |B| + (4-n) = (n-3) + (4-n) = 1.\end{aligned}$$

So $\overline{E}_2(\mathcal{T}^*) > \overline{E}_2(\mathcal{T})$. By the procedure described above, the value of $\overline{E}_2(\mathcal{T})$ is increased. If $\mathcal{T}^* \cong P_n$, then $\overline{E}_2(\mathcal{T}) < \overline{E}_2(\mathcal{T}^*) = \overline{E}_2(P_n)$, and the inequality in right-hand side of Equation (7) holds. If $\mathcal{T}^* \ncong P_n$, then the procedure can be continued as follows. Select a pendent vertex $(\neq v_1, v_k)$ from $\mathcal{T}^*$, etc. Repeat the process sufficiently, we get a tree having the maximum degree 2, which is the path P_n. □

Lemma 4.5. *For each edge $e_\Gamma = a_\Gamma b_\Gamma \in E(\Gamma)$ for which $\Gamma - e_\Gamma$ is connected,*

$$\overline{E}_2(\Gamma - e_\Gamma) > \overline{E}_2(\Gamma).$$

Proof. It was proved in [22] that, for each $u_\Gamma \in V(\Gamma - e_\Gamma) = V(\Gamma)$, $\varepsilon_{\Gamma - e_\Gamma}(u_\Gamma) \geq \varepsilon_\Gamma(u_\Gamma)$. On the other hand, $E(\overline{\Gamma - e_\Gamma}) = E(\overline{\Gamma}) \cup \{e_\Gamma\}$ and $\varepsilon_{\Gamma - e_\Gamma}(a_\Gamma), \varepsilon_{\Gamma - e_\Gamma}(b_\Gamma) \geq 2$, as $e_\Gamma = a_\Gamma b_\Gamma \notin E(\Gamma - e_\Gamma)$. Now from the definition of the SZEC, we have

$$\begin{aligned}\overline{E}_2(\Gamma - e_\Gamma) &= \sum_{u_\Gamma v_\Gamma \notin E(\Gamma - e_\Gamma)} \varepsilon_{\Gamma - e_\Gamma}(u_\Gamma)\varepsilon_{\Gamma - e_\Gamma}(v_\Gamma) \\ &= \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \varepsilon_{\Gamma - e_\Gamma}(u_\Gamma)\varepsilon_{\Gamma - e_\Gamma}(v_\Gamma) + \varepsilon_{\Gamma - e_\Gamma}(a_\Gamma)\varepsilon_{\Gamma - e_\Gamma}(b_\Gamma) \\ &\geq \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma) + 4 = \overline{E}_2(\Gamma) + 4 > \overline{E}_2(\Gamma),\end{aligned}$$

and the proof is completed. □

Theorem 4.6. *For any connected graph Γ on n vertices,*

$$\overline{E}_2(K_n) \leq \overline{E}_2(\Gamma) \leq \overline{E}_2(P_n). \tag{8}$$

Moreover, the equality case in left-hand side (right-hand side, resp.) of Equation (8) happens if and only if $\Gamma \cong K_n$ ($\Gamma \cong P_n$, resp.).

Proof. The proof of the left-hand side inequality in Equation (8) is obvious by considering the fact that $\overline{E}_2(\Gamma) \geq 0 = \overline{E}_2(K_n)$, with equality if and only if $\Gamma \cong K_n$. To prove the right-hand side inequality in Equation (8), suppose $\mathcal{T}$ is a spanning tree of Γ. By Lemma 4.5, $\overline{E}_2(\Gamma) \leq \overline{E}_2(\mathcal{T})$ and the equality case occurs if and only if $\Gamma = \mathcal{T}$. By Theorem 4.4, $\overline{E}_2(\mathcal{T}) \leq \overline{E}_2(P_n)$ and the equality case occurs if and only if $\mathcal{T} \cong P_n$. Hence $\overline{E}_2(\Gamma) \leq \overline{E}_2(P_n)$ and the equality case occurs in Equation (8) if and only if $\Gamma \cong P_n$. □

