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Research Article

On Mostar and Edge Mostar Indices of Graphs

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Let G be a graph with edge set $E(G)$ and $e = uv \in E(G)$. Define $n_u(e, G)$ and $m_u(e, G)$ to be the number of vertices of G closer to u than to v and the number of edges of G closer to u than to v, respectively. The numbers $n_v(e, G)$ and $m_v(e, G)$ can be defined in an analogous way. The Mostar and edge Mostar indices of G are new graph invariants defined as $Mo(G) = \sum_{uv\in E(G)} |n_u(uv, G) - n_v(uv, G)|$ and $Mo_e(G) = \sum_{uv\in E(G)} |m_u(uv, G) - m_v(uv, G)|$, respectively. In this paper, an upper bound for the Mostar and edge Mostar indices of a tree in terms of its diameter is given. Next, the trees with the smallest and the largest Mostar and edge Mostar indices are also given. Finally, a recent conjecture of Liu, Song, Xiao, and Tang (2020) on bicyclic graphs with a given order, for which extremal values of the edge Mostar index are attained, will be proved. In addition, some new open questions are presented.

1. Introduction

In this paper, graph means undirected and connected finite graph without loops or multiple edges. The vertex and edge sets of such a graph G will be denoted by $V = V(G)$ and $E = E(G)$, respectively. We use the notations $\deg_G(v)$ and $N[v, G]$ for the degree of a vertex v and the set of all vertices adjacent to v, respectively. Suppose e is an edge and x and y are two nonadjacent vertices of G. Then, $G - e$ is the subgraph of G obtained by deleting the edge e and $G + xy$ is a graph obtained from G by adding an edge connecting x and y.

If H and G are graphs such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$, then we call H to be a subgraph of G. The subgraph P with vertex set $\{v_0, v_1, \ldots, v_r\}$ and edge set $\{v_0v_1, v_1v_2, \ldots, v_{r-1}v_r\}$ is called a pendent path of G if $\deg_G(v_0) \geq 3$, $\deg_G(v_r) = 1$ and $\deg_G(v_1) = \deg_G(v_2) = \cdots = \deg_G(v_{r-1}) = 2$, when $r \geq 2$. While, a subgraph Q with vertex set $\{u_0, u_1, \ldots, u_s\}$ and edge set $\{u_0u_1, u_1u_2, \ldots, u_{s-1}u_s\}$ is called an internal path if $\deg_G(v_0), \deg_G(v_s) \geq 3$ and $\deg_G(v_1) = \deg_G(v_2) = \cdots = \deg_G(v_{s-1}) = 2$, when $s \geq 2$. An edge incident to a pendent vertex is called a pendent edge.

Suppose G is a connected graph with two vertices u and v. The distance $d_G(u, v)$ is defined as the number of edges in a shortest path connecting u and v. The cyclomatic number of G, $\gamma(G)$, is defined to be $\gamma(G) = |E(G)| - |V(G)| + 1$. If $\gamma(G) = 0, 1, 2, 3, 4, 5$, then the graph G is said to be tree, unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic, respectively. We refer the readers to consult the famous book of West [1] for our graph theory notions and notations.

In a recent paper, Došlic et al. [2] introduced a new bond-additive structural invariant as a quantitative refinement of the distance nonbalancedness and also a measure of peripherality in graphs. They used the name Mostar index for this invariant which is defined as $Mo(G) = \sum_{uv\in E(G)} |n_u(uv, G) - n_v(uv, G)|$, where $n_u(uv, G)$ is the number of vertices of G closer to u than to v, and similarly, $n_v(uv, G)$ is the number of vertices closer to v than to u. They determined the extremal values of this invariant and characterized extremal trees and unicyclic graphs with respect to the Mostar index. Arockiaraj et al. [3] introduced the edge Mostar of the graph G as $Mo_e(G) = \sum_{e=uv\in E(G)} |m_u(e, G) - m_v(e, G)|$, where $m_u(e, G)$ and $m_v(e, G)$ are the number of edges of G lying closer to the vertex u than v and the number of edges of G lying closer to the vertex v than to the vertex u. They computed the Mostar and edge Mostar indices of the family of coronoid and carbon nanocones. Imran et al. [4] computed the edge Mostar index of some graph operations. As a consequence of these calculations, they obtained the edge Mostar index of several classes of chemical graphs and nanostructures.

Deng and Li [5] determined the catacondensed hexagonal systems with the least and the second-least Mostar indices. In another paper [6], these authors computed the extremal trees

with respect to the Mostar index. Ghorbani et al. [7] proved that a graph G with $Mo(G) = 1$ has no cut edge and computed the Mostar index of the pentagonal nanocones. A connected graph with this property, in which any two graph cycles have no edge in common, is called a cactus graph. Hayat and Zhou [8] determined all n–vertex cacti with maximum Mostar index and gave a sharp upper bound for the Mostar index of n–vertex cacti containing k cycles. The same authors in [9] constructed n–vertex trees with maximum Mostar index and fixed the maximum degree, diameter, or number of pendent vertices. Huang et al. [10] found the extremal hexagonal chains with respect to Mostar index, and Xiao et al. [11] computed the first three minimum of Mostar index in the class of hexagonal chains. Finally, Tepeh [12] proved a conjecture of Došlić et al. [2] about the characterization of bicyclic graphs with a given number of vertices, for which extremal values of the Mostar index are attained.

