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Research Article

On the Reformulated Multiplicative First Zagreb Index of Trees and Unicyclic Graphs

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The multiplicative first Zagreb index of a graph H is defined as the product of the squares of the degrees of vertices of H. The line graph of a graph H is denoted by $L(H)$ and is defined as the graph whose vertex set is the edge set of H where two vertices of $L(H)$ are adjacent if and only if they are adjacent in H. The multiplicative first Zagreb index of the line graph of a graph H is referred to as the reformulated multiplicative first Zagreb index of H. This paper gives characterization of the unique graph attaining the minimum or maximum value of the reformulated multiplicative first Zagreb index in the class of all (i) trees of a fixed order (ii) connected unicyclic graphs of a fixed order.

1. Introduction

A numerical quantity of a graph that remains the same under graph isomorphism is known as a graph invariant. For a graph H, denote by $V(H)$ and $E(H)$, its vertex set and edge set, respectively. For a vertex $v \in V(H)$, denote by $d_v(H)$ and $N_H(v)$, the degree of v and the set of all those vertices of H that are adjacent to v, respectively. The members of $N_H(v)$ are known as neighbors of v. For $u, v \in V(G)$, the edge with its end-vertices u and v is denoted by uv and the degree of uv is defined as $d_u(H) + d_v(H) - 2$. In the following, we drop the symbol "(H)" from "$d_v(H)$" whenever there is no confusion about the graph under consideration. Also, in the present paper, we consider only connected graphs. The notation and terminology used in this paper, but not defined here, can be found in standard (chemical) graph-theoretical books, such as [1–3].

Denote by $M_1(H)$ the sum of the squares of the degrees of vertices of H, that is,

$$M_1(H) = \sum_{v \in V(H)} (d_v)^2. \tag{1}$$

The graph invariant M_1, known as the first Zagreb index, was appeared in the first quarter of 1970s within a study of chemical modeling [4]. The first Zagreb index can be considered as one of the most studied graph invariants, especially in chemical graph theory [5–11].

The line graph of a graph H is denoted by $L(H)$ and is defined as the graph whose vertex set is the edge set of H where two vertices of $L(H)$ are adjacent if and only if they are adjacent in H. The first Zagreb index of the line graph of a graph H is known as the reformulated first Zagreb index [12] of H, and for simplicity, it is denoted as $EM_1(H)$. Thus,

$$EM_1(H) = M_1(L(H)) = \sum_{uv \in E(H)} (d_u + d_v - 2)^2. \tag{2}$$

Details about the mathematical properties of the reformulated first Zagreb index can be found in [13–16].

The multiplicative version of the first Zagreb index is defined [17, 18] as

$$\Pi_1(H) = \prod_{v\in V(H)} (d_v)^2. \tag{3}$$

The multiplicative first Zagreb index also gained a considerable attention from researchers, and hence, many investigations on this graph invariant have been conducted; for example, see [19, 20] and the related references included therein. Here, it should be pointed out that the multiplicative first Zagreb index is actually the square of the well-known Narumi–Katayama index [21], see, for example, [22], for details about the Narumi–Katayama index.

This paper is concerned with the graph invariant $\Pi_1(L(H))$ that is the product of the squares of the degrees of edges of H. We call the invariant $\Pi_1(L(H))$ as the reformulated multiplicative first Zagreb index of $L(H)$ and denote it by $\Pi_{1,e}(H)$ for simplicity. Thus,

$$\Pi_{1,e}(H) = \Pi_1(L(H)) = \prod_{uv\in E(H)} (d_u + d_v - 2)^2. \tag{4}$$

Throughout this paper, whenever we consider a class of graphs of the same order, we assume that all the graphs of the considered class are pairwise nonisomorphic. A graph containing exactly one cycle is known as a unicyclic graph. By an n-vertex graph, we mean a graph of order n. For $n \geq 4$, denote by $\mathcal{T}_n$ the class of all n-vertex trees and let $\mathcal{U}_n$ be the class of all n-vertex connected unicyclic graphs. In this paper, the unique graph having the maximum or minimum value of the reformulated multiplicative first Zagreb index is characterized from each of the classes $\mathcal{T}_n$ and $\mathcal{U}_n$ for every fixed integer n greater than 3.

