Iranian Journal of Mathematical chemistry

IJMC

DOI: 10.22052/IJMC.2024.253967.1793
Vol. 15, No. 3, 2024, pp. 203–225
Research Paper

On the Multiplicative Reformulated First Zagreb Index of n-Vertex Trees with Respect to Matching Number

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Keywords:

Multiplicative reformulated first Zagreb index,
Tree,
Unicyclic graphs,
Matching,
Perfect matching

AMS Subject Classification (2020):

05C09; 05C90; 05C92

Article History:

Received: 8 December 2023
Accepted: 23 March 2024

Abstract

The multiplicative first Zagreb index is the product of the square of the degree of vertices in a graph $\mathbb{G}$. The multiplicative reformulated first Zagreb index is defined as $\prod_{1,e}(\mathbb{G}) = \prod_{x_1x_2\in E(\mathbb{G})}(d_{\mathbb{G}}(x_1) + d_{\mathbb{G}}(x_1) - 2)^2$, where $E(\mathbb{G})$ is the edge set of a graph $\mathbb{G}$ and $d_{\mathbb{G}}(x_1)$ is the degree of a vertex x_1 in a graph $\mathbb{G}$. In this paper, we characterize the minimum and maximum trees and unicyclic graphs with respect to matching and perfect matching using this graph invariant $\prod_{1,e}(\mathbb{G})$ among the collection of all n-vertex graphs.

1 Introduction

Let $\mathbb{G}$ be a simple, connected and finite graph that has a vertex set $V(\mathbb{G})$ and an edge set $E(\mathbb{G})$. The books [1, 2] contain notation and terminology that are not specified here. Topological indices are important in many domains, including chemistry, materials science, pharmaceutical sciences, and engineering, since they connect with the physical and chemical characteristics of molecules, chemical compound modeling, and biological activities. The Zagreb indices are well-known topological indices that express chemical compounds through trees and unicyclic graphs. They were proposed in the last decade of the 19^{th} century. The Zagreb index was the first degree-based topological index created in 1972. The topological indices that depend on vertex degree are the first Zagreb index $\mathcal{M}_1(\mathbb{G})$ and the second Zagreb index $\mathcal{M}_2(\mathbb{G})$. In a publication [3], Gutman and Trinajstić introduced these indices. Other well-known and most used degree-based topological indices include the hyper-Zagreb index [4], reduced second Zagreb index [5] and reduced first Zagreb index [6]. These indices are extensively researched in (chemical) graph theory. In addition to Zagreb indices, readers who are interested in some recent assessments on the topic are referred to [7]. Another invariant of the Zagreb index is the

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Academic Editor: Petra Žigert Pleteršek

reformulated first Zagreb index [8], which is defined in terms of edge degrees rather than vertex degrees. The mathematical properties of the reformulated first Zagreb indices were investigated in this paper [9]. These indices represent the degree of branching of the molecular carbon-atom skeleton and may thus be used to describe molecular structure. For more detail on trees and unicyclic graphs, see [10–24]. The multiplicative definition of the first Zagreb index is defined in [25]. The paper [26] aims to identify a graph that achieves the highest or lowest possible value of the reformulated multiplicative first Zagreb index. The invariant $\prod_1(\mathbb{G})$ is known as the multiplicative reformulated first Zagreb index in [27]. It is denoted by $\prod_{1,e}(\mathbb{G})$ and is defined as:

$$\prod_{1,e}(\mathbb{G}) \quad = \prod_{x_1,x_2 \in E(\mathbb{G})} (deg(x_1) + deg(x_2) - 2)^2.$$

We denote the collection of all extremal trees by $\mathbb{MT}_{n,\alpha}$ of n-vertex and α-matching number. We further define the subclasses of trees that minimize and maximize multiplicative reformulated first Zagreb as $\mathbb{MT}_{min,n,\alpha}$ and $\mathbb{MT}_{max,n,\alpha}$. For $\alpha = 1$, the collection $\mathbb{MT}_{n,1}$ has unique elements $\mathbb{P}_2$, $\mathbb{P}_3$ and $\mathbb{MT}_{n,\alpha} = \emptyset$ for $\lfloor \frac{n}{2} \rfloor < \alpha \leq n$. Therefore, the class of trees under consideration is $\mathbb{MT}_{n,\alpha}$ with $2 \leq \alpha \leq \lfloor \frac{n}{2} \rfloor$ and $n \geq 4$. The minimal tree is the path $\mathbb{P}_n$, whereas the maximal tree is a star-like graph $\mathbb{S}_{n,\alpha}$. Let us suppose that $\mathbb{MU}_{n,\alpha}$ is the collection of n-order unicyclic

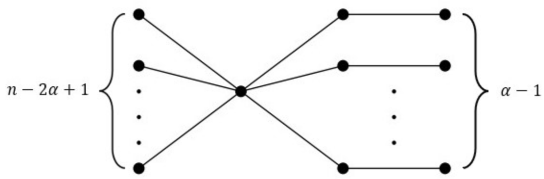


Figure 1: $\mathbb{MT}_{max,n,\alpha}$.

graph having an α-matching. The characterization of unicyclic graph that gives the minimum $\mathbb{MU}_{min,n,\alpha}$ and maximum value $\mathbb{MU}_{max,n,\alpha}$ with respect to matching and perfect matching about multiplicative reformulated first Zagreb index are discussed here. If $\alpha = 1$, then $\mathbb{MU}_{n,1}$ has a unique cycle of length 3 and $\mathbb{MU}_{n,\alpha} = \emptyset$ for $\lfloor \frac{n}{2} \rfloor < \alpha \leq n$. Let $\mathcal{C}_q$ be a cycle of length q for $3 \geq q \geq n$. For the minimum value of multiplicative reformulated first Zagreb index, the unicyclic graph has $\mathbb{MU}_{min,n,\alpha} = \mathcal{C}_n$, on the other hand, the maximum value of the multiplicative reformulated first Zagreb index, unicyclic graph can be obtained by connecting $n - 2\alpha + 1$ pendant vertices and $\alpha - 2$ paths of length 2 to one of the three vertices of $\mathcal{C}_3$.

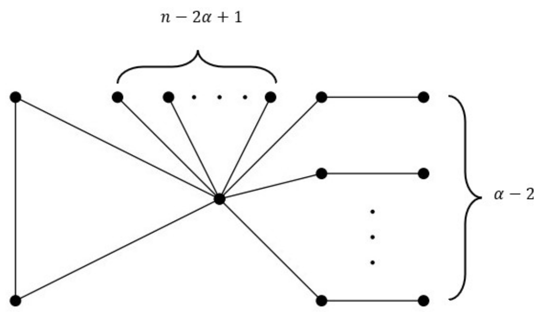


Figure 2: $\mathbb{MU}_{max,n,\alpha}$.

2 Preliminaries

The order of a graph $\mathbb{G}$ represents the total number of vertices it contains. The number of edges that are incident to a vertex x_1 in $V(\mathbb{G})$ is the degree of the vertex, which is represented by $deg_{\mathbb{G}}(x_1)$. If vertex x_1 is an endpoint of edge e then x_1 is said to be incident on e and e is incident on x_1. If there is an edge between two vertices x_1 and x_2, then we say that these vertices are adjacent to each other. When the degree of a vertex is 1, then it is known as a pendant vertex. A branching vertex is a vertex that has a degree of at least 3. Let $\mathbb{P}_n$, $\mathbb{S}_n$ and $\mathbb{C}_n$ denote the path, cycle and star of n vertices respectively. A path is a chain of distinct vertices such that two consecutive vertices are adjacent. If one end vertex of graph $\mathbb{G}$ is of degree greater or equal to 3, the other end vertex is the pendant vertex and (if an internal vertex exists), every internal vertex with a degree of exactly 2 is known as pendant path. An undirected connected graph is a tree that contains no cycles. If two distinct edges have a common vertex; they are said to be adjacent edges or neighbouring point. A vertex x_1 is a neighbor of x_2 if x_1 and x_2 are adjacent. The neighbourhood is the set of all neighbours of vertex x_1 and denoted by $\mathcal{N}(x_1)$. If the maximum degree of a vertex of a tree is four, then it is called a chemical(molecular) tree. A connected graph is a unicyclic graph in which it has only one cycle. In a graph $\mathbb{G}$, a matching $\mathbb{M}$ is a collection of distinct edges. Maximum matching is the set of the largest non-adjacent edges. Maximal matching is the collection of the smallest possible collection of non-adjacent edges. The number of edges in a maximum matching of a graph G is known as the matching number. Perfect matching occurs when every vertex of a graph $\mathbb{G}$ is connected by exactly one edge. If each vertex in $V(\mathbb{G})$ is on an edge of $\mathbb{M}$, a set of vertices in a graph $\mathbb{G}$ is said to be saturated by matching $\mathbb{M}$; otherwise it is $\mathbb{M}$-unsaturated.