Our calculations are done with the aid of Nauty [13] and Matlab [14]. Our codes are accessible from the authors upon request.

2. Mostar Index

A vertex v in a given graph G is called a starlike vertex if $\deg_G(v) \geq 2$ and $|\{u\colon uv \in E(G) \text{ and } \deg_G(u) = 1\}| \geq \deg_G(v) - 1$. The set of all such vertices is denoted by $SV(G)$, and we use the name starlike set for $SV(G)$.

Transformation 1. We assume that T is a tree and $v \in SV(T)$. We also assume that $uv \in E(T)$, $\deg_G(u) \neq 1$, and $\{x\colon xv \in E(T) \text{ and } x \neq u\} = \{v_1, v_2, \ldots, v_{\deg_G(v)-1}\}$. Define $T' = T - \{vv_i\colon i = 1, 2, \ldots, \deg_G(v) - 1\} + \{uv_i\colon i = 1, 2, \ldots, \deg_G(v) - 1\}$. The resulting tree has been illustrated in Figure 1.

Lemma 1. *Let T and T' be the n–vertex trees described in Transformation 1. Then, $Mo(T) < Mo(T')$.*

Proof. By definition, $Mo(T) - Mo(T') = |n_u(uv, T) - n_v(uv, T)| - (n-2)$. Since $\deg_T(v)$, $\deg_T(u) \geq 2$, and $|n_u(uv, T) - n_v(uv, T)| < n - 2$. Therefore, $Mo(T) - Mo(T') < 0$.

A caterpillar is a tree in which all the vertices are within distance 1 of a central path [15]. Let T be a caterpillar with the central path $P_k\colon = v_1v_2, \ldots, v_k$ and d_i, $1 \leq i \leq k$, be the number of pendent vertices that are in distance 1 of a vertex v_i. Then, we use the notation $P_k[1^{d_1}, 2^{d_2}, \ldots, k^{d_k}]$ instead of T. Note that if $d_i = 0$, $1 \leq i \leq k$, then we refuse to write i^{d_i} in $P_k[1^{d_1}, 2^{d_2}, \ldots, k^{d_k}]$, see Figure 2. □

Transformation 2. We assume that T_c is a caterpillar with the longest path $P\colon = v_1v_2, \ldots, v_k$. We also assume that $Q\colon = v_lv_{l+1}, \ldots, v_j$, $1 < l < j < k-1$, is an internal path in T_c such that $n_{v_{j-1}}(v_{j-1}v_j, T_c) \leq n_{v_j}(v_{j-1}v_j, T_c)$ and $\{x\colon xv_l \in E(T_c) \text{ and } x \notin \{v_{l-1}, v_{l+1}\}\} = \{w_1, w_2, \ldots, w_{\deg_{T_c}(v_l)-2}\}$. Define

$$T_c' = T_c - \{w_iv_l\colon i = 1, 2, \ldots, \deg_{T_c}(v_l) - 2\} + \{w_iv_j\colon i = 1, 2, \ldots, \deg_{T_c}(v_l) - 2\}. \tag{1}$$

The resulting tree has been illustrated in Figure 3.

Lemma 2. *Let T_c and T_c' be two trees in Transformation 2 with n vertices. Then, $Mo(T_c) < Mo(T_c')$.*

Proof. We consider two cases as follows:

(1) $j = l + 1$. By definition of T_c and T_c', we have

$$\begin{aligned} Mo(T_c) - Mo(T_c') = {} & n_{v_j}(v_lv_j, T_c) - n_{v_l}(v_lv_j, T_c) - \Big[n_{v_j}(v_lv_j, T_c) + \deg_{T_c}(v_l) - 2 \\ & - n_{v_l}(v_lv_j, T_c) + \deg_{T_c}(v_l) - 2\Big] = 4 - 2\deg_{T_c}(v_l) < 0. \end{aligned} \tag{2}$$

