Iranian Journal of Mathematical Chemistry

IJMC

DOI: 10.22052/IJMC.2024.253802.1781
Vol. 15, No. 1, 2024, pp. 17–25
Research Paper

Some Basic Properties of the Second Multiplicative Zagreb Eccentricity Index

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(Dedicated to the memory of Professor Ali Reza Ashrafi.)

Keywords:
Topological index,
Vertex eccentricity,
Tree,
Extremal problem,
Bound

AMS Subject Classification (2020):
05C12; 05C35; 05C05

Article History:
Received: 2 November 2023
Accepted: 23 December 2023

Abstract

The second multiplicative Zagreb eccentricity index $E_2^*(G)$ of a simple connected graph G is expressed as the product of the weights $\varepsilon_G(a)\varepsilon_G(b)$ over all edges ab of G, where $\varepsilon_G(a)$ stands for the eccentricity of the vertex a in G. In this paper, some extremal problems on the E_2^* index over some special graph classes including trees, unicyclic graphs and bicyclic graphs are examined, and the corresponding extremal graphs are characterized. Besides, the relationships between this vertex-eccentricity-based graph invariant and some well-known parameters of graphs and existing graph invariants such as the number of vertices, number of edges, minimum vertex degree, maximum vertex degree, eccentric connectivity index, connective eccentricity index, first multiplicative Zagreb eccentricity index and second multiplicative Zagreb index are investigated.

1 Introduction

In this paper, our focus is on graphs that are finite, simple, and connected. For a given graph G, the symbols $V(G)$ and $E(G)$ show the vertex set and the edge set of G, respectively. The degree $d_G(a)$ of $a \in V(G)$ is the number of vertices joined to a with an edge. By δ and Δ, we mean the minimum degree and maximum degree of G, respectively. A vertex $a \in V(G)$ is said pendant if $d_G(a) = 1$. If $d_G(a) = d_G(b)$ for all $a, b \in V(G)$, then G is said to be regular. If, in addition, $\Delta = r$, then G is called r-regular. For positive integers r_1, r_2, $r_1 \neq r_2$, we call G is (r_1, r_2)-semi-regular if the set $V(G)$ can be partitioned to the nonempty subsets V_1 and V_2, where $V_i = \{a \in V(G) : d_G(a) = r_i\}$, $i \in \{1, 2\}$. The distance $d_G(a, b)$ between $a, b \in V(G)$ is the length of any shortest $a - b$ path in G. The eccentricity $\varepsilon_G(a)$ of $a \in V(G)$ is defined as $\varepsilon_G(a) = \max\{d_G(b, a) : b \in V(G)\}$. The diameter $d(G)$ and the radius $r(G)$ are defined to

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Academic Editor: Saeid Alikhani

be the sets $d(G) = \max\{\varepsilon_G(a) : a \in V(G)\}$ and $r(G) = \min\{\varepsilon_G(a) : a \in V(G)\}$. The total eccentricity of G is $\zeta(G) = \sum_{a\in V(G)} \varepsilon_G(a)$. A non-isolated vertex $a \in V(G)$ is called universal if $\varepsilon_G(a) = 1$. If $\varepsilon_G(a) = \varepsilon_G(b)$ for all $a, b \in V(G)$, then G is said to be self-centered. If, in addition, $d(G) = s$, then G is called s-self-centered.

A *topological index* is a real-valued parameter that describes the topology of a graph and remains invariant by any isomorphism of a graph. Topological indices are used in organic chemistry as effective tools in QSAR[1], QSPR[2] and QSTR[3] investigations [1, 2].

The best-known topological index which is dependent on the eccentricity and degree of vertices in graph is the *eccentric connectivity index*. This invariant was suggested by Sharma et al. [3] in 1997 and formulated by

$$\xi^c(G) = \sum_{a\in V(G)} d_G(a)\varepsilon_G(a) = \sum_{ab\in E(G)} (\varepsilon_G(a) + \varepsilon_G(b)).$$

The ξ^c index has been successfully applied to mathematical models of biological activities of different natures. For its basic and general properties and applications, refer to [4–11].