3 Results

This section discusses the structure of extremal trees and unicyclic graphs and identifies the lower and upper bounds on multiplicative reformulated first Zagreb index in relation to perfect matching and the matching number α.

3.1 Characterization of trees with respect to matching

We will discuss the lower and upper bounds on multiplicative reformulated first Zagreb index for n-vertex trees with respect to perfect matching and matching number α.

Theorem 3.1. *If $\mathbb{MT} \in \mathbb{MT}_{min,n,\alpha}$, where $\alpha \geq 2$ and $n \geq 4$ then we have:*

$$\prod_{1,e}(\mathbb{MT}) \quad \geq \quad 4^{n-3},$$

with equality if and only if $\mathbb{MT}$ is $\mathbb{P}_n$.

Now we will discuss the cases for $\alpha \geq 2$ and $n \geq 5$.

Theorem 3.2. *Let $\mathbb{MT} \in \mathbb{MT}_{min,2\alpha,\alpha}$, where $\alpha \geq 2$ then we have:*

$$\prod_{1,e}(\mathbb{MT}) \quad \geq \quad 4^{2\alpha-3},$$

with equality if and only if $\mathbb{MT}$ is $\mathbb{P}_{2\alpha}$.

Proof. For α=2, only $\mathbb{P}_4$ is the tree of 2α=4 vertices. We have $\prod_{1,e}(\mathbb{P}_4) = 4$ and this satisfies the given bound. Thus, this result is true for α=2. We know that for $n = 2\alpha \geq 4$ the path $\mathbb{P}_{2\alpha}$ is only the tree with the smallest $\prod_{1,e}$ index among trees with 2α vertices (using Theorem 3.1). The path $\mathbb{P}_{2\alpha}$ has $4^{2\alpha-3}$ vertices of degree 2 and two vertices of degree 1 because $\mathbb{P}_{2\alpha}$ has a perfect matching, $\mathbb{P}_{2\alpha}$ is the only tree having the smallest $\prod_{1,e}$ index among trees with perfect matching, therefore

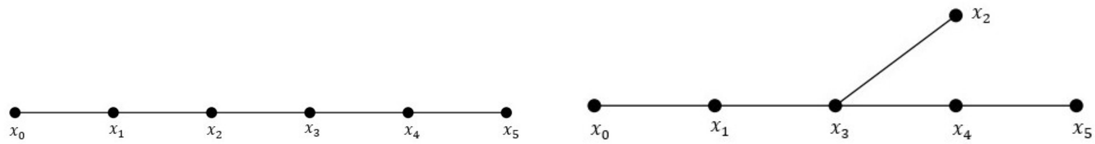
$$\prod_{1,e}(\mathbb{MT}) = 4^{2\alpha-3}.1.1 = 4^{2\alpha-3}.$$

■

Now, we characterize the structure of the maximal tree $\mathbb{MT}_{max,n,\alpha}$ with respect to perfect matching and matching number α of order n.

Lemma 3.3. *If* $\mathbb{MT} \in \mathbb{MT}_{max,n,\alpha}$, *where* $(n \geq 5, \alpha \geq 2)$ *then* $\mathbb{MT}$ *is not a path.*

Proof. Suppose on contrary that $\mathbb{MT} = x_0x_1...x_{n-1}$ is a path. Construct $\mathbb{MT}' = \mathbb{MT} + \{x_1x_3\} - \{x_1x_2\}$ then $\mathbb{MT}' \in \mathbb{MT}_{max,n,\alpha}$. For $n = 5$,

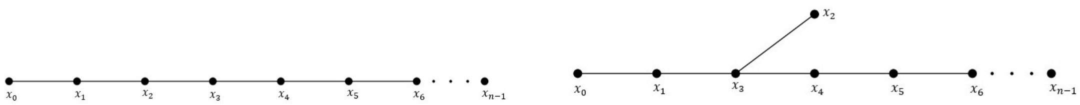


(a) $\mathbb{MT}$ (b) $\mathbb{MT}'$

Figure 3: For $n = 5$.

$$\begin{aligned}\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (1+2-2)^2(2+3-2)^2(3+1-2)^2(3+1-2)^2 \\ &\quad -(1+2-2)^2(2+2-2)^2(2+2-2)^2(2+1-2)^2 \\ &= 128 > 0,\end{aligned}$$

which is a contradiction (see Figure 3). For $n \geq 6$,



(a) $\mathbb{MT}$ (b) $\mathbb{MT}'$

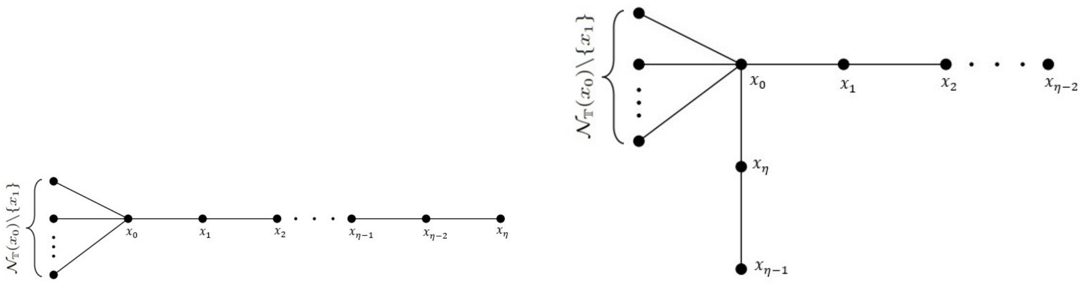
Figure 4: For $n \geq 6$.

$$\begin{aligned}\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (1+2-2)^2(2+3-2)^2(2+3-2)^2(3+1-2)^2 \\ &\times\ (2+2-2)^{2(n-5)} - (1+2-2)^2(2+2-2)^{2(n-2)} \\ &= (65)(4^{n-4}) > 0,\end{aligned}$$

which is a contradiction to our supposition (see Figure 4). Therefore $\mathbb{MT}$ is not a path. ■

Lemma 3.4. *Let $\mathbb{P}$ is a pendant path of $\mathbb{MT} \in \mathbb{MT}_{max,n,\alpha}$ then $|\mathbb{P}| \leq 2$.*

Proof. Suppose on contrary that $\mathbb{P} = x_0x_1...x_\eta$ is a pendant path of length $\eta \geq 3$ with $deg_{\mathbb{MT}}(x_0) = \omega \geq 3$, $deg_{\mathbb{MT}}(x_\eta) = 1$ and $deg_{\mathbb{MT}}(x_1)$=$deg_{\mathbb{MT}}(x_2) = \cdots = deg_{\mathbb{MT}}(x_{\eta-1})$=2. Construct $\mathbb{MT}' = \mathbb{MT}+\{x_0x_\eta\}-\{x_{\eta-2}x_{\eta-1}\}$ (as shown in Figure 5) then we have $\mathbb{MT}' \in \mathbb{MT}_{max,n,\alpha}$. For $\eta > 3$, let $\mathcal{N}_0 = \mathcal{N}_{\mathbb{MT}}(x_0)\backslash\{x_1\}$,