(2) $j \geq l + 2$. Again by definition of T_c and T_c', we have

$$\begin{aligned} Mo(T_c) - Mo(T_c') = {} & \sum_{i=l}^{j-1}\Big[\big(n_{v_{i+1}}(v_iv_{i+1}, T_c) + (j-i)\big) - \big(n_{v_i}(v_iv_{i+1}, T_c) + (i-l)\big)\Big] \\ & - \sum_{i=l}^{j-1}\Big[\big(n_{v_{i+1}}(v_iv_{i+1}, T_c) + (j-i) + \deg_{T_c}(v_l) - 2\big) \\ & - \big(n_{v_i}(v_iv_{i+1}, T_c) + (i-l) - \deg_{T_c}(v_l) + 2\big)\Big] \\ = {} & \sum_{i=l}^{j-1}\big[4 - 2\deg_{T_c}(v_l)\big] < 0, \end{aligned} \tag{3}$$

proving the lemma. □

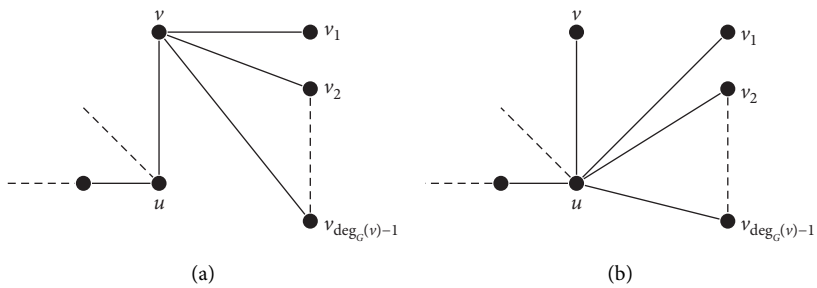

Figure 1: The trees (a) T and (b) T' in Transformation 1.

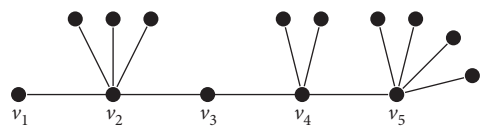

Figure 2: The caterpillar $P_5[2^3, 4^2, 5^4]$.

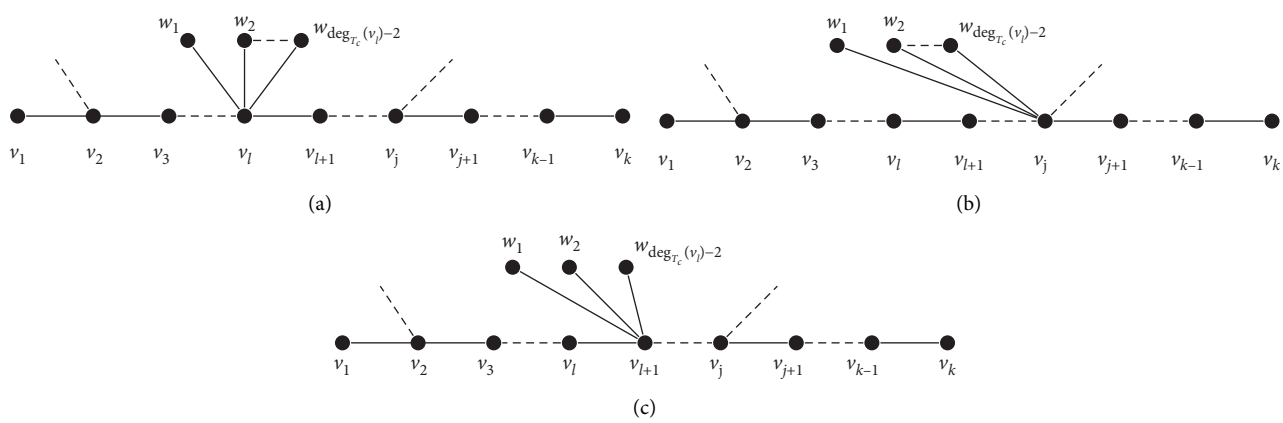

Figure 3: The trees (a) T_c, (b) T_c', and (c) T_c'' in Transformations 2 and 3.

Transformation 3. We assume that T_c, P, Q, and $\{w_1, w_2, \ldots, w_{\deg_{T_c}(v_l)-2}\}$ are defined in Transformation 2. We also assume that $j \geq l+2$ and $n_{v_l}(v_l v_{l+1}, T_c) < n_{v_{l+1}}(v_l v_{l+1}, T_c)$. Define

$$\begin{aligned} T_c'' = T_c &- \left\{w_i v_l \colon i = 1, 2, \ldots, \deg_{T_c}(v_l) - 2\right\} \\ &+ \left\{w_i v_{l+1} \colon i = 1, 2, \ldots, \deg_{T_c}(v_l) - 2\right\}. \end{aligned} \tag{4}$$

The resulting tree has been illustrated in Figure 3.