After the introduction of the ξ^c index, several modifications of this index have been put forward in the literature. The foremost ones are the *first and second Zagreb eccentricity indices* which have been considered by Vukičević and Graovac [12] in 2010. They are formulated for graph G as

$$E_1(G) = \sum_{a\in V(G)} \varepsilon_G(a)^2 \quad \text{and} \quad E_2(G) = \sum_{ab\in E(G)} \varepsilon_G(a)\varepsilon_G(b).$$

These indices are considered as the eccentricity version of the well-known first and second Zagreb indices [13, 14]. Further results on them can be seen in [15–22].
The multiplicative version of E_1 and E_2 indices were proposed by De [23] in 2012 as:

$$E_1^*(G) = \prod_{a\in V(G)} \varepsilon_G(a)^2 \quad \text{and} \quad E_2^*(G) = \prod_{ab\in E(G)} \varepsilon_G(a)\varepsilon_G(b).$$

The second one, E_2^*, can also be formulated by

$$E_2^*(G) = \prod_{a\in V(G)} \varepsilon_G(a)^{d_G(a)}.$$

De [23] obtained several bounds on E_1^* and E_2^* indices in terms of certain graph parameters. Luo and Wu [24] studied these graph invariants for some families of product graphs. In this paper, our focus is on some basic mathematical properties of the E_2^* index. At first, we compute the values of E_2^* index for some specific graphs. Then, we solve some extremal problems concerning to E_2^* index over some collections of graphs like trees, unicyclic graphs and bicyclic graphs. In addition, we give several new and sharp bounds (upper and lower) on the E_2^* index which clarify its connection to some previously-introduced indices.

2 Extremal properties

In this section, we study some extremal problems on the E_2^* index over certain graph classes including trees, unicyclic graphs and bicyclic graphs and characterize the extremal graphs.

[1]Quantitative Structure-Activity Relationship
[2]Quantitative Structure-Property Relationship
[3]Quantitative Structure-Toxicity Relationship

In the rest of the paper, $\mathcal{T}_n$, $\mathcal{U}_n$, $\mathcal{B}_n$, $\mathcal{G}_n$, $\mathcal{G}_m$ and $\mathcal{G}_{n,m}$, stand for the set of trees on n vertices, the set of unicyclic graphs on n vertices, the set of bicyclic graphs on n vertices, the set of connected graphs on n vertices, the set of connected graphs on m edges, and the set of connected graphs on n vertices and m edges, respectively.

The values of the E_2^* index for cycle, star, and complete graph on n vertices were given in [23] as follows:

$$E_2^*(C_n) = \lfloor \frac{n}{2} \rfloor^{2n},\ E_2^*(S_n) = 2^{n-1},\ E_2^*(K_n) = 1.$$

In the following lemma, we give the values of this invariant for a path on n vertices and the complete bipartite graph on $r+s$ vertices. The results can be deduced straightforwardly from the definition and their proofs are hence not given.

Lemma 2.1. *The following relations hold.*

(i) $E_2^*(P_n) = \begin{cases} (n-1)^2 \prod_{i=1}^{\frac{n}{2}-1} (n-(i+1))^4 & 2 \mid n, \\ \frac{1}{4} \prod_{i=1}^{\frac{n-1}{2}} (n-i)^4 & 2 \nmid n; \end{cases}$

(ii) $E_2^*(K_{r,s}) = 4^{rs}$.

Theorem 2.2. *Let $T \in \mathcal{T}_n$ and $n \geq 3$. Then*

$$E_2^*(T) \geq E_2^*(S_n), \tag{1}$$

with equality if and only if $T \cong S_n$.