(a) $\mathbb{MT}$ (b) $\mathbb{MT}'$

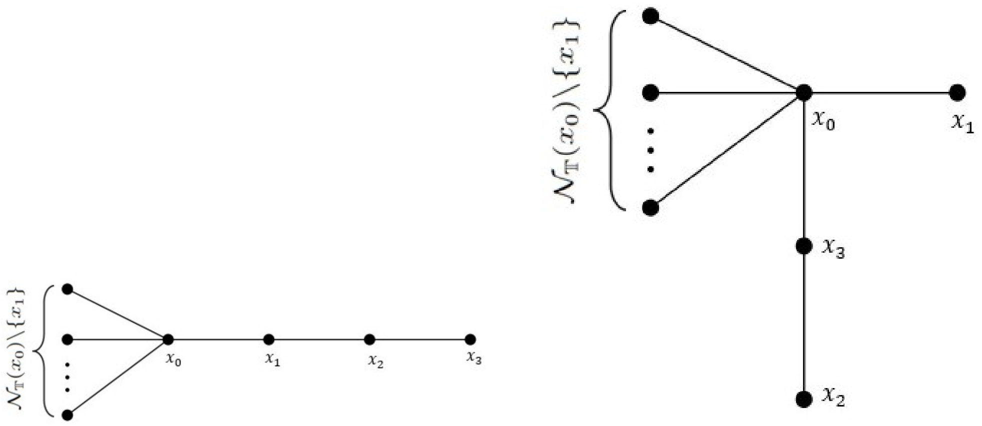
Figure 5: For $\eta > 3$.

$$\begin{aligned}
\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (2+1-2)^2(2+1-2)^2(\omega+1+2-2)^2(\omega+1+2-2)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0}(\omega+1+d_{\mathbb{MT}}(x_i)-2)^2 - (2+2-2)^2(2+2-2)^2 \\
&\times (2+1-2)^2(\omega+2-2)^2 \prod_{x_i \in \mathcal{N}_0}(\omega+d_{\mathbb{MT}}(x_i)-2)^2 \\
&= (\omega+1)^4 \prod_{x_i \in \mathcal{N}_0}(\omega+d_{\mathbb{MT}}(x_i)-1)^2 - 16\omega^2 \\
&\times \prod_{x_i \in \mathcal{N}_0}(\omega+d_{\mathbb{MT}}(x_i)-2)^2 > 0.
\end{aligned}$$

Note that for $\omega \geq 3$ we obviously have:

$$\prod_{x_i \in \mathcal{N}_0}(\omega+d_{\mathbb{MT}}(x_i)-1)^2 > \prod_{x_i \in \mathcal{N}_0}(\omega+d_{\mathbb{MT}}(x_i)-2)^2, \ (\omega+1)^2 \geq 16, \ (\omega+1)^2 > \omega^2.$$

For $\eta = 3$ (see Figure 6),



(a) $\mathbb{MT}$ (b) $\mathbb{MT}'$

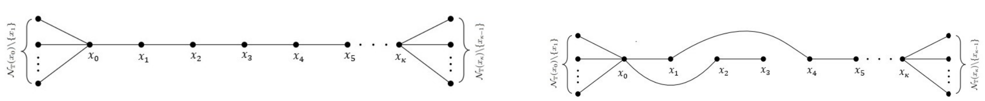
Figure 6: For $\eta = 3$.

$$\begin{aligned}\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (2+1-2)^2(\omega+1+2-2)^2(\omega+1+1-2)^2\\ &\times \prod_{x_i\in\mathcal{N}_0}(\omega+1+d_{\mathbb{MT}}(x_i)-2)^2 - (2+2-2)^2(2+1-2)^2\\ &\times (\omega+2-2)^2\prod_{x_i\in\mathcal{N}_0}(\omega+d_{\mathbb{MT}}(x_i)-2)^2\\ &= \omega^2(\omega+1)^2\prod_{x_i\in\mathcal{N}_0}(\omega+d_{\mathbb{MT}}(x_i)-1)^2 - 4\omega^2\\ &\times \prod_{x_i\in\mathcal{N}_0}(\omega+d_{\mathbb{MT}}(x_i)-2)^2 > 0.\end{aligned}$$

In above equation, note that we used $(\omega+1)^2 > 4$, $\omega \geq 3$. Thus, $\prod_{1,e}(\mathbb{MT}') > \prod_{1,e}(\mathbb{MT})$, which is a contradiction to our supposition. Therefore $\mathbb{MT}$ is a pendant path of length 2. ■

Lemma 3.5. *Let $\mathbb{P}_I$ is an internal path of $\mathbb{MT} \in \mathbb{MT}_{max,n,\alpha}$ then $|\mathbb{P}_I| < 1$.*

Proof. Suppose on contrary that $\mathbb{P}_I = x_0x_1...x_\kappa$ has an internal path of length $\kappa \geq 1$ of $\mathbb{MT}$ with $deg_{\mathbb{MT}}(x_0) = t \geq 3$, $deg_{\mathbb{MT}}(x_\kappa) = s \geq 3$ and $deg_{\mathbb{MT}}(x_1)$=$deg_{\mathbb{MT}}(x_2) = \cdots = deg_{\mathbb{MT}}(x_{\kappa-1})$=2. Let $\mathcal{N}_0 = \mathcal{N}_{\mathbb{MT}}(x_0)\backslash\{x_1\}$ and $\mathcal{N}_1 = \mathcal{N}_{\mathbb{MT}}(x_\kappa)\backslash\{x_{\kappa-1}\}$.
Case 1. For $\kappa \geq 5$, construct $\mathbb{MT}' = \mathbb{MT} + \{x_0x_2, x_1x_4\} - \{x_1x_2, x_3x_4\}$ (see Figure 7) then we have $\mathbb{MT}' \in \mathbb{MT}_{max,n,\alpha}$ and

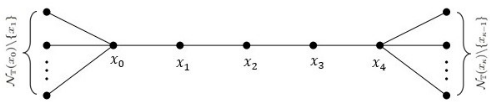


(a) $\mathbb{MT}$ (b) $\mathbb{MT}'$

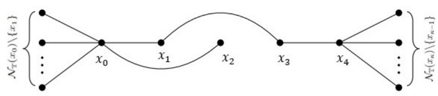
Figure 7: For $\kappa \geq 5$.

$$\begin{aligned}
\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (2+2-2)^2(2+1-2)^2(t+1+2-2)^2(t+1+2-2)^2 \\
&\times \prod_{x_i\in\mathcal{N}_0}(t+1+d_{\mathbb{MT}}(x_i)-2)^2 - (2+2-2)^2(2+2-2)^2 \\
&\times (2+2-2)^2(t+2-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MT}}(x_i)-2)^2 \\
&= 4(t+1)^4 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MT}}(x_i)-1)^2 - 64t^2 \\
&\times \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MT}}(x_i)-2)^2 > 0,
\end{aligned}$$

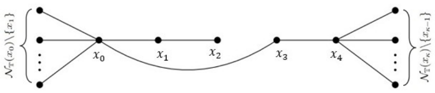
which is a contradiction. Note that here for $t \geq 3$ we obviously have $4(t+1)^2 \geq 64$ and $(t+1)^2 > t^2$.



(a) **Case** 2.



(b) **Subcase** 2.1



(c) **Subcase** 2.2

Figure 8: For $\kappa = 4$.