Lemma 3. *Let T_c and $T_c^{''}$ be two trees in Transformation 3 with n vertices. Then, $Mo(T_c) < Mo(T_c'')$.*

Proof. By definition of T_c and T_c'',

$$\begin{aligned} Mo(T_c) - Mo(T_c'') = n_{v_{l+1}}(v_l v_{l+1}, T_c) - n_{v_l}(v_l v_{l+1}, T_c) - \Big[n_{v_{l+1}}(v_l v_{l+1}, T_c) + \deg_{T_c}(v_l) - 2 \\ - n_{v_l}(v_l v_{l+1}, T_c) + \deg_{T_c}(v_l) - 2\Big] = 4 - 2\deg_{T_c}(v_l) < 0, \end{aligned} \tag{5}$$

proving the lemma. □

Lemma 4. *Let n, k, and r be three positive integers such that $k < n$ and $1 \le r \le n-k$. If $r < \lceil (n-k)/2 \rceil$, then $Mo(P_{n-k}[r^k]) < Mo(P_{n-k}[(r+1)^k])$.*

Proof. By definition, $Mo(P_{n-k}[r^k]) - Mo(P_{n-k}[(r+1)^k]) = |r + k - (n-k-r)| - (n-2r) \le \max\{-2(n-k-2r), -2k\} < 0$, as desired. □

Proposition 1. *Let T be a tree on n vertices. If $T \cong P_r[s^t]$, where $r = diam(T)+1$, $s = \lceil (diam(T)+1)/2 \rceil$, and $t = n-r$, then*

$$Mo(T) = \begin{cases} n^2 - 3n - \frac{1}{2}\operatorname{diam}(T)^2 + \operatorname{diam}(T) + 2, & 2 \mid \operatorname{diam}(T), \\ n^2 - 3n - \frac{1}{2}\operatorname{diam}(T)^2 + \operatorname{diam}(T) + \frac{3}{2}, & 2 \mid \operatorname{diam}(T) - 1. \end{cases} \tag{6}$$

Proof. Suppose $\operatorname{diam}(T) = d$. By definition of caterpillar,

$$Mo(T) = \begin{cases} 2((n-2) + (n-4) + \cdots + (n-d)) + (n-d-1)(n-2), & 2|d, \\ 2((n-2) + (n-4) + \cdots + (n-d+1)) + (n-d-1)(n-1), & 2|d-1, \end{cases} \tag{7}$$

and by simple calculations,

$$Mo(T) = \begin{cases} n^2 - 3n - \frac{1}{2}d^2 + d + 2, & 2|d, \\ n^2 - 3n - \frac{1}{2}d^2 + d + \frac{3}{2}, & 2|d-1, \end{cases} \tag{8}$$

proving the lemma. □

Theorem 1. *Let T be a tree with n vertices. Then,*

$$Mo(T) \le \begin{cases} n^2 - 3n - \frac{1}{2}\operatorname{diam}(T)^2 + \operatorname{diam}(T) + 2, & 2|\operatorname{diam}(T), \\ n^2 - 3n - \frac{1}{2}\operatorname{diam}(T)^2 + \operatorname{diam}(T) + \frac{3}{2}, & 2|\operatorname{diam}(T) - 1, \end{cases} \tag{9}$$

with equality if and only if $T \cong P_r[s^t]$, where $r = diam(T)+1$, $s = \lceil (diam(T)+1)/2 \rceil$, and $t = n-r$.

Proof. If $T \cong P_r[s^t]$, where $r = \operatorname{diam}(T)+1$, $s = \lceil (\operatorname{diam}(T)+1)/2 \rceil$, and $t = n-r$, then Proposition 1 gives the result. Otherwise, we assume that $P: = v_1 v_2, \ldots, v_{\operatorname{diam}(T)+1}$ is the longest path in T. At first, by repeated applications of Transformation 1 on vertices of $SV(T) \backslash \{v_2, v_{\operatorname{diam}(T)}\}$, we arrive at a caterpillar T_c with central path P. We now apply Lemma 1 to deduce that $Mo(T) \le Mo(T_c)$. Next, by the repeated applications of Transformations 2 and 3 on the internal paths in T_c, we arrive at a caterpillar $P_r[s^t]$, where $r = \operatorname{diam}(T)+1$, $2 \le s \le \operatorname{diam}(T)$, and $t = n-r$. Apply Lemmas 2 and 3 to prove that $Mo(T) \le Mo(T_c) \le Mo(P_r[s^t])$. Finally, by Lemma 4,

$$Mo(T) \le \begin{cases} n^2 - 3n - \frac{1}{2}\operatorname{diam}(T)^2 + \operatorname{diam}(T) + 2, & 2|\operatorname{diam}(T), \\ n^2 - 3n - \frac{1}{2}\operatorname{diam}(T)^2 + \operatorname{diam}(T) + \frac{3}{2}, & 2|\operatorname{diam}(T) - 1, \end{cases} \tag{10}$$

with equality if and only if $T \cong P_r[s^t]$, where $r = \operatorname{diam}(T)+1$, $s = \lceil (\operatorname{diam}(T)+1)/2 \rceil$, and $t = n-r$. □

Lemma 5. *Let n and r be two positive integers. If $1 \le r \le n-r-4$, then,*

$$Mo\left(P_4\left[2^{r-1}, 3^{n-r-3}\right]\right) = Mo\left(P_4\left[2^{r}, 3^{n-r-4}\right]\right) + 2. \quad (11)$$

Proof. By definition, $Mo(P_4[2^{r-1}, 3^{n-r-3}]) - Mo(P_4[2^r, 3^{n-r-4}]) = n - r - 1 - (r+1) - (n - r - 2 - (r+2)) = 2.$ □