Theorem 4.7. *Let Γ be a connected bipartite graph on n vertices with bipartition R_Γ and S_Γ, where $|R_\Gamma| = r > 1$ and $|S_\Gamma| = s > 1$. Then*

$$\overline{E}_2(K_{r,s}) \leq \overline{E}_2(\Gamma) \leq \overline{E}_2(P_n). \tag{9}$$

Moreover, the equality in left-hand side (right-hand side, resp.) of Equation (9) happens if and only if $\Gamma \cong K_{r,s}$ ($\Gamma \cong P_n$, resp.).

Proof. From Theorem 4.6, the inequality in right-hand side of Equation (9) holds and the equality case occurs if and only if $\Gamma \cong P_n$. If $\Gamma \cong K_{r,s}$, then the equality in left-hand side of Equation (9) holds trivially. If $\Gamma \ncong K_{r,s}$, then by Lemma 4.5, $\overline{E}_2(\Gamma) \geq \overline{E}_2(K_{r,s} - e) > \overline{E}_2(K_{r,s})$, for each $e \in E(K_{r,s})$ and hence the inequality in left-hand side of Equation (9) holds. □

5. Comparison Between Coindices

In this section, we make a comparison between the SZEC and ECC.

Theorem 5.1. *For any connected graph* Γ,

$$\overline{E}_2(\Gamma) \geq \overline{\xi}^c(\Gamma), \tag{10}$$

and the equality case occurs if and only if $d(\Gamma) \leq 2$.

Proof. Since for any $u_\Gamma v_\Gamma \notin E(\Gamma)$, $\varepsilon_\Gamma(u_\Gamma), \varepsilon_\Gamma(v_\Gamma) \geq 2$, so $\varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma) \geq \varepsilon_\Gamma(u_\Gamma) + \varepsilon_\Gamma(v_\Gamma)$, for each $u_\Gamma v_\Gamma \notin E(\Gamma)$, and the equality case occurs if and only if $\varepsilon_\Gamma(u_\Gamma) = \varepsilon_\Gamma(v_\Gamma) = 2$. The inequality in Equation (10) now follows by summing both sides of the previous inequality over all non-adjacent vertex pairs of Γ. The equality case occurs in Equation (10) if and only if for any $u_\Gamma v_\Gamma \notin E(\Gamma)$, $\varepsilon_\Gamma(u_\Gamma) = \varepsilon_\Gamma(v_\Gamma) = 2$, which is equivalent to $d(\Gamma) \leq 2$. □

Theorem 5.2. *For any connected graph* Γ,

$$\overline{E}_2(\Gamma) \leq \frac{d(\Gamma)}{2}\overline{\xi}^c(\Gamma), \tag{11}$$

and the equality case occurs if and only if Γ *is self-centered or* $r(\Gamma) = 1$ *and* $d(\Gamma) = 2$.

Proof. Evidently, for each $u_\Gamma \in V(\Gamma)$, $\varepsilon_\Gamma(u_\Gamma) \leq d(\Gamma)$. Now by arithmetic-geometric mean inequality, we get

$$\begin{aligned}\overline{E}_2(\Gamma) = \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma) &= \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \sqrt{\varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma)}\sqrt{\varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma)} \\ &\leq \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \sqrt{d(\Gamma)d(\Gamma)}\sqrt{\varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma)} \\ &\leq d(\Gamma) \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \frac{\varepsilon_\Gamma(u_\Gamma) + \varepsilon_\Gamma(v_\Gamma)}{2} = \frac{d(\Gamma)}{2}\overline{\xi}^c(\Gamma).\end{aligned}$$