Case 2. For $\kappa = 4$, to prove this case there are two possibilities (see Figure 8).
Subcase 2.1. In this subcase x_2 is $\mathbb{M}$-unsaturated then x_1 and x_3 must be $\mathbb{M}$-saturated. Let $\mathbb{MT}' = \mathbb{MT} + \{x_0x_2, x_1x_3\} - \{x_1x_2, x_2x_3\}$ then we have $\mathbb{MT}' \in \mathbb{MT}_{max,n,\alpha}$ and

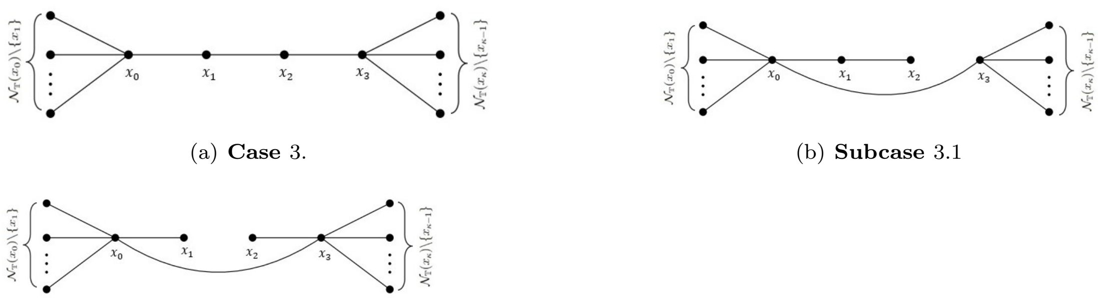
$$\begin{aligned}
\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (2+2-2)^2(t+1+2-2)^2(t+1+1-2)^2 \\
&\times \prod_{x_i\in\mathcal{N}_0}(t+1+d_{\mathbb{MT}}(x_i)-2)^2 - (2+2-2)^2(2+2-2)^2 \\
&\times (t+2-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MT}}(x_i)-2)^2 \\
&= 4t^2(t+1)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MT}}(x_i)-1)^2 - 16t^2 \\
&\times \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MT}}(x_i)-2)^2 > 0,
\end{aligned}$$

which is a contradiction.
Subcase 2.2. In this subcase x_2 is $\mathbb{M}$-saturated and let $x_1x_2 \in \mathbb{M}$ then let at least one from x_0 and x_3 is $\mathbb{M}$-saturated. Define $\mathbb{MT}' = \mathbb{MT} + \{x_0x_3\} - \{x_2x_3\}$ then we have $\mathbb{MT}' \in \mathbb{MT}_{max,n,\alpha}$

and

$$\begin{aligned}\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (2+1-2)^2(t+1+2-2)^2(t+1+2-2)^2 \\ &\times \prod_{x_i \in \mathcal{N}_0} (t+1+d_{\mathbb{MT}}(x_i)-2)^2 - (2+2-2)^2(2+2-2)^2 \\ &\times (t+2-2)^2 \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-2)^2 \\ &= (t+1)^4 \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-1)^2 - 16t^2 \\ &\times \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-2)^2 > 0,\end{aligned}$$

which is a contradiction.



(a) **Case** 3. (b) **Subcase** 3.1 (c) **Subcase** 3.2

Figure 9: For $\kappa = 3$.

Case 3. For $\kappa = 3$ (see Figure 9).
Subcase 3.1. $x_1x_2 \in \mathbb{M}$. Define $\mathbb{MT}' = \mathbb{MT} + \{x_0x_3\} - \{x_2x_3\}$ then we have $\mathbb{MT}' \in \mathbb{MT}_{max,n,\alpha}$ and

$$\begin{aligned}\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (2+1-2)^2(t+1+2-2)^2(t+1+s-2)^2 \\ &\times \prod_{x_i \in \mathcal{N}_0} (t+1+d_{\mathbb{MT}}(x_i)-2)^2 - (2+2-2)^2(2+s-2)^2 \\ &\times (t+2-2)^2 \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-2)^2 \\ &= (t+1)^2(t+s-1)^2 \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-1)^2 - 4t^2s^2 \\ &\times \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-2)^2 > 0.\end{aligned}$$

which is a contradiction. Note that here for $t \geq 3$ and $s \geq 3$ we obviously have:

$$\prod_{x_i \in \mathcal{N}_0} (t + d_{\mathbb{MT}}(x_i) - 1)^2 > 4 \prod_{x_i \in \mathcal{N}_0} (t + d_{\mathbb{MT}}(x_i) - 2)^2,$$
$$(t + s - 1)^2 > s^2,$$
$$(t + 1)^2 > t^2.$$

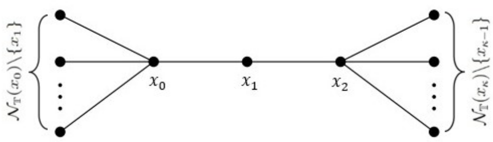
Subcase 3.2. x_1x_2 does not belongs to $\mathbb{M}$. Define $\mathbb{MT}' = \mathbb{MT} + \{x_0x_3\} - \{x_1x_2\}$ then we have $\mathbb{MT}' \in \mathbb{MT}_{max,n,\alpha}$ and

$$\begin{aligned}
\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (t+1+1-2)^2(t+1+s+1-2)^2(1+s+1-2)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (t+1+d_{\mathbb{MT}}(x_i)-2)^2 \prod_{x_j \in \mathcal{N}_1} (s+1+d_{\mathbb{MT}}(x_j)-2)^2 \\
&\quad -(2+2-2)^2(2+s-2)^2(t+2-2)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-2)^2 \prod_{x_j \in \mathcal{N}_1} (s+d_{\mathbb{MT}}(x_j)-2)^2 \\
&= t^2s^2(t+s)^2 \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-1)^2 \prod_{x_j \in \mathcal{N}_1} (s+d_{\mathbb{MT}}(x_j)-1)^2 \\
&\quad -4t^2s^2 \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-2)^2 \prod_{x_j \in \mathcal{N}_1} (s+d_{\mathbb{MT}}(x_j)-2)^2 > 0,
\end{aligned}$$

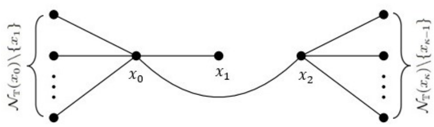
which is a contradiction. Note that here for $t \geq 3$ and $s \geq 3$ we obviously have:

$$\prod_{x_i \in \mathcal{N}_0} (t + d_{\mathbb{MT}}(x_i) - 1)^2 > \prod_{x_i \in \mathcal{N}_0} (t + d_{\mathbb{MT}}(x_i) - 2)^2,$$
$$\prod_{x_j \in \mathcal{N}_1} (s + d_{\mathbb{MT}}(x_j) - 1)^2 > \prod_{x_j \in \mathcal{N}_1} (s + d_{\mathbb{MT}}(x_j) - 2)^2,$$
$$(t+s)^2 > 4.$$

Case 4. For $\kappa = 2$ (see Figure 10).



(a) **Case** 4.



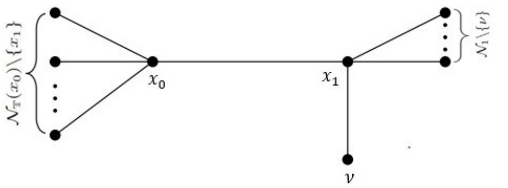
(b) **Subcase** 4.1 **and** 4.2

Figure 10: For $\kappa = 2$.

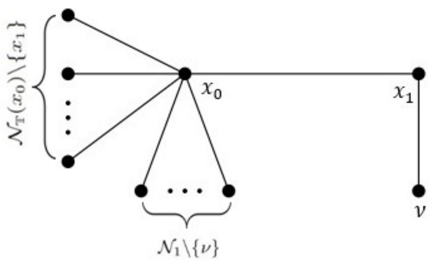
Subcase 4.1. In this subcase, x_1 is $\mathbb{M}$-unsaturated then let both x_0 and x_2 be $\mathbb{M}$-saturated. Define $\mathbb{MT}' = \mathbb{MT} + \{x_0x_2\} - \{x_1x_2\}$, we have $\mathbb{MT}' \in \mathbb{MT}_{max,n,\alpha}$ and as we know $\mathbb{M}$ is maximum matching of $\mathbb{MT}$ then

$$\begin{aligned}\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (t+1+1-2)^2(t+1+s-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+1+d_{\mathbb{MT}}(x_i)-2)^2 \\ &\quad -(2+s-2)^2(t+2-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MT}}(x_i)-2)^2 \\ &= t^2(t+s-1)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MT}}(x_i)-1)^2 - t^2s^2 \\ &\times \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MT}}(x_i)-2)^2 > 0,\end{aligned}$$

which is a contradiction.
Subcase 4.2. Here, x_1 is $\mathbb{M}$-saturated then let both x_0x_1 is form $\mathbb{M}$. To prove this subcase we can use the same transformation as in Subcase 4.1 then also we get a contradiction.