Theorem 2. *Let T be an n–vertex tree and*

$$T \notin \left\{P_3\left[2^{n-3}\right], P_4\left[2^{n-4}\right], P_4\left[2^{n-5}, 3^1\right], P_5\left[3^{n-5}\right]\right\}. \quad (12)$$

See Figure 4, for details. Then,

$$Mo(T) < Mo\left(P_5\left[3^{n-5}\right]\right) = Mo\left(P_4\left[2^{n-5}, 3^1\right]\right) < Mo\left(P_4\left[2^{n-4}\right]\right) < Mo\left(P_3\left[2^{n-3}\right]\right). \quad (13)$$

Proof. By definition,

$$Mo\left(P_5\left[3^{n-5}\right]\right) = Mo\left(P_4\left[2^{n-5}, 3^1\right]\right) = n^2 - 3n - 2, Mo\left(P_4\left[2^{n-4}\right]\right) = n(n-3), Mo\left(P_3\left[2^{n-3}\right]\right) = (n-1)(n-2), \quad (14)$$

so $Mo(P_5[3^{n-5}]) = Mo(P_4[2^{n-5}, 3^1]) < Mo(P_4[2^{n-4}]) < Mo(P_3[2^{n-3}])$. Since $T \notin \{P_3[2^{n-3}], P_4[2^{n-4}], P_4[2^{n-5}, 3^1], P_5[3^{n-5}]\}$, $\operatorname{diam}(T) \geq 3$. If $\operatorname{diam}(T) = 3$, then, by Lemma 5, $Mo(T) < Mo(P_4[2^{n-5}, 3^1])$. If $\operatorname{diam}(T) \geq 4$, then, by repeated applications of Transformation 1 on elements of $SV(T)$, we arrive at a tree T_x with $\operatorname{diam}(T_x) = 4$. By Lemma 1, $Mo(T) \leq Mo(T_x)$, and by Theorem 1, $Mo(T_x) \leq Mo(P_5[3^{n-5}])$. The equality holds if and only if $T_x \cong P_5[3^{n-5}]$, as desired. □

Lemma 6. *Let a, b, and c be three positive integers such that $a < b$. Then, $|a + c - b| < |b + c - a|$.*

Proof. Suppose $\iota = b - a$. Then, $|a + c - b| - |b + c - a| = |c - \iota| - |c + \iota| < 0$. □

Transformation 4. (see [16]). Suppose that w is a vertex in a connected graph G with at least two vertices and $N[w, G] = \left\{x_1, x_2, \ldots, x_{d_G(w)}\right\}$. In addition, we assume that P: $u_k u_{k-1}, \ldots, u_2 u_1$ and Q: $v_\ell v_{\ell-1}, \ldots, v_2 v_1$, are two paths of lengths k and ℓ, $k \geq \ell \geq 1$, respectively. Let G_1 be the graph obtained from G, P, and Q by attaching edges $v_\ell w$, $w u_k$, and $G_2 = G_1 - \{w x_i \colon x_i \in N[w, G]\} + \{v_\ell x_i \colon x_i \in N[w, G]\}$. The graphs G_1 and G_2 have been illustrated in Figure 5.

Lemma 7. *Let G_1 and G_2 be two graphs in Transformation 3 on n vertices. Then, $Mo(G_2) < Mo(G_1)$.*

Proof. Suppose $|V(G)| = c$. By definition of G_1 and G_2, we have

$$\begin{aligned} Mo(G_1) - Mo(G_2) &= |k + c - l| - |l + (c-1) - (k+1)| \\ &= |(k+1) + (c-1) - l| \\ &\quad - |l + (c-1) - (k+1)|, \end{aligned} \quad (15)$$

and Lemma 6 gives the result. □

Remark 1. In Transformation 4, if we replace the path P by a tree on k vertices, then again Lemma 7 is valid.

Corollary 1. *The path P_n and the caterpillar $P_{n-1}[2^1]$ have the first and second minimum Mostar index among all trees on n vertices, respectively.*

Proposition 2. *Let $n \geq 8$ be a positive integer.*

(1) If n is odd, then $Mo(P_{n-2}[2^2]) = (1/2)(n-1)^2 + 6$, $Mo(P_{n-2}[2^1, 3^1]) = (1/2)(n-1)^2 + 8$, $Mo(P_{n-2}[2^1, (n-3)^1]) = (1/2)(n-1)^2 + 4$, $Mo(P_{n-2}[3^1, (n-3)^1]) = (1/2)(n-1)^2 + 6$, $Mo(P_{n-1}[1^1]) = (1/2)(n-1)^2$, $Mo(P_{n-1}[2^1]) = (1/2)(n-1)^2 + 2$, $Mo(P_{n-1}[3^1]) = (1/2)(n-1)^2 + 4$, and $Mo(P_{n-1}[4^1]) = (1/2)(n-1)^2 + 6$.