2. Reformulated Multiplicative First Zagreb Index of Trees

This section is concerned with the characterization of the unique graph attaining the maximum or minimum value of the reformulated multiplicative first Zagreb index over the class of all trees of a fixed order $n \geq 4$.

A vertex of degree one is called a pendent vertex. A nontrivial path P: $v_1v_2\ldots v_r$ in a graph G is said to be a pendent path if $\min(d_{v_1}, d_{v_r}) = 1$ and $\max(d_{v_1}, d_{v_r}) \geq 3$, and every other vertex (if exists) of P has degree 2. Two pendent paths having the same vertex of degree greater than 2 are known as adjacent pendent paths. By an (n,m)-graph, we mean a graph of order n and size m.

Lemma 1. *If G is a connected (n,m)-graph containing at least one pair of adjacent pendent paths, then there exists at least one connected (n,m)-graph G' such that*

$$\Pi_{1,e}(G') < \Pi_{1,e}(G). \tag{5}$$

Proof. Let $vu_1u_2\ldots u_q$ and $vw_1w_2\ldots w_r$ be two adjacent pendent paths in G having lengths q and r, respectively. Without loss of generality, we assume that $q \geq r$. Let G' be the graph deduced from G by deleting the edge w_1v and inserting the edge u_qw_1 (see Figure 1). Throughout this proof, by d_u, we mean the degree of the vertex $u \in V(G) = V(G')$ in G. By the definition of the reformulated multiplicative first Zagreb index, there exists a positive integer z such that

$$\Pi_{1,e}(G) - \Pi_{1,e}(G') = z\left(\Gamma_1 \prod_{w\in N_G(v)\setminus\{u_1,w_1\}} (d_w + d_v - 2)^2 - \Gamma_2 \prod_{w\in N_G(v)\setminus\{u_1,w_1\}} (d_w + d_v - 3)^2\right), \tag{6}$$

where

$$\Gamma_1 = \begin{cases} (d_v - 1)^4, & \text{if } q = r = 1, \\ d_v^2(d_v - 1)^2, & \text{if } q > 1 \text{ and } r = 1, \\ d_v^4, & \text{if } q > 1 \text{ and } r > 1, \end{cases}$$
$$\Gamma_2 = \begin{cases} (d_v - 1)^2, & \text{if } q = r = 1, \\ 4(d_v - 1)^2, & \text{if } q > 1 \text{ and } r = 1, \\ 16(d_v - 1)^2, & \text{if } q > 1 \text{ and } r > 1. \end{cases} \tag{7}$$

From the inequality $d_v > 2$ (which gives $d_v^2 > 4(d_v - 1)$, that is, $d_v^4 > 16(d_v - 1)^2$) and equation (6), it follows that

$$\Pi_{1,e}(G) - \Pi_{1,e}(G') > 0. \tag{8}$$

□

Theorem 1. *Among all trees of a fixed order $n \geq 4$, path P_n is the unique graph with the minimum value of $\Pi_{1,e}$. In other words, if T is any tree of order $n \geq 4$, then*

$$\Pi_{1,e}(T) \geq \Pi_{1,e}(P_n), \tag{9}$$

with equality if and only if T is isomorphic to the path graph P_n.

Proof. Let T^* be a tree with the minimum value of $\Pi_{1,e}$ among all trees of a fixed order $n \geq 4$. We claim that T^* is isomorphic to P_n. Contrarily, we assume that T^* is not isomorphic to P_n. Then, T^* contains at least two adjacent pendent paths, and hence by Lemma 1, there exists at least one tree T' such that

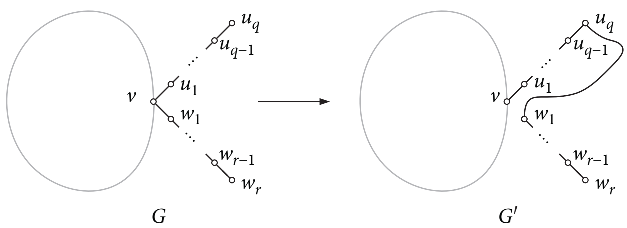

FIGURE 1: The graph transformation used in the proof of Lemma 1.