(a) **Case** 5



(b) **Subcase** 5.1

Figure 11: For $\kappa = 1$.

Case 5. For $\kappa = 1$ (see Figure 11), at vertex x_1 there exist $\nu \in \mathcal{N}_1$ with $deg_{\mathbb{MT}}(\nu) \geq 1$ then we have the following possibilities.
Subcase 5.1. If $\nu = 1$, then let

$$\mathbb{MT}' = \mathbb{MT} + \bigcup_{x_j\in\mathcal{N}_1\setminus\{\nu\}}\{x_0x_j\} - \bigcup_{x_j\in\mathcal{N}_1\setminus\{\nu\}}\{x_1x_j\}.$$

We have $\mathbb{MT}' \in \mathbb{MT}_{max,n,\alpha}$ and then

$$\begin{aligned}
\prod_{1,e}(\mathbb{MT}') - \prod_{1,e}(\mathbb{MT}) &= (t+s-2+2-2)^2(2+1-2)^2 \\
&\times \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (t+s-2+d_{\mathbb{MT}}(x_j)-2)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (t+s-2+d_{\mathbb{MT}}(x_i)-2)^2 - (t+s-2)^2(s+1-2)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-2)^2 \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (s+d_{\mathbb{MT}}(x_j)-2)^2 \\
&= (t+s-2)^2 \prod_{x_i \in \mathcal{N}_0} (t+s+d_{\mathbb{MT}}(x_i)-4)^2 \\
&\times \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (t+s+d_{\mathbb{MT}}(x_j)-2)^2 - (t+s-2)^2(s-1)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-2)^2 \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (s+d_{\mathbb{MT}}(x_j)-2)^2 > 0
\end{aligned}$$

which is a contradiction. Note that here for $t \geq 3$ and $s \geq 3$ we obviously have:

$$\prod_{x_i \in \mathcal{N}_0} (t+s+d_{\mathbb{MT}}(x_i)-4)^2 > (s-1)^2 \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MT}}(x_i)-2)^2,$$
$$\prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (t+s+d_{\mathbb{MT}}(x_j)-4)^2 > \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (s+d_{\mathbb{MT}}(x_j)-2)^2.$$

Subcase 5.2. Let $\nu > 1$. To prove this subcase we can use the same transformation as in Subcase 5.1 then also we get a contradiction. ■

Lemma 3.3, Lemma 3.4, and Lemma 3.5 characterize the structure of extremal trees that maximize the aforementioned index.

Theorem 3.6. *Let* $\mathbb{MT} \in \mathbb{MT}_{max,n,\alpha}$, *where* $\alpha \geq 2$ *and* $n \geq 5$ *then we have*

$$\prod_{1,e}(\mathbb{MT}) \leq (n-\alpha)^{2(\alpha-1)}(n-\alpha-1)^{2(n-2\alpha+1)},$$

with equality if and only if $\mathbb{MT}$ *has the structure of Figure 1.*

Proof. If $n = 2\alpha$ or $n > 2\alpha$, then from Lemma 3.3, Lemma 3.4, and Lemma 3.5, the extremal tree $\mathbb{MT}$ is unique and

$$\prod_{1,e}(\mathbb{MT}) \leq (n-\alpha)^{2(\alpha-1)}(n-\alpha-1)^{2(n-2\alpha+1)}, n > 2\alpha,$$

and

$$\prod_{1,e}(\mathbb{MT}) \leq (\alpha)^{2(\alpha-1)}(\alpha-1)^2,\ n = 2\alpha.$$

■

3.2 Characterization of unicyclic graphs with respect to matching

The characterization of a unicyclic graph that gives the minimum $\mathbb{MU}_{min,n,\alpha}$ and maximum value $\mathbb{MU}_{max,n,\alpha}$ with respect to perfect matching and matching number α and order n about the multiplicative reformulated first Zagreb index is discussed here. The following results are required to demonstrate our key findings:

Theorem 3.7. *Let* $\mathbb{MU} \in \mathbb{MU}_{min,n,\alpha}$*, where* $\alpha \geq 2$ *and* $n \geq 4$ *then we have:*

$$\prod_{1,e}(\mathbb{MU}) \quad \geq \quad 4^{n-1},$$

with equality if and only if $\mathbb{MU}$ *is* $\mathcal{C}_n$*.*

Theorem 3.8. *Let* $\mathbb{MU} \in \mathbb{MU}_{min,2\alpha,\alpha}$*, where* $\alpha \geq 2$ *then we have:*

$$\prod_{1,e}(\mathbb{MU}) \geq 4^{2\alpha-1}.$$

Proof. Let $\mathbb{MU}$ be a unicyclic graph with 2α vertices, a cycle of length p, and matching number α with the smallest $\prod_{1,e}$ index. Let $\mathcal{C}_q = c_0c_1c_2...c_qc_0$ be the cycle in $\mathbb{MU}$. Then $\mathbb{MU}$ has only cycle $\mathcal{C}_q$.

For $\alpha = 2$, the only unicyclic graph with $2\alpha = 4$ vertices is $\mathbb{MU}_4$. We have $\prod_{1,e}(\mathbb{MU}_4) = 64$ and this satisfies the given bound. Thus, this result is true for α=2. For $n = 2\alpha \geq 4$, $\mathbb{MU}_{2\alpha}$ is the only graph with the smallest $\prod_{1,e}$ index among unicyclic graphs with 2α vertices (using Theorem 3.7). The unicyclic graph has $4^{2\alpha-1}$ vertices of degree 2 having the smallest $\prod_{1,e}$ index among trees with 2α vertices with perfect matching. Therefore,

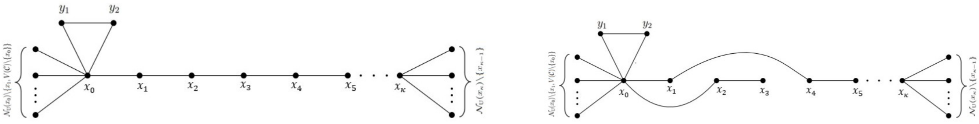
$$\prod_{1,e}(\mathbb{MU}) \geq 4^{2\alpha-1}.$$

■

Now, we characterize the structure of the maximum unicyclic graph $\mathbb{MU}_{max,n,\alpha}$ with respect to perfect matching and matching number α of order n.

Lemma 3.9. *Let* $\mathbb{MU} \in \mathbb{MU}_{max,n,\alpha}$ *then* $\mathbb{MU}$ *has an internal path of length* < 1.

Proof. Let $\mathbb{UP}_I$ be an internal path of $\mathbb{MU}$. Suppose on contrary that $\mathbb{UP}_I = x_0x_1...x_\kappa$ is an internal path of length $\kappa \geq 1$ of $\mathbb{MU}$ with $deg_{\mathbb{MU}}(x_0) = t \geq 3$, $deg_{\mathbb{MU}}(x_\kappa) = s \geq 3$ and $deg_{\mathbb{MU}}(x_1)$=$deg_{\mathbb{MU}}(x_2) = \cdots = deg_{\mathbb{MU}}(x_{\kappa-1})$=2.
Let $\mathcal{N}_0 = \mathcal{N}_{\mathbb{MU}}(x_0)\backslash\{x_1, V(\mathcal{C})\backslash\{x_0\}\}$, $\mathcal{N}_1 = \mathcal{N}_{\mathbb{MU}}(x_\kappa)\backslash\{x_{\kappa-1}\}$ and $\mathcal{N}_2 = \{y_m; y_m \in V(\mathcal{C})$ which is adjacent to $x_0\}$.
Case 1. For $\kappa \geq 5$ (see Figure 12). Construct $\mathbb{MU}' = \mathbb{MU} + \{x_0x_2, x_1x_4\} - \{x_1x_2, x_3x_4\}$ then



(a) $\mathbb{MU}$ (b) $\mathbb{MU}'$

Figure 12: For $\kappa \geq 5$.