The equality case occurs if and only if for each $u_\Gamma v_\Gamma \notin E(\Gamma)$, $\varepsilon_\Gamma(u_\Gamma) = \varepsilon_\Gamma(v_\Gamma) = d(\Gamma)$. In case Γ is self-centered or $r(\Gamma) = 1$ and $d(\Gamma) = 2$, the equality case occurs in Equation (11). Now let the equality hold in Equation (11). If $r(\Gamma) = d(\Gamma) = 1$, then Γ is self-centered. If $r(\Gamma) = 1$ and $d(\Gamma) = 2$, then there exists nothing to prove. Now suppose that, $r(\Gamma) \geq 2$. Let u_Γ denote a vertex of Γ such that $\varepsilon_\Gamma(u_\Gamma) = r(\Gamma) \geq 2$. Then there is a vertex $v_\Gamma \in V(\Gamma)$ with $u_\Gamma v_\Gamma \notin E(\Gamma)$. Thus $r(\Gamma) = \varepsilon_\Gamma(u_\Gamma) = \varepsilon_\Gamma(v_\Gamma) = d(\Gamma)$, which means that Γ is self-centered. □

Theorem 5.3. *For any connected graph* Γ *on* n *vertices and* m *edges,*

$$\overline{\xi}^c(\Gamma)^2 \leq \overline{m}\Big((n-1)E_1(\Gamma) - \xi^{(2)}(\Gamma) + 2\overline{E}_2(\Gamma)\Big), \tag{12}$$

and the equality case occurs if and only if Γ *is self-centered or* $r(\Gamma) = 1$ *and* $d(\Gamma) = 2$.

Proof. By definition of ECC and Cauchy-Schwartz inequality, we get

$$\begin{aligned}
\overline{\xi}^{c}(\Gamma)^{2} =&\Big(\sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \big(\varepsilon_\Gamma(u_\Gamma)+\varepsilon_\Gamma(v_\Gamma)\big)\Big)^{2} \leq \overline{m} \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \big(\varepsilon_\Gamma(u_\Gamma)+\varepsilon_\Gamma(v_\Gamma)\big)^{2}\\
=&\overline{m} \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \big(\varepsilon_\Gamma(u_\Gamma)^2+\varepsilon_\Gamma(v_\Gamma)^2+2\varepsilon_\Gamma(u_\Gamma)\varepsilon_\Gamma(v_\Gamma)\big)\\
=&\overline{m}\Big(\sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \big(\varepsilon_\Gamma(u_\Gamma)^2+\varepsilon_\Gamma(v_\Gamma)^2\big)+2\overline{E}_2(\Gamma)\Big)\\
=&\overline{m}\Big(\sum_{u_\Gamma \in V(\Gamma)} \big(n-1-d_\Gamma(u_\Gamma)\big)\varepsilon_\Gamma(u_\Gamma)^2+2\overline{E}_2(\Gamma)\Big)\\
=&\overline{m}\Big((n-1)E_1(\Gamma)-\xi^{(2)}(\Gamma)+2\overline{E}_2(\Gamma)\Big).
\end{aligned}$$

By Cauchy-Schwartz inequality, the equality case occurs in Equation (12) if and only if for any $u_\Gamma v_\Gamma, z_\Gamma t_\Gamma \notin E(\Gamma)$, $\varepsilon_\Gamma(u_\Gamma)+\varepsilon_\Gamma(v_\Gamma) = \varepsilon_\Gamma(z_\Gamma)+\varepsilon_\Gamma(t_\Gamma)$. If Γ is self-centered or $r(\Gamma) = 1$ and $d(\Gamma) = 2$, then the equality case in Equation(12) occurs. Now let the equality hold in Equation (12). If $r(\Gamma) = d(\Gamma) = 1$, then Γ is self-centered. If $r(\Gamma) = 1$ and $d(\Gamma) = 2$, then there exists nothing to prove. Now consider the case that, $r(\Gamma) \geq 2$. Then there are $x_\Gamma, y_\Gamma \in V(\Gamma)$ such that $x_\Gamma y_\Gamma \notin E(\Gamma)$ and $\varepsilon_\Gamma(x_\Gamma) = r(\Gamma)$. On the other hand, there exist $a_\Gamma, b_\Gamma \in V(\Gamma)$ with $a_\Gamma b_\Gamma \notin E(\Gamma)$ and $\varepsilon_\Gamma(a_\Gamma) = \varepsilon_\Gamma(b_\Gamma) = d(\Gamma)$. Since the equality holds in Equation (12), $\varepsilon_\Gamma(a_\Gamma)+\varepsilon_\Gamma(b_\Gamma) = \varepsilon_\Gamma(x_\Gamma)+\varepsilon_\Gamma(y_\Gamma)$, and we obtain