$$\Pi_{1,e}(T^*) > \Pi_{1,e}(T'), \tag{10}$$

which contradicts the definition of T^*. Thus, $T^* \cong P_n$. □

Lemma 2. *Let G be a connected (n, m)-graph. Let $uv \in E(G)$ be an edge such that it does not lie on any triangle of G and $d_u(G) \geq d_v(G) \geq 2$, and $N_G(v) = \{u, w_1, w_2, \ldots, w_p\}$. If G' is the graph formed from G by deleting the edges $w_1v, w_2v, \ldots, w_pv$ and inserting the edges $w_1u, w_2u, \ldots, w_pu$, then*

$$\Pi_{1,e}(G) < \Pi_{1,e}(G'). \tag{11}$$

Proof. In this proof, by d_x, we mean the degree of the vertex $x \in V(G) = V(G')$ in G. By the definition of the reformulated multiplicative first Zagreb index, there exists a positive integer z such that

$$\Pi_{1,e}(G) - \Pi_{1,e}(G') = z\left(\prod_{i=1}^{p}\left(d_v + d_{w_i} - 2\right)^2 \prod_{y \in N_G(u)\setminus\{v\}}\left(d_u + d_y - 2\right)^2 - \prod_{i=1}^{p}\left(d_u + d_{w_i} + p - 2\right)^2 \prod_{y \in N_G(u)\setminus\{v\}}\left(d_u + d_y + p - 2\right)^2\right). \tag{12}$$

Since $d_v \leq d_u$, the right hand side of equation (12) is negative. □

Theorem 2. *Among all trees of a fixed order $n \geq 4$, star graph S_n uniquely attains the maximum value of $\Pi_{1,e}$. In other words, if T is any tree of order $n \geq 4$, then*

$$\Pi_{1,e}(T) \leq \Pi_{1,e}(S_n), \tag{13}$$

with equality if and only if T is isomorphic to the star graph S_n.

Proof. Let T^* be a tree with the maximum value of $\Pi_{1,e}$ among all trees of a fixed order $n \geq 4$. Let Δ be the maximum degree of T^*. We claim that T^* is isomorphic to S_n. Contrarily, we assume that T^* is not isomorphic to S_n. Then, $\Delta \leq n-2$, and hence by Lemma 2, there exists at least one n-vertex tree T' such that

$$\Pi_{1,e}(T^*) < \Pi_{1,e}(T'), \tag{14}$$

which contradicts the definition of T^*. Thus, $T^* \cong S_n$. □

3. Reformulated Multiplicative First Zagreb Index of Unicyclic Graphs

This section is concerned with the maximum and minimum values of the reformulated multiplicative first Zagreb index over the class of all unicyclic graphs of a fixed order.

Theorem 3. *Among all connected unicyclic graphs of a fixed order $n \geq 4$, the cycle graph C_n attains uniquely the minimum value of $\Pi_{1,e}$. In other words, if G is any connected unicyclic graphs of order $n \geq 4$, then*

$$\Pi_{1,e}(G) \geq \Pi_{1,e}(C_n), \tag{15}$$

with equality if and only if T is isomorphic to C_n.

Proof. Let G^* be a graph attaining the minimum value of $\Pi_{1,e}$ in the class of all connected unicyclic graphs of a fixed order $n \geq 4$. If G^* contains at least two adjacent pendent paths, then by Lemma 1, there exists at least one connected unicyclic graph G' of order n such that

$$\Pi_{1,e}(G) > \Pi_{1,e}(G'), \tag{16}$$

which is a contradiction to the definition of G^*. Thus, G^* does not have any pair of adjacent pendent paths, which implies that the maximum degree of G^* is at most 3.

We claim that the maximum degree of G^* is 2, that is, $G^* \cong C_n$. Contrarily, assume that $uu_1u_2\ldots u_r$ is a pendent path in G^*, where u has degree 3 and u_r has degree 1. Let v be a neighbor of u different from u_1. Let G'' be the graph formed from G^* by deleting the edge uv and inserting the edge u_rv (see Figure 2). In the following, by d_x, we mean the degree of the vertex $x \in V(G^*) = V(G'')$ in G^*. By the definition of the reformulated multiplicative first Zagreb index, there exists a positive integer z such that

$$\Pi_{1,e}(G^*) - \Pi_{1,e}(G'') = z\left(\Gamma_1 \prod_{w \in N_{G^*}(u)\setminus\{u_1, v\}}(d_w + 1)^2 - \Gamma_2 \prod_{w \in N_{G^*}(u)\setminus\{u_1, v\}} d_w^2\right), \tag{17}$$

where

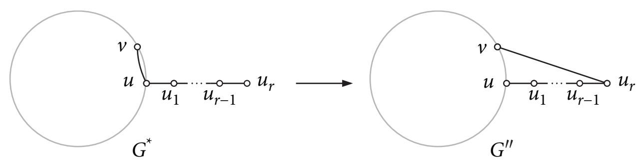

FIGURE 2: The graph transformation used in the proof of Theorem 3.