Proof. Note that T has no edge ab with $\varepsilon_T(a) = \varepsilon_T(b) = 1$, as T contains no cycle and $n \geq 3$. Hence for each $ab \in E(T)$, $\varepsilon_T(a)\varepsilon_T(b) \geq 2$ and we arrive at

$$E_2^*(T) = \prod_{ab \in E(T)} \varepsilon_T(a)\varepsilon_T(b) \geq \prod_{ab \in E(T)} 2 = 2^{n-1} = E_2^*(S_n),$$

and (1) follows. The equality occurs in (1) if and only if for each $ab \in E(T)$, $\varepsilon_T(a) = 1$ and $\varepsilon_T(b) = 2$, which implies that $T \cong S_n$. ■

Theorem 2.3. *For each $T \in \mathcal{T}_n$,*

$$E_2^*(T) \leq E_2^*(P_n), \tag{2}$$

with equality if and only if $T \cong P_n$.

Proof. Let $V(T) = \{b_1, b_2, ..., b_n\}$ and d is the diameter of T. If $T \cong P_n$, then there is not anything to prove. Hence, suppose that $T \ncong P_n$. Then $n \geq 4$, $d \leq n-2$, and T contains more than two pendant vertices. Let $P_{d+1} : b_1 b_2 ... b_{d+1}$ be a path of length d in T. Let ε_i denote the eccentricity of vertex b_i in T, $1 \leq i \leq n$. Thus $\varepsilon_i = \max\{d_T(b_i, b_1), d_T(b_i, b_{d+1})\}$. As T is a tree, vertices b_1 and b_{d+1} must be pendant. Let b_k $(k \neq 1, d+1)$ be a pendant vertex incident with b_l in T. Let $T' \in T_n$ be derived from T by removing the edge $b_k b_l$ and joining the vertices b_{d+1} and b_k by an edge. So $V(T') = V(T)$ and $E(T') = (E(T) \setminus \{b_k b_l\}) \cup \{b_k b_{d+1}\}$. Thus the path $P_{d+2} : b_1 b_2 ... b_{d+1} b_k$ whose length is $d+1$ has the maximum length in T'. Let $\varepsilon'_i = \varepsilon_{T'}(b_i)$, $1 \leq i \leq n$. Then for each $1 \leq i \leq n$, $i \neq k$, we have

$$\begin{aligned} \varepsilon'_i = \max\{d_{T'}(b_i, b_1), d_{T'}(b_i, b_k)\} &= \max\{d_T(b_i, b_1), d_T(b_i, b_{d+1}) + 1\} \\ &\geq \max\{d_T(b_i, b_1), d_T(b_i, b_{d+1})\} = \varepsilon_i, \end{aligned}$$

and $\varepsilon'_k = d+1 > d \geq \varepsilon_k$. This implies that, for each $b_r b_s \in E(T) \setminus \{b_k b_l\}$, $\varepsilon'_r \varepsilon'_s \geq \varepsilon_r \varepsilon_s$, and $\varepsilon'_k \varepsilon'_{d+1} = (d+1)d > d^2 \geq \varepsilon_k \varepsilon_l$. Now the definition of the E_2^* index implies,

$$\begin{aligned} E_2^*(T') = & \prod_{b_r b_s \in (E(T)\setminus\{b_k b_l\}) \cup \{b_k b_{d+1}\}} \varepsilon'_r \varepsilon'_s = \varepsilon'_k \varepsilon'_{d+1} \times \prod_{b_r b_s \in E(T)\setminus\{b_k b_l\}} \varepsilon'_r \varepsilon'_s \\ > & \varepsilon_k \varepsilon_l \times \prod_{b_r b_s \in E(T)\setminus\{b_k b_l\}} \varepsilon_r \varepsilon_s = \prod_{b_r b_s \in E(T)} \varepsilon_r \varepsilon_s = E_2^*(T). \end{aligned}$$

So $E_2^*(T') > E_2^*(T)$. Based on the aforementioned construction, the amount of $E_2^*(T)$ has been increased. If $T' \cong P_n$, then $E_2^*(T) < E_2^*(T') = E_2^*(P_n)$, and (2) holds. If $T' \ncong P_n$, then by repetition of the process as many as necessary, we reach a tree whose maximum degree equals 2, which is P_n. ■

Theorem 2.4. *Let $G \in \mathcal{G}_{n,m}$ and k indicate the number of universal vertices of G. Then*

$$E_2^*(G) \geq 2^{2m-k(n-1)}, \tag{3}$$

with equality if and only if G has a diameter at most 2.