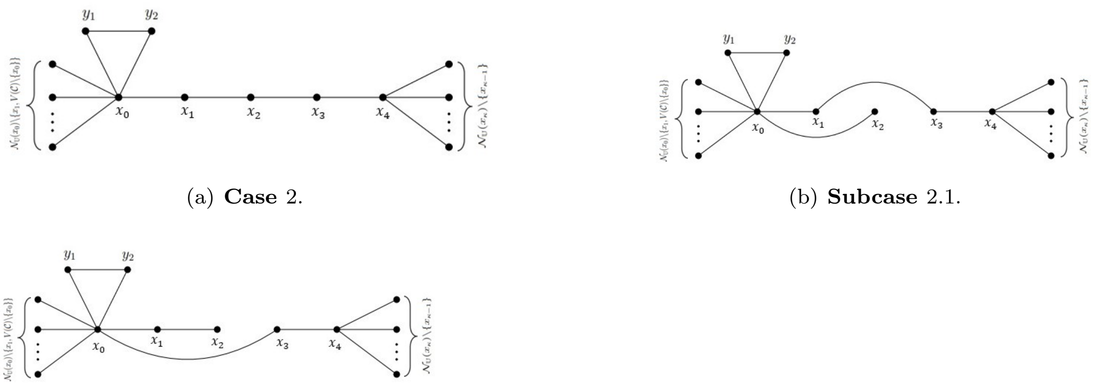
we have $\mathbb{MU}' \in \mathbb{MU}_{max,n,\alpha}$ and

$$\begin{aligned}
\prod_{1,e}(\mathbb{MU}') - \prod_{1,e}(\mathbb{MU}) &= (2+1-2)^2(2+2-2)^2(t+1+2-2)^2(t+1+2-2)^2 \\
&\times \prod_{y_m \in \mathcal{N}_2}(t+1+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i \in \mathcal{N}_0}(t+1+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\quad -(2+2-2)^2(2+2-2)^2(2+2-2)^2(t+2-2)^2 \\
&\times \prod_{y_m \in \mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i \in \mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \\
&= 4(t+1)^4 \prod_{x_i \in \mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-1)^2 \prod_{y_m \in \mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-1)^2 \\
&\quad -64t^2 \prod_{x_i \in \mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \prod_{y_m \in \mathcal{N}_0}(t+d_{\mathbb{MU}}(y_m)-2)^2 \\
&> 0,
\end{aligned}$$

which is a contradiction. Note that for $t \geq 3$ it obvious that:

$$\prod_{x_i \in \mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-1)^2 > \prod_{x_i \in \mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2,$$
$$\prod_{y_m \in \mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-1)^2 > \prod_{y_m \in \mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2,$$
$$4(t+1)^2 \geq 64, \ (t+1)^2 > t^2.$$

Case 2. For $\kappa = 4$ (see Figure 13). To prove this case there are two possibilities.
Subcase 2.1. In this subcase, x_2 is $\mathbb{M}$-unsaturated then x_1 and x_3 must be $\mathbb{M}$-saturated. Let



(a) **Case** 2. (b) **Subcase** 2.1.

(c) **Subcase** 2.2.

Figure 13: For $\kappa = 4$.

$\mathbb{MU}' = \mathbb{MU} + \{x_0x_2, x_1x_3\} - \{x_1x_2, x_2x_3\}$ then we have $\mathbb{MU}' \in \mathbb{MU}_{max,n,\alpha}$ and

$$
\begin{aligned}
\prod_{1,e}(\mathbb{MU}') - \prod_{1,e}(\mathbb{MU}) &= (2+2-2)^2(t+1+1-2)^2(t+1+2-2)^2 \\
&\times \prod_{y_m \in \mathcal{N}_2}(t+1+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i \in \mathcal{N}_0}(t+1+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\quad -(2+2-2)^2(2+2-2)^2(t+2-2)^2 \\
&\times \prod_{y_m \in \mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i \in \mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \\
&= 4t^2(t+1)^2 \prod_{x_i \in \mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-1)^2 \prod_{y_m \in \mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-1)^2 \\
&\quad -16t^2 \prod_{x_i \in \mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \prod_{y_m \in \mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 \\
&> 0,
\end{aligned}
$$

which is a contradiction.

Subcase 2.2. In this subcase x_2 is $\mathbb{M}$-saturated and let $x_1x_2 \in \mathbb{M}$ and assume that at least one of x_0 or x_3 is $\mathbb{M}$-saturated. Define $\mathbb{MU}' = \mathbb{MU} + \{x_0x_3\} - \{x_2x_3\}$ then we have $\mathbb{MU}' \in \mathbb{MU}_{max,n,\alpha}$

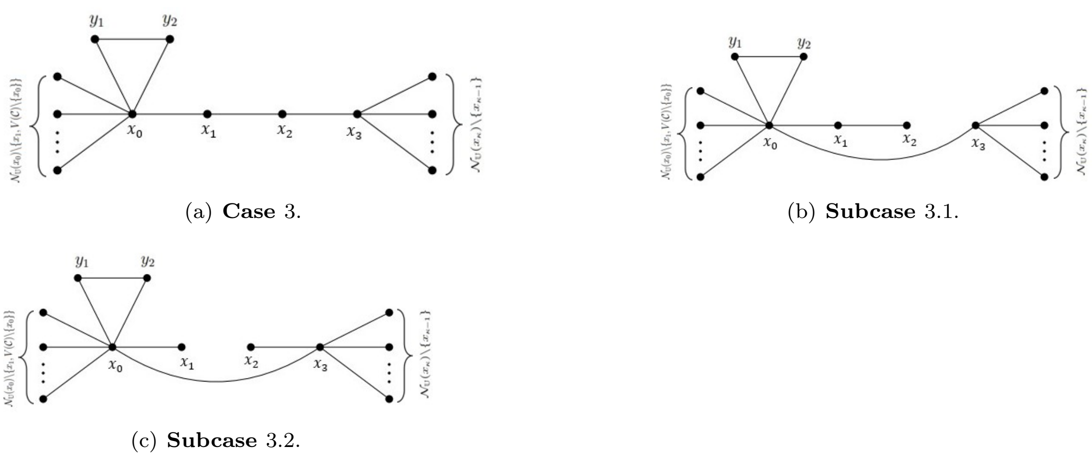
and

$$\begin{aligned}
\prod_{1,e}(\mathbb{MU}') - \prod_{1,e}(\mathbb{MU}) &= (2+1-2)^2(t+1+2-2)^2(t+1+2-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+1+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+1+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\quad -(2+2-2)^2(2+2-2)^2(t+2-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \\
&= (t+1)^4 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-1)^2 \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-1)^2 \\
&\quad -16t^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 \\
&> 0,
\end{aligned}$$

which is a contradiction.

Case 3. For $\kappa = 3$ (see Figure 14).

Subcase 3.1. $x_1x_2 \in \mathbb{M}$. Define $\mathbb{MU}' = \mathbb{MU} + \{x_0x_3\} - \{x_2x_3\}$ then we have $\mathbb{MU}' \in \mathbb{MU}_{max,n,\alpha}$



(a) **Case** 3.

(b) **Subcase** 3.1.

(c) **Subcase** 3.2.