$$\Gamma_1 = \begin{cases} 4(d_v+1)^2, & \text{if } r = 1, \\ 9(d_v+1)^2, & \text{if } r \ge 2, \end{cases}$$
$$\Gamma_2 = \begin{cases} 4d_v^2, & \text{if } r = 1, \\ 16d_v^2, & \text{if } r \ge 2. \end{cases} \quad (18)$$

Since $d_v \le 3$, it holds that $9(d_v+1)^2 \ge 16d_v^2$; this together with equation (17) implies that

$$\Pi_{1,e}(G^*) - \Pi_{1,e}(G'') > 0, \quad (19)$$

which is again a contradiction to the definition of G^*. Therefore, $G^* \cong C_n$. □

Theorem 4. *Among all connected unicyclic graphs of a fixed order $n \ge 4$, the graph obtained from the star S_n by adding an edge attains uniquely the maximum value of $\Pi_{1,e}$. In other words, if G is any connected unicyclic graphs of order $n \ge 4$, then*

$$\Pi_{1,e}(G) \le \Pi_{1,e}(S_n^+), \quad (20)$$

with equality if and only if T is isomorphic to S_n^+, where S_n^+ is the graph obtained from the star S_n by adding an edge.

Proof. Let G^* be a graph attaining the maximum value of $\Pi_{1,e}$ in the class of all connected unicyclic graphs of a fixed order $n \ge 4$. From Lemma 2, it follows that the removal of all the vertices of degree 1 of G^* results in C_3 (the cycle of order 3), that is, G^* is isomorphic to the graph $G^\dagger$ depicted in Figure 3. By routine calculations, one gets

$$\Pi_{1,e}(G^\dagger) = (p_1+1)^{2p_1}(p_2+1)^{2p_2}(p_3+1)^{2p_3}(p_1+p_2+2)^2 (p_1+p_3+2)^2(p_2+p_3+2)^2, \quad (21)$$

where $p_1 + p_2 + p_3 = n - 3$. Without loss of generality, we assume that $p_1 \ge p_2 \ge p_3 \ge 0$. Thus, $n - p_2 - p_3 - 3 \ge p_2 \ge p_3$, and hence, $((2n-6)/3) \ge p_2 + p_3$. Equation (21) is equivalent to

$$\Pi_{1,e}(G^\dagger) = (n-p_2-p_3-2)^{2(n-p_2-p_3-3)}(p_2+1)^{2p_2} (p_3+1)^{2p_3}(n-p_2-1)^2(n-p_3-1)^2(p_2+p_3+2)^2, \quad (22)$$

with the condition $p_2 + p_3 \le ((2n-6)/3)$. For a fixed integer $n \ge 4$, since the function f defined by

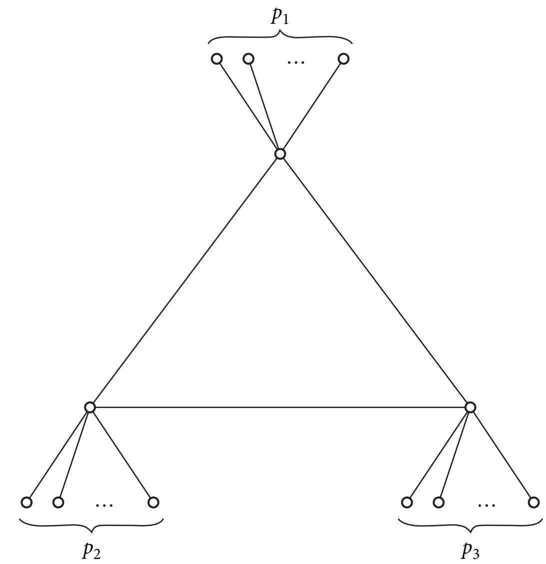

FIGURE 3: The graph $G^\dagger$ used in the proof of Theorem 4.