Proof. From the definition of the E_2^* index,

$$\begin{aligned} E_2^*(G) = & \prod_{a \in V(G)} \varepsilon_G(a)^{d_G(a)} = \prod_{\substack{a \in V(G): \\ \varepsilon_G(a)=1}} 1^{n-1} \times \prod_{\substack{a \in V(G): \\ \varepsilon_G(a) \geq 2}} \varepsilon_G(a)^{d_G(a)} \\ \geq & \prod_{\substack{a \in V(G): \\ \varepsilon_G(a) \geq 2}} 2^{d_G(a)} = 2^{\sum_{\substack{a \in V(G): \\ \varepsilon_G(a) \geq 2}} d_G(a)} = 2^{2m - \sum_{\substack{a \in V(G): \\ \varepsilon_G(a)=1}} d_G(a)} \\ = & 2^{2m-k(n-1)}, \end{aligned}$$

from that (3) follows. The equality happens in (3) if and only if vertices of G have eccentricity 1 or 2 which implies that G has diameter at most two. ■

As a result of Theorem 2.4, we obtain:

Corollary 2.5. *Let $G \in \mathcal{G}_m$ have a radius of at least 2. Then*

$$E_2^*(G) \geq 4^m,$$

with equality if and only if G is a 2-self-centered graph.

Now we apply Corollary 2.5 to get a Nordhaus-Gaddum result for the E_2^* index.

Theorem 2.6. *Let $G \in \mathcal{G}_n$ with $n \geq 4$ and connected complement $\overline{G}$. Then*

$$E_2^*(G)E_2^*(\overline{G}) \geq 2^{n(n-1)}, \tag{4}$$

with equality if and only if both G and $\overline{G}$ are 2-self-centered.

Proof. Let G have m edges. Since G and $\overline{G}$ are connected graphs, both of them have a radius of at least 2. Now by Corollary 2.5, we have

$$E_2^*(G)E_2^*(\overline{G}) \geq 4^m \times 4^{\binom{n}{2}-m} = 2^{n(n-1)},$$

from that the inequality (4) follows. Based on Corollary 2.5, the equality holds in (4) if and only if G and $\overline{G}$ both are 2-self centered. ■

It is obvious that, for any $G \in \mathcal{G}_n$, $E_2^*(G) \geq E_2^*(K_n)$, with equality if and only if $G \cong K_n$. Hence, among the members of $\mathcal{G}_n$, K_n is the unique graph having the minimum amount of the E_2^* index.

Theorem 2.7. *Let $G \in \mathcal{U}_n$ and $n \geq 4$. Then*

$$E_2^*(G) \geq 2^{n+1},$$

and the equality occurs if and only if G is derived from S_n by adding an edge between two pendant vertices.

Proof. The unique member of $\mathcal{U}_n$ with $n \geq 4$ vertices and radius 1 is the graph derived from S_n by adding an edge between two pendant vertices for which we have:

$$E_2^*(G) = (2 \times 2)(1 \times 2)^{n-1} = 2^{n+1}.$$

If $r(G) \geq 2$, then by Corollary 2.5 we have

$$E_2^*(G) \geq 4^n = 2^{2n} > 2^{n+1},$$

from which the result holds. ■

Theorem 2.8. *Let $G \in \mathcal{B}_n$ and $n \geq 5$. Then*

$$E_2^*(G) \geq 2^{n+3},$$

with equality if and only if G is the graph derived from S_n by adding two edges.