(2) If n is even, then $Mo(P_{n-2}[2^2]) = (1/2)(n-1)^2 + (11/2)$, $Mo(P_{n-2}[2^1, 3^1]) = (1/2)(n-1)^2 + (15/2)$, $Mo(P_{n-2}[2^1, (n-3)^1]) = (1/2)(n-1)^2 + (7/2)$, $Mo(P_{n-2}[3^1, (n-3)^1]) = (1/2)(n-1)^2 + (11/2)$, $Mo(P_{n-1}[1^1]) = (1/2)(n-1)^2 - (1/2)$, $Mo(P_{n-1}[2^1]) = (1/2)(n-1)^2 + (3/2)$, $Mo(P_{n-1}[3^1]) = (1/2)(n-1)^2 + (7/2)$, and $Mo(P_{n-1}[4^1]) = (1/2)(n-1)^2 + (11/2)$.

Theorem 3. *Let T be a tree on $n \geq 8$ vertices. If*

$$T \notin \left\{P_{n-1}\left[i^1\right] | 1 \leq i \leq 4\right\} \cup \left\{P_{n-2}\left[2^2\right], P_{n-2}\left[2^1, (n-3)^1\right], P_{n-2}\left[3^1, (n-3)^1\right]\right\}, \quad (16)$$

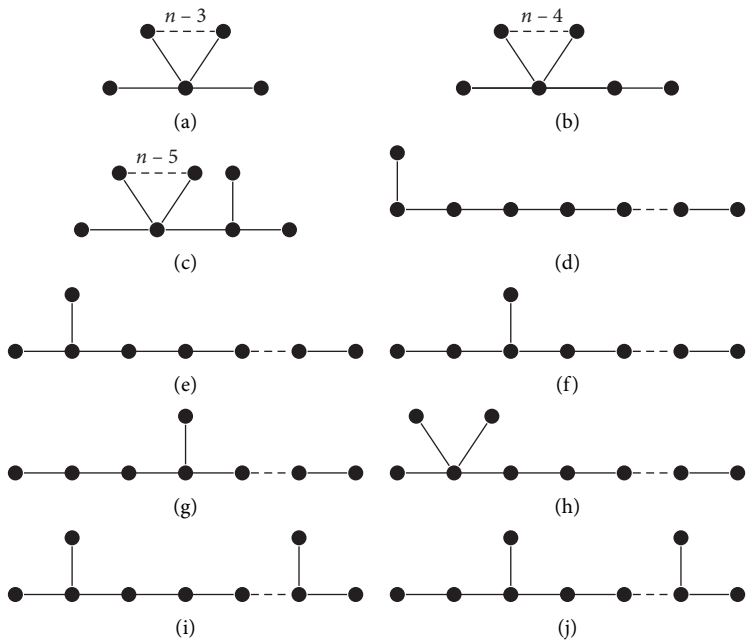

Figure 4: The trees in Theorems 2 and 3. (a) $P_3[2^{n-3}]$. (b) $P_4[2^{n-4}]$. (c) $P_4[2^{n-5}, 3^1]$. (d) $P_{n-1}[1^1]$. (e) $P_{n-1}[2^1]$. (f) $P_{n-1}[3^1]$. (g) $P_{n-1}[4^1]$. (h) $P_{n-2}[2^2]$. (i) $P_{n-2}[2^1, (n-3)^1]$. (j) $P_{n-2}[3^1, (n-3)^1]$.

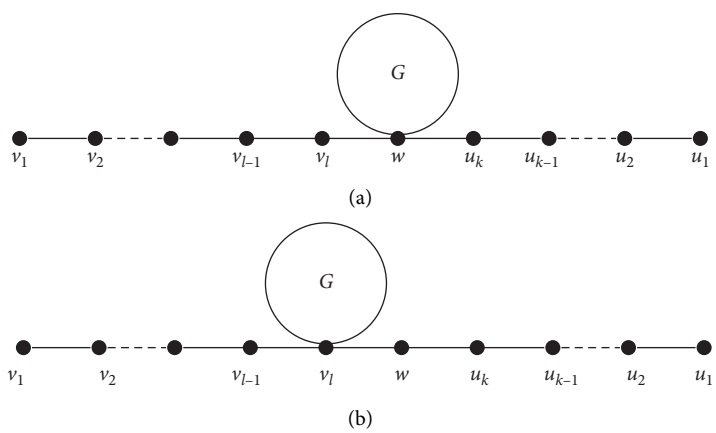

Figure 5: The graphs P, Q, G, G_1, and G_2 in Transformation 4. (a) G_1. (b) G_2.

then

$$\begin{aligned} Mo\left(P_{n-1}\left[1^1\right]\right) &< Mo\left(P_{n-1}\left[2^1\right]\right) < Mo\left(P_{n-1}\left[3^1\right]\right) = Mo\left(P_{n-2}\left[2^1, (n-3)^1\right]\right) < Mo\left(P_{n-1}\left[4^1\right]\right) \\ &= Mo\left(P_{n-2}\left[3^1, (n-3)^1\right]\right) = Mo\left(P_{n-2}\left[2^2\right]\right) < Mo(T). \end{aligned} \tag{17}$$