$$\begin{aligned}
[d(\Gamma)-r(\Gamma)]+[d(\Gamma)-\varepsilon_\Gamma(y_\Gamma)] =&[\varepsilon_\Gamma(a_\Gamma)-\varepsilon_\Gamma(x_\Gamma)]+[\varepsilon_\Gamma(b_\Gamma)-\varepsilon_\Gamma(y_\Gamma)]\\
=&[\varepsilon_\Gamma(a_\Gamma)+\varepsilon_\Gamma(b_\Gamma)]-[\varepsilon_\Gamma(x_\Gamma)+\varepsilon_\Gamma(y_\Gamma)] = 0.
\end{aligned}$$

Using the fact that $d(\Gamma)-r(\Gamma),\ d(\Gamma)-\varepsilon_\Gamma(y_\Gamma) \geq 0$, we get $d(\Gamma) = r(\Gamma)$, hence Γ is self-centered. □

By substituting Equation (2) in Equation (12), we arrive at:

Corollary 5.4. *For any connected graph* Γ *on* n *vertices and* m *edges,*

$$\overline{\xi}^{c}(\Gamma)^{2} \leq \overline{m}\Big((n-1)E_1(\Gamma)-2(E_2(\Gamma)-\overline{E}_2(\Gamma))-E_3(\Gamma)\Big),$$

and the equality case occurs if and only if Γ *is self-centered or* $r(\Gamma) = 1$ *and* $d(\Gamma) = 2$.

6. Concluding Remarks

In this paper, we introduced the SZEC as the eccentricity version of the second Zagreb coindex. We also considered the recently-introduced ECC which is the eccentricity version of the first Zagreb coindex and studied some primary mathematical properties of these invariants. Furthermore, we studied the extremal problems of the SZEC for connected graphs, connected bipartite graphs, trees, and unicyclic graphs of a given number of vertices and for connected graphs of a given number of vertices and edges, and made a comparison between the SZEC and ECC. In particular, we prove that, among all n-vertex trees, the SZEC uniquely gets its maximum value at P_n and its minimum value at S_n. From this fact, this new invariant satisfies a necessary condition for a topological index to be an admissible measure of branching (see [9]).

There exists several open questions for further researches. For instance, one could try to derive exact formulae for the value of the SZEC on certain specific classes of graphs. It would also be interesting to obtain bounds on the SZEC in terms of parameters and invariants of graphs. It is also useful to explore some applications of SZEC to other fields of science including chemistry, biology, computer science, etc. Finally, there exists a class of vertex-eccentricity-based graph invariants of a connected graph Γ as follows:

$$\mathcal{I}(\Gamma) = \sum_{u_\Gamma v_\Gamma \in E(\Gamma)} h(\varepsilon_\Gamma(u_\Gamma), \varepsilon_\Gamma(v_\Gamma)),$$

where $h(u,v)$ is a two-variable real function of u and v with $h(u,v) \geq 0$ and $h(u,v) = h(v,u)$.

If $h(u,v) = u+v$, then $\mathcal{I}(\Gamma) = \xi^c(\Gamma)$, the eccentric connectivity index of Γ.

If $h(u,v) = uv$, then $\mathcal{I}(\Gamma) = E_2(\Gamma)$, the second Zagreb eccentricity index of Γ.