Proof. The unique member of $\mathcal{B}_n$ with $n \geq 5$ vertices and radius 1 is the graph derived by adding two edges to S_n for which we have:

$$E_2^*(G) = (2 \times 2)^2(1 \times 2)^{n-1} = 2^{n+3}.$$

If $r(G) \geq 2$, then Corollary 2.5 implies,

$$E_2^*(G) \geq 4^{n+1} = 2^{2n+2} > 2^{n+3},$$

and the proof is completed. ■

3 Relations with other invariants

In this section, some new and sharp bounds on the E_2^* index are given. These bounds will reveal the connection between E_2^* and a number of previously-introduced indices.

Theorem 3.1. *For each connected graph G,*

$$E_1^*(G)^{\frac{\delta}{2}} \leq E_2^*(G) \leq E_1^*(G)^{\frac{\Delta}{2}}. \tag{5}$$

The equality holds on both sides of (5) if and only if G is regular.

Proof. Considering the fact that for each vertex $a \in V(G)$, $\delta \leq d_G(a) \leq \Delta$, we get

$$E_2^*(G) = \prod_{a\in V(G)} \varepsilon_G(a)^{d_G(a)} \leq \prod_{a\in V(G)} \varepsilon_G(a)^{\Delta} = \prod_{a\in V(G)} \left(\varepsilon_G(a)^2\right)^{\frac{\Delta}{2}} = E_1^*(G)^{\frac{\Delta}{2}},$$

$$E_2^*(G) \geq \prod_{a\in V(G)} \varepsilon_G(a)^{\delta} = \prod_{a\in V(G)} \left(\varepsilon_G(a)^2\right)^{\frac{\delta}{2}} = E_1^*(G)^{\frac{\delta}{2}}.$$

The equality holds in (5) if and only if for each $a \in V(G)$, $d_G(a) = \Delta = \delta$, that is G is regular. ■

Theorem 3.2. *For any nontrivial graph $G \in \mathcal{G}_n$,*

$$E_2^*(G) \leq E_1^*(G)^{\frac{n-2}{2}}, \tag{6}$$

with equality if and only if $G \cong K_n$ or G is $(n-2)$-regular or $(n-1, n-2)$-semi-regular.

Proof. By definition of the E_2^* index,

$$\begin{aligned} E_2^*(G) &= \prod_{a\in V(G)} \varepsilon_G(a)^{d_G(a)} \\ &= \prod_{\substack{a\in V(G):\\ \varepsilon_G(a)=1}} 1^{n-1} \times \prod_{\substack{a\in V(G):\\ \varepsilon_G(a)\geq 2}} \varepsilon_G(a)^{d_G(a)} \\ &\leq \prod_{\substack{a\in V(G):\\ \varepsilon_G(a)\geq 2}} \varepsilon_G(a)^{n-2} = \prod_{\substack{a\in V(G):\\ \varepsilon_G(a)\geq 2}} \left(\varepsilon_G(a)^2\right)^{\frac{n-2}{2}} = E_1^*(G)^{\frac{n-2}{2}}, \end{aligned}$$

and the inequality (6) is deduced. The equality holds in (6) if and only if for each vertex $a \in V(G)$, with $\varepsilon_G(a) \geq 2$, $d_G(a) = n-2$. This happens if and only if the degrees of vertices of G are either $n-1$ or $n-2$, from which we deduce that, $G \cong K_n$ or G is $(n-2)$-regular or $(n-1, n-2)$-semi-regular. ■

It is interesting to note that, for graphs with radius at least 2, the upper bound presented in (5) is stronger than the one given in (6), while for non-complete graphs with radius 1, the bound in (6) is better than the one in (5).

Theorem 3.3. *For a nontrivial graph $G \in \mathcal{G}_m$,*

$$E_2^*(G) \leq \left(\frac{\xi^c(G)}{2m}\right)^{2m}, \tag{7}$$

with equality if and only if G is self-centered.