Proof. By Proposition 2,

$$\begin{aligned} Mo\left(P_{n-1}\left[1^1\right]\right) &< Mo\left(P_{n-1}\left[2^1\right]\right) < Mo\left(P_{n-1}\left[3^1\right]\right) = Mo\left(P_{n-2}\left[2^1, (n-3)^1\right]\right) < Mo\left(P_{n-1}\left[4^1\right]\right) \\ &= Mo\left(P_{n-2}\left[3^1, (n-3)^1\right]\right) = Mo\left(P_{n-2}\left[2^2\right]\right). \end{aligned} \tag{18}$$

We now apply repeated applications of Transformation 4 on the pendent paths in T to arrive at a caterpillar T_c in the set $\{P_{n-1}[4^1], P_{n-2}[2^2], P_{n-2}[3^1, (n-3)^1]\}$ (Figure 4). Now, by Lemma 7, $Mo(T_c) < Mo(T)$. Therefore, by Proposition 2,

$$Mo\left(P_{n-1}\left[4^1\right]\right) = Mo\left(P_{n-2}\left[3^1, (n-3)^1\right]\right) = Mo\left(P_{n-2}\left[2^2\right]\right) < Mo(T), \tag{19}$$

and this gives the result. □

3. Edge Mostar Index

The aim of this section is to compare the Mostar and edge Mostar indices of trees and unicyclic graphs. We also present a proof for Conjecture 5.5 of Liu et al. [17]. In the end of this section, conjectures on the minimum of edge Mostar index of tricyclic, tetracyclic, and pentacyclic graphs are presented. Suppose G is a connected graph and $E' \subseteq E(G)$. Define $Mo(E') = \sum_{e=uv\in E'} |n_u(e,G) - n_v(e,G)|$ and $Mo_e(E') = \sum_{e=uv\in E'} |m_u(e,G) - m_v(e,G)|$.

Proposition 3. *If T is a tree, then $Mo_e(T) = Mo(T)$.*

Proof. Suppose $e = uv \in (T)$ and the trees T_u and T_v are components of $T - e$ such that $u \in V(T_u)$ and $v \in V(T_v)$. By definition, $m_u(e,T) = |E(T_u)|$, $m_v(e,T) = |E(T_v)|$, $n_u(e,T) = |V(T_u)|$, and $n_v(e,T) = |V(T_v)|$. The result follows from these facts that $|E(T_u)| = |V(T_u)| - 1$ and $|E(T_v)| = |V(T_v)| - 1$. □

Remark 2. Suppose T is a tree. In Proposition 3, it is proved that the Mostar and edge Mostar indices of trees are equal. This shows that the edge version of all results in Section 2 containing Lemmas 1– 5, 7, Theorems 1–3, and Corollary 1 are correct.

Note that the converse of Proposition 3 is not generally correct. For example, $Mo(C_n) = Mo_e(C_n) = 0$, for each cycle C_n of length n.

Suppose G is connected graph which is not a tree, $e = uv$ is a cut edge of G and G_u and G_v are components of $G - e$. If one of G_u or G_v is a tree, then the edge e is said to be a tree-like cut edge of G and the number of vertices in the acyclic component of $G - e$ is denoted by $w(e)$. Furthermore, the set of all tree-like cut edges of G is denoted by $CT(G)$. A tree-like cut edge of G is said to be strong (weak), if the number of vertices in the acyclic component of $G - e$ is greater than (less than) the number of vertices in another component of $G - e$. The set of all strong and weak tree-like cut edges of G are denoted by $CT_{St}(G)$ and $CT_W(G)$, respectively.

Proposition 4. *If G is not acyclic graph, $e_1 = x_1y_1$ and $e_2 = x_2y_2 \in CT_{St}(G)$, then $w(e_1) \neq w(e_2)$*

Proof. Suppose G_{x_1} and G_{y_1} are two components of $G - e_1$ and G_{x_2} and G_{y_2} are two components of $G - e_2$. Without loss of generality, we can assume that G_{y_1} and G_{y_2} are trees. Since $e_1, e_2 \in CT_{St}(G)$, G_{y_1} is a subgraph of G_{y_2} or G_{y_2} is a subgraph of G_{y_1}, as desired. □

Proposition 5. *If G is not an acyclic graph and $|CT_{St}(G)| \geq 1$, then $G[CT_{St}(G)]$ is a path.*

Proof. Suppose $CT_{St}(G) = \{e_1 = x_1y_1, e_2 = x_2y_2, \ldots, e_k = x_ky_k\}$ and $w(e_1) > w(e_2) > \cdots > w(e_k)$. We also assume that G_{x_1} and G_{y_1} are two components of $G - e_1$. Without loss of generality, we can assume that G_{y_1} is a tree. Since all edges of a tree is a cut edge, $e_2 \in CT_{St}(G)$ and $w(e_2) = \max\{w(e_2), w(e_3), \ldots, w(e_k)\}$, it can be proved that $x_2 = y_1$ or $y_2 = y_1$. Choose the edge e_2 and repeat this process to complete the proof. □