$$f(y,z) = (n-y-z-2)^{2(n-y-z-3)}(y+1)^{2y}(z+1)^{2z} (n-y-1)^2(n-z-1)^2(y+z+2)^2, \quad (23)$$

with $y \ge z \ge 0$ and $y + z \le ((2n-6)/3)$ is strictly decreasing in y and z, we conclude that the maximum value of $\Pi_{1,e}(G^\dagger)$ is attained if and only if $p_2 = p_3 = 0$. Therefore, $G^\dagger$ is isomorphic to the graph S_n^+. □

Data Availability

The data used to support the findings of this study are available from the authors upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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References

[1] J. A. Bondy and U. S. R. Murty, *Graph Theory*, Springer, London, UK, 2008.
[2] G. Chartrand, L. Lesniak, and P. Zhang, *Graphs & Digraphs*, CRC Press, Boca Raton, FL, USA, 2016.
[3] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL, USA, 1992.
[4] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.
[5] A. Ali, I. Gutman, E. Milovanović, and I. Milovanović, "Sum of powers of the degrees of graphs: extremal results and

bounds," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 80, pp. 5–84, 2018.

[6] B. Borovićanin, K. C. Das, B. Furtula, and I. Gutman, "Bounds for Zagreb indices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 78, pp. 17–100, 2017.

[7] I. Gutman, "Degree-based topological indices," *Croatica Chemica Acta*, vol. 86, no. 4, pp. 351–361, 2013.

[8] I. Gutman and K. C. Das, "The first Zagreb index 30 years after," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 50, pp. 83–92, 2004.

[9] I. Gutman, E. Milovanović, and I. Milovanović, "Beyond the Zagreb indices," *AKCE International Journal of Graphs and Combinatorics*, vol. 17, no. 1, pp. 74–85, 2020.

[10] S. Noureen, A. Ali, and A. A. Bhatti, "On the extremal Zagreb indices of n-vertex chemical trees with fixed number of segments or branching vertices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 84, pp. 513–534, 2020.

[11] T. Réti, A. Ali, P. Varga, and E. Bitay, "Some properties of the neighborhood first Zagreb index," *Discrete Mathematics Letters*, vol. 2, pp. 10–17, 2019.

[12] A. Miličević, S. Nikolić, and N. Trinajstić, "On reformulated Zagreb indices," *Molecular Diversity*, vol. 8, pp. 393–399, 2004.

[13] A. Ali and D. Dimitrov, "On the extremal graphs with respect to bond incident degree indices," *Discrete Applied Mathematics*, vol. 238, pp. 32–40, 2018.

[14] A. Ali, D. Dimitrov, Z. Du, and F. Ishfaq, "On the extremal graphs for general sum-connectivity index (χ_α) with given cyclomatic number when $\alpha > 1$," *Discrete Applied Mathematics*, vol. 257, pp. 19–30, 2019.

[15] A. Ilić and B. Zhou, "On reformulated Zagreb indices," *Discrete Applied Mathematics*, vol. 160, pp. 204–209, 2012.

[16] S. Ji, X. Li, and B. Huo, "On reformulated Zagreb indices with respect to acyclic, unicyclic and bicyclic graphs," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 72, pp. 723–732, 2014.

[17] I. Gutman, "Multiplicative Zagreb indices of trees," *Bulletin of International Mathematical Virtual Institute*, vol. 1, pp. 13–19, 2011.

[18] R. Todeschini and V. Consonni, "New local vertex invariants and molecular descriptors based on functions of the vertex degrees," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 64, pp. 359–372, 2010.

[19] I. Gutman, I. Milovanovic, and E. Milovanovic, "Relations between ordinary and multiplicative degree-based topological indices," *Filomat*, vol. 32, no. 8, pp. 3031–3042, 2018.

[20] A. Iranmanesh, M. Hosseinzadeh, and I. Gutman, "On multiplicative Zagreb indices of graphs," *Iranian Journal of Mathematical Chemistry*, vol. 3, pp. 145–154, 2012.

[21] H. Narumi and M. Katayama, "Simple topological index: a newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons," *Memoirs of the Faculty of Engineering, Hokkaido University*, vol. 16, pp. 209–214, 1984.

[22] M. Azari, "Sharp lower bounds on the Narumi-Katayama index of graph operations," *Applied Mathematics and Computation*, vol. 239, pp. 409–421, 2014.