Proof. Applying the arithmetic-geometric mean inequality gives

$$E_2^*(G) = \prod_{a\in V(G)} \varepsilon_G(a)^{d_G(a)} \leq \left(\frac{\sum_{a\in V(G)} d_G(a)\varepsilon_G(a)}{\sum_{a\in V(G)} d_G(a)}\right)^{\sum_{a\in V(G)} d_G(a)} = \left(\frac{\xi^c(G)}{2m}\right)^{2m},$$

and (7) holds. The equality holds in (7) if and only if for each $a \in V(G)$, $\varepsilon_G(a)$ is constant. This happens if and only if G is self-centered. ■

The *second multiplicative Zagreb index* was put forward by Todeschini and Consonni [25] in 2010 and formulated for graph G as:

$$\Pi_2(G) = \prod_{ab\in E(G)} d_G(a)d_G(b) = \prod_{a\in V(G)} d_G(a)^{d_G(a)}.$$

The subsequent theorem provides an upper bound on $E_2^*(G)$ in terms of $\Pi_2(G)$.

Theorem 3.4. *For any $G \in \mathcal{G}_m$,*

$$E_2^*(G) \leq \Pi_2(G)\Big(\frac{\zeta(G)}{2m}\Big)^{2m}, \tag{8}$$

with equality if and only if for any $a \in V(G)$, $\frac{\varepsilon_G(a)}{d_G(a)}$ is constant.

Proof. Application of arithmetic-geometric mean inequality gives,

$$\begin{aligned}\frac{E_2^*(G)}{\Pi_2(G)} =& \frac{\prod_{a\in V(G)} \varepsilon_G(a)^{d_G(a)}}{\prod_{a\in V(G)} d_G(a)^{d_G(a)}} = \prod_{a\in V(G)} \Big(\frac{\varepsilon_G(a)}{d_G(a)}\Big)^{d_G(a)} \\ \leq& \Big(\frac{\sum_{a\in V(G)} d_G(a) \times \frac{\varepsilon_G(a)}{d_G(a)}}{\sum_{a\in V(G)} d_G(a)}\Big)^{\sum_{a\in V(G)} d_G(a)} = \Big(\frac{\zeta(G)}{2m}\Big)^{2m}.\end{aligned}$$

Then inequality in (8) is concluded. The equality holds in (8) if and only if for any $a \in V(G)$, $\frac{\varepsilon_G(a)}{d_G(a)}$ is constant. ∎

The *connective eccentricity index* of G was formulated by Gupta et al. [26] in 2000 by

$$\xi^{ce}(G) = \sum_{a\in V(G)} \frac{d_G(a)}{\varepsilon_G(a)} = \sum_{ab\in E(G)} \Big(\frac{1}{\varepsilon_G(a)} + \frac{1}{\varepsilon_G(b)}\Big).$$

The theorem below contains a lower bound on $E_2^*(G)$ based on $\xi^{ce}(G)$.

Theorem 3.5. *For any nontrivial graph $G \in \mathcal{G}_m$,*

$$E_2^*(G) \geq \Big(\frac{2m}{\xi^{ce}(G)}\Big)^{2m}, \tag{9}$$

with equality if and only if G is self-centered.

Proof. Application of the geometric-harmonic mean inequality implies,

$$\sqrt[2m]{E_2^*(G)} = \sqrt[2m]{\prod_{a\in V(G)} \varepsilon_G(a)^{d_G(a)}} \geq \frac{2m}{\sum_{a\in V(G)} \frac{d_G(a)}{\varepsilon_G(a)}} = \frac{2m}{\xi^{ce}(G)},$$

from which the inequality (9) holds with equality if and only if G is self-centered. ∎

Conflicts of Interest. The author declares that she has no conflicts of interest regarding the publication of this article.

Acknowledgment. The author would like to thank the editor and referee for their valuable comments which improved the presentation of the paper.

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