Figure 14: For $\kappa = 3$.

and

$$\begin{aligned}
\prod_{1,e}(\mathbb{MU}') - \prod_{1,e}(\mathbb{MU}) &= (2+1-2)^2(t+1+2-2)^2(t+1+s-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+1+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+1+d_{\mathbb{MU}}(x_i)-2)^2 \\
&-(2+2-2)^2(2+s-2)^2(t+2-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \\
&= (t+1)^2(t+s-1)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-1)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-1)^2 - 4t^2s^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 > 0,
\end{aligned}$$

which is a contradiction. Note that for $t \geq 3$ and $s \geq 3$ it is obvious that

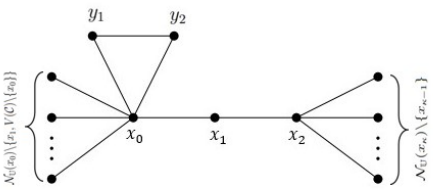
$$\begin{aligned}
\prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-1)^2 &> 4\prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2, \\
\prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-1)^2 &> \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2, \\
(t+s-1)^2 > s^2,\ & (t+1)^2 > t^2.
\end{aligned}$$

Subcase 3.2. x_1x_2 does not belongs to $\mathbb{M}$. Define $\mathbb{MU}' = \mathbb{MU} + \{x_0x_3\} - \{x_1x_2\}$ then we have $\mathbb{MU}' \in \mathbb{MU}_{max,n,\alpha}$ and

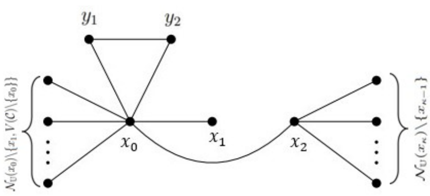
$$\begin{aligned}
\prod_{1,e}(\mathbb{MU}') - \prod_{1,e}(\mathbb{MU}) &= (t+1+1-2)^2(t+1+s+1-2)^2(1+s+1-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+1+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+1+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\times \prod_{x_j\in\mathcal{N}_1}(s+1+d_{\mathbb{MU}}(x_j)-2)^2 - (2+2-2)^2(2+s-2)^2 \\
&\times (t+2-2)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_j\in\mathcal{N}_1}(s+d_{\mathbb{MU}}(x_j)-2)^2 \\
&= t^2s^2(t+s)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-1)^2 \prod_{x_j\in\mathcal{N}_1}(s+d_{\mathbb{MU}}(x_j)-1)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-1)^2 - 4t^2s^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\times \prod_{x_j\in\mathcal{N}_1}(s+d_{\mathbb{MU}}(x_j)-2)^2 \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 > 0,
\end{aligned}$$

which is a contradiction.

Case 4. For $\kappa = 2$ (see Figure 15).



(a) **Case** 4.



(b) **Subcase** 4.1 **and** 4.2.

Figure 15: For $\kappa = 2$.

Subcase 4.1. In this subcase x_1 be $\mathbb{M}$-unsaturated then let both x_0 and x_2 is $\mathbb{M}$-saturated. Define $\mathbb{MU}' = \mathbb{MU} + \{x_0x_2\} - \{x_1x_2\}$, we have $\mathbb{MU}' \in \mathbb{MU}_{max,n,\alpha}$ and as we know $\mathbb{M}$ is maximum matching of $\mathbb{MU}$ then

$$\begin{aligned}
\prod_{1,e}(\mathbb{MU}') - \prod_{1,e}(\mathbb{MU}) &= (t+1+1-2)^2(t+1+s-2)^2 \\
&\times \prod_{x_i\in\mathcal{N}_0}(t+1+d_{\mathbb{MU}}(x_i)-2)^2 \prod_{y_m\in\mathcal{N}_2}(t+1+d_{\mathbb{MU}}(y_m)-2)^2 \\
&\quad -(2+s-2)^2(t+2-2)^2 \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-1)^2 \\
&\times \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \\
&= t^2(t+s-1)^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-1)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-1)^2 - t^2s^2 \prod_{x_i\in\mathcal{N}_0}(t+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(t+d_{\mathbb{MU}}(y_m)-2)^2 > 0,
\end{aligned}$$

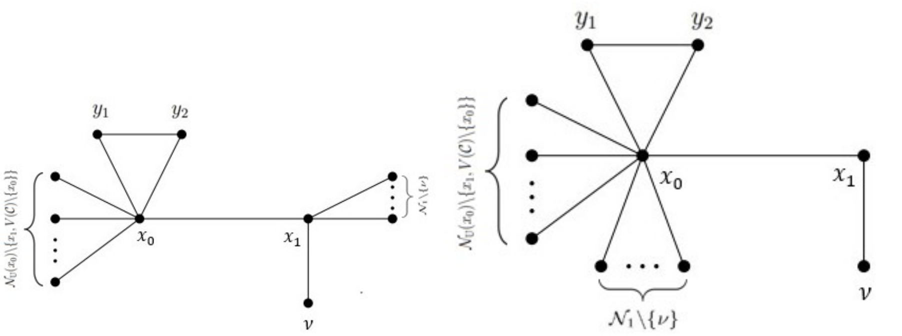
which is a contradiction.

Subcase 4.2. x_1 is $\mathbb{M}$-saturated then let both x_0x_1 is form $\mathbb{M}$. To prove this subcase we can use the same transformation as in Subcase 4.1 then also we get a contradiction.

Case 5. For $\kappa = 1$ (see Figure 16), at vertex x_1 there exist $\nu \in \mathcal{N}_1$ with $deg_{\mathbb{MU}}(\nu) \geq 1$ then we have the following possibilities.

Subcase 5.1. If $\nu = 1$. Let

$$\mathbb{MU}' = \mathbb{MU} + \bigcup_{x_j\in\mathcal{N}_1\setminus\{\nu\}}\{x_0x_j\} - \bigcup_{x_j\in\mathcal{N}_1\setminus\{\nu\}}\{x_1x_j\},$$



(a) **Case** 5. (b) **Subcase** 5.1.

Figure 16: For $\kappa = 1$.

we have $\mathbb{MU}' \in \mathbb{MU}_{max,n,\alpha}$ and then

$$\begin{aligned}
\prod_{1,e}(\mathbb{MU}') - \prod_{1,e}(\mathbb{MU}) &= (t+s-2+2-2)^2(2+1-2)^2 \\
&\times \prod_{y_m \in \mathcal{N}_2} (t+s-2+d_{\mathbb{MU}}(y_m)-2)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (t+s-2+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\times \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (t+s-2+d_{\mathbb{MU}}(x_j)-2)^2 \\
&\quad -(t+s-2)^2(s+1-2)^2 \prod_{x_i \in \mathcal{N}_0} (t++d_{\mathbb{MU}}(x_i)-2)^2 \\
&\times \prod_{y_m \in \mathcal{N}_2} (t+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (s+d_{\mathbb{MU}}(x_j)-2)^2 \\
&= (t+s-2)^2 \prod_{x_i \in \mathcal{N}_0} (t+s+d_{\mathbb{MU}}(x_i)-4)^2, \\
&\times \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (t+s+d_{\mathbb{MU}}(x_j)-4)^2 \\
&\times \prod_{y_m \in \mathcal{N}_2} (t+s+d_{\mathbb{MU}}(y_m)-4)^2 - (t+s-2)^2(s-1)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (t+d_{\mathbb{MU}}(x_i)-2)^2 \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (s+d_{\mathbb{MU}}(x_j)-2)^2 \\
&\times \prod_{y_m \in \mathcal{N}_2} (t+d_{\mathbb{MU}}(y_m)-2)^2 > 0,
\end{aligned}$$

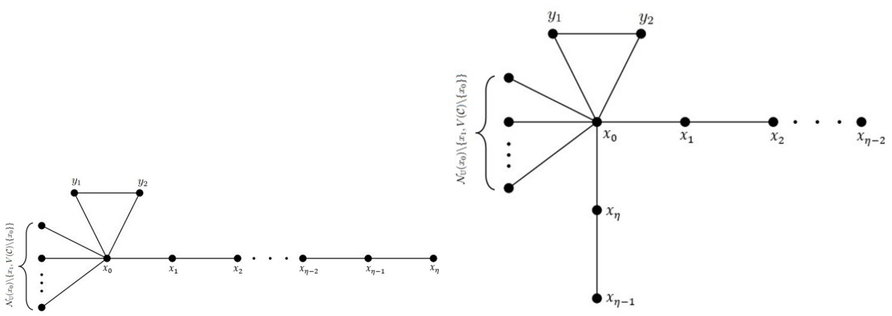
which is a contradiction. Note that for $t \geq 3$ and $s \geq 3$ we obviously have:

$$\prod_{x_i \in \mathcal{N}_0} (t + s + d_{\mathbb{MU}}(x_i) - 4)^2 > (s-1)^2 \prod_{x_i \in \mathcal{N}_0} (t + d_{\mathbb{MU}}(x_i) - 2)^2,$$
$$\prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (t + s + d_{\mathbb{MU}}(x_j) - 4)^2 > \prod_{x_j \in \mathcal{N}_1 \setminus \{\nu\}} (s + d_{\mathbb{MU}}(x_j) - 2)^2,$$
$$\prod_{y_m \in \mathcal{N}_2} (t + s + d_{\mathbb{MU}}(y_m) - 4)^2 > \prod_{y_m \in \mathcal{N}_2} (t + d_{\mathbb{MU}}(y_m) - 2)^2,$$

Subcase 5.2. If $\nu > 1$, to prove this subcase, we can use the same transformation as in Subcase 5.1. Then also we get a contradiction. ■

Lemma 3.10. *If* $\mathbb{MU} \in \mathbb{MU}_{max,n,\alpha}$, *then the pendant path is attached to most one end vertex of the cycle having a maximum length of* 2.