If $h(u,v) = u^2+v^2$, then $\mathcal{I}(\Gamma) = \xi^{(2)}(\Gamma)$, the second eccentric connectivity index of Γ.

If $h(u,v) = |u-v|$, then $\mathcal{I}(\Gamma) = E_3(\Gamma)$, the third Zagreb eccentricity index of Γ.

If $h(u,v) = \frac{1}{u} + \frac{1}{v}$, then $\mathcal{I}(\Gamma) = \xi^{ec}(\Gamma)$, the *total reciprocal edge eccentricity* or *connective eccentricity index* of Γ (see [15]).

If $h(u,v) = \frac{2}{u+v}$, then $\mathcal{I}(\Gamma) = H_4(\Gamma)$, the *fourth harmonic index* or *eccentric harmonic index* of Γ (see [12]).

If $h(u,v) = \frac{\sqrt{uv}}{\frac{1}{2}(u+v)}$, then $\mathcal{I}(\Gamma) = GA_4(\Gamma)$, the *fourth geometric-arithmetic index* of Γ (see [14]).

If $h(u,v) = \sqrt{\frac{u+v-2}{uv}}$, then $\mathcal{I}(\Gamma) = ABC_5(\Gamma)$, the *fifth atom-bond connectivity index* of Γ (see [13]).

Then we can define the coindex $\overline{\mathcal{I}}(\Gamma)$ of Γ as

$$\overline{\mathcal{I}}(\Gamma) = \sum_{u_\Gamma v_\Gamma \in E(\overline{\Gamma})} h(\varepsilon_\Gamma(u_\Gamma), \varepsilon_\Gamma(v_\Gamma)) = \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} h(\varepsilon_\Gamma(u_\Gamma), \varepsilon_\Gamma(v_\Gamma)).$$

If $h(u,v) = u+v$, then $\overline{\mathcal{I}}(\Gamma) = \overline{\xi}^c(\Gamma)$, the ECC of Γ and for $h(u,v) = uv$, $\overline{\mathcal{I}}(\Gamma) = \overline{E}_2(\Gamma)$, the SZEC of Γ. It is interesting to consider other vertex-eccentricity-based coindices such as the second eccentric connectivity coindex $\overline{\xi}^{(2)}(\Gamma)$, third Zagreb eccentricity coindex $\overline{E}_3(\Gamma)$, connective eccentricity coindex $\overline{\xi}^{ec}(\Gamma)$, fourth geometric-arithmetic coindex $\overline{GA_4}(\Gamma)$, and fifth atom-bond connectivity coindex $\overline{ABC_5}(\Gamma)$, and derive all those results for these coindices too. In particular, one could try to find some relations between $\overline{\xi}^{c}(\Gamma)$ or $\overline{E}_2(\Gamma)$ and other vertex-eccentricity-based coindices. As an illustration, a lower bound on $\overline{\xi}^{c}(\Gamma)$ in terms of $\overline{E}_3(\Gamma)$ is presented.

Theorem 6.1. *For any connected graph* Γ *on* n *vertices,*

$$\overline{\xi}^{c}(\Gamma) \geq \overline{E}_3(\Gamma), \tag{13}$$

and the equality case occurs if and only if Γ *is isomorphic to* K_n.

Proof. If $\Gamma \cong K_n$, then $\overline{\xi}^{c}(\Gamma) = \overline{E}_3(\Gamma) = 0$ and the equality in Equation (13) holds. If $\Gamma \ncong K_n$, then

$$\overline{\xi}^{c}(\Gamma) = \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} \big(\varepsilon_\Gamma(u_\Gamma) + \varepsilon_\Gamma(v_\Gamma)\big) > \sum_{u_\Gamma v_\Gamma \notin E(\Gamma)} |\varepsilon_\Gamma(u_\Gamma) - \varepsilon_\Gamma(v_\Gamma)| = \overline{E}_3(\Gamma),$$

from which the inequality in Equation (13) holds. □

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