Proposition 6. *If G is not acyclic, then $|CT_{St}(G)| \leq |CT_W(G)|$.*

Proof. Suppose $CT_{St}(G) = \{e_1 = x_1y_1, e_2 = x_2y_2, \ldots, e_k = x_ky_k\}$ and $w(e_1) > w(e_2) > \cdots > w(e_k)$. We also assume that G_{x_k} and G_{y_k} are two components of $G - e_k$. Without loss of generality, it can be assumed that G_{y_k} is a tree. Since $e_k \in CT_{St}(G)$, $|V(G_{x_k})| < |V(G_{y_k})|$. On the contrary, $w(e_k) = \min\{w(e_1), w(e_2), w(e_3), \ldots, w(e_k)\}$ and $e \in E(G_{y_k})$ implies that $e \in CT_W(G)$. Apply Proposition 5 and the fact that a cut edge cannot be on a cycle to complete our argument. □

Corollary 2. *Suppose γ is the cyclomatic number of a connected graph G with $|CT_{St}(G)| \geq 1$; then,*

(1) If $\gamma = 1$, then $|CT_{St}(G)| \leq |CT_W(G)| - 2$.

(2) If $\gamma = 2$, then $|CT_{St}(G)| \leq |CT_W(G)| - 3$.

Lemma 8. *Let G be γ–cyclic graph such that $|CT(G)| \geq 1$; then,*

(1) If $\gamma = 1$, then $Mo_e(CT(G)) \geq Mo(CT(G)) + 1$.

(2) If $\gamma = 2$, then $Mo_e(CT(G)) \geq Mo(CT(G)) + 2$.

Proof. Suppose $e = uv \in CT(G)$; G_u and G_v are components of $G - e$ such that $u \in V(G_u)$, $v \in V(G_v)$, and G_u is a tree. By definition, $m_u(e,T) = |E(G_u)|$, $m_v(e,G) = |E(G_v)|$, $n_u(e,G) = |V(G_u)|$, and $n_v(e,G) = |V(G_v)|$. Our main proof will consider two cases as follows:

(1) $\gamma = 1$. In this case, $|E(G_u)| = |V(G_u)| - 1$ and $|E(G_v)| = |V(T_v)|$. Thus,

$$\begin{aligned} Mo_e(CT(G)) &= Mo_e(CT_{St}(G)) + Mo_e(CT_W(G)) \\ &= \sum_{e=uv\in CT_{St}(G)} \left|n_u(e,G) - 1 - n_v(e,G)\right| + \sum_{e=uv\in CT_W(G)} \left|n_u(e,G) - 1 - n_v(e,G)\right| \\ &= \sum_{e=uv\in CT_{St}(G)} \left|n_u(e,G) - n_v(e,G)\right| - 1 + \sum_{e=uv\in CT_W(G)} \left|n_u(e,G) - n_v(e,G)\right| + 1 \\ &= Mo(CT(G)) - \sum_{e=uv\in CT_{St}(G)} 1 + \sum_{e=uv\in CT_W(G)} 1. \end{aligned} \tag{20}$$

Now, by Corollary 2, $Mo_e(CT(G)) \geq Mo(CT(G)) + 1$.

(2) $\gamma = 2$. In this case, $|E(G_u)| = |V(G_u)| - 1$ and $|E(G_v)| = |V(T_v)| + 1$. Hence,

$$\begin{aligned} Mo_e(CT(G)) &= Mo_e(CT_{St}(G)) + Mo_e(CT_W(G)) \\ &= \sum_{e=uv\in CT_{St}(G)} \left|n_u(e,G) - 1 - n_v(e,G) - 1\right| \\ &\quad + \sum_{e=uv\in CT_W(G)} \left|n_u(e,G) - 1 - n_v(e,G) - 1\right| \\ &\geq \sum_{e=uv\in CT_{St}(G)} \left|n_u(e,G) - n_v(e,G)\right| - 2 + \sum_{e=uv\in CT_W(G)} \left|n_u(e,G) - n_v(e,G)\right| + 2 \\ &= Mo(CT(G)) - \sum_{e=uv\in CT_{St}(G)} 2 + \sum_{e=uv\in CT_W(G)} 2. \end{aligned} \tag{21}$$

Again by Corollary 2, $Mo_e(CT(G)) \geq Mo(CT(G)) + 2$.

This completes the proof.

Suppose $k \geq 3$ is a positive integer and T_i, $1 \leq i \leq k$, is a tree with a given vertex v_i. Define the unicyclic graph Γ_k with vertex set $V(\Gamma_k) = \cup_{i=1}^{k} V(T_i)$ and edge set $E(\Gamma_k) = \cup_{i=1}^{k} E(T_i) \bigcup \