Proof. Let $\mathbb{UP}$ is the pendant path of $\mathbb{MU}$. Suppose on contrary that $\mathbb{UP} = x_0x_1...x_\eta$ is a pendant path of length $\eta \geq 3$ with $deg_{\mathbb{MU}}(x_0) = \omega \geq 3$, $deg_{\mathbb{MU}}(x_\eta) = 1$ and $deg_{\mathbb{MU}}(x_1)$=$deg_{\mathbb{MU}}(x_2)$=...=$deg_{\mathbb{MU}}(x_{\eta-1})$=2. Construct



(a) $\mathbb{MU}$. (b) $\mathbb{MU}'$.

Figure 17: For $\eta > 3$.

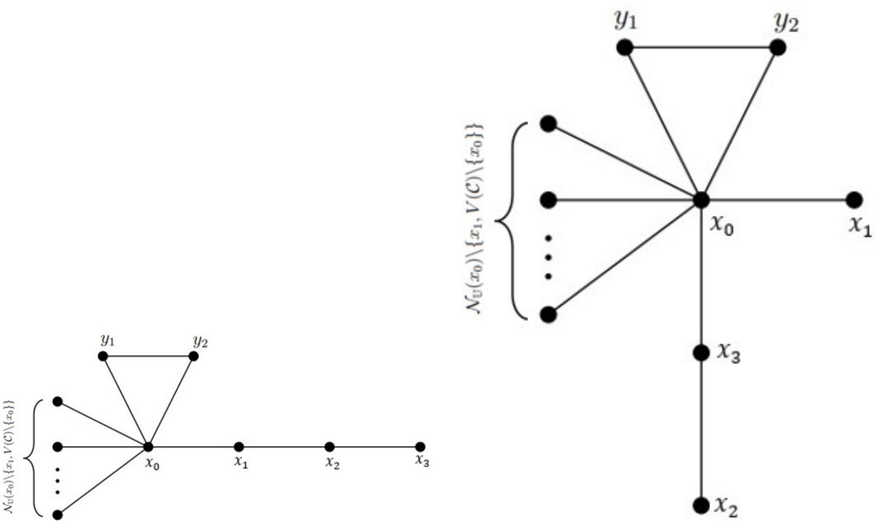
$$\mathbb{MU}' = \mathbb{MU} + \{x_0x_\eta\} - \{x_{\eta-2}x_{\eta-1}\},$$

then we have $\mathbb{MU}' \in \mathbb{MU}_{n,\alpha}$.
For $\eta > 3$ (see Figure 17), let $\mathcal{N}_0 = \mathcal{N}_{\mathbb{MU}}(x_0) \setminus \{x_1, V(\mathcal{C}) \setminus \{x_0\}\}$, where $\mathcal{N}_2 = \{y_m; y_m \in V(\mathcal{C})$

which is adjacent to $x_0\}$.

$$\begin{aligned}
\prod_{1,e}(\mathbb{MU}') - \prod_{1,e}(\mathbb{MU}) &= (2+1-2)^2(2+1-2)^2(\omega+1+2-2)^2(\omega+1+2-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(\omega+1+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i\in\mathcal{N}_0}(\omega+1+d_{\mathbb{MU}}(x_i)-2)^2 \\
&\quad -(2+2-2)^2(2+2-2)^2(2+1-2)^2(\omega+2-2)^2 \\
&\times \prod_{y_m\in\mathcal{N}_2}(\omega+d_{\mathbb{MU}}(y_m)-2)^2 \prod_{x_i\in\mathcal{N}_0}(\omega+d_{\mathbb{MU}}(x_i)-2)^2 \\
&= (\omega+1)^4 \prod_{x_i\in\mathcal{N}_0}(\omega+d_{\mathbb{MU}}(x_i)-1)^2 \prod_{y_m\in\mathcal{N}_2}(\omega+d_{\mathbb{MU}}(y_m)-1)^2 \\
&\quad -16\omega^2 \prod_{x_i\in\mathcal{N}_0}(\omega+d_{\mathbb{MU}}(x_i)-2)^2 \prod_{y_m\in\mathcal{N}_2}(\omega+d_{\mathbb{MU}}(y_m)-2)^2 \\
&> 0.
\end{aligned}$$

Note that for $\omega \geq 3$, we obviously have $(\omega+1)^2 > \omega^2$ and $(\omega+1)^2 \geq 16$.



(a) $\mathbb{MU}$. (b) $\mathbb{MU}'$.

Figure 18: For $\eta = 3$.

For $\eta = 3$, (see Figure 18),

$$\begin{aligned}
\prod_{1,e}(\mathbb{MU}') - \prod_{1,e}(\mathbb{MU}) &= (2+1-2)^2(\omega+1+2-2)^2(\omega+1+1-2)^2 \\
&\times \prod_{y_m \in \mathcal{N}_2} (\omega+1+d_{\mathbb{MU}}(y_m)-2)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (\omega+1+d_{\mathbb{MU}}(x_i)-2)^2 - (2+2-2)^2(2+1-2)^2 \\
&\times (\omega+2-2)^2 \prod_{y_m \in \mathcal{N}_2} (\omega+d_{\mathbb{MU}}(y_m)-2)^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (\omega+d_{\mathbb{MU}}(x_i)-2)^2 \\
&= \omega^2(\omega+1)^2 \prod_{x_i \in \mathcal{N}_0} (\omega+d_{\mathbb{MU}}(x_i)-1)^2, \\
&\times \prod_{y_m \in \mathcal{N}_2} (\omega+d_{\mathbb{MU}}(y_m)-1)^2 - 4\omega^2 \\
&\times \prod_{x_i \in \mathcal{N}_0} (\omega+d_{\mathbb{MU}}(x_i)-2)^2 \prod_{y_m \in \mathcal{N}_2} (\omega+d_{\mathbb{MU}}(y_m)-2)^2 > 0,
\end{aligned}$$

which is a contradiction to our supposition. Therefore $\mathbb{MU}$ has a pendant path of length 2. ■

Lemma 3.10 and Lemma 3.9 characterize the structure of extremal unicyclic graph that maximizes aforementioned index.

Theorem 3.11. *Let $\mathbb{MU} \in \mathbb{MU}_{max,n,\alpha}$, where $\alpha \geq 2$ and $n \geq 5$ then we have*

$$\prod_{1,e}(\mathbb{MU}) \leq (n-\alpha)^{2(n-2\alpha+1)}(n-\alpha+1)^{2(n)},$$

with equality if and only if $\mathbb{MU}$ has the structure of Figure 2.

Proof. If $n = 2\alpha$ or $n > 2\alpha$, then from Lemma 3.10 and Lemma 3.9, the extremal unicyclic graph $\mathbb{MU}$ is unique and

$$\prod_{1,e}(\mathbb{MU}) \leq (n-\alpha)^{2(n-2\alpha+1)}(n-\alpha+1)^{2(n)}, \quad n > 2\alpha,$$

and

$$\prod_{1,e}(\mathbb{MU}) \leq (\alpha)^2(\alpha+1)^{2\alpha}, \quad n = 2\alpha.$$

■

4 Conclusion

The study focuses on characterizing the extremal in the collection of all n-vertex trees using multiplicative reformulated first Zagreb index and under specific conditions. It provides sharp lower and upper bounds for the multiplicative reformulated first Zagreb index among trees with a given order n, matching number α and perfect matching.

Conflicts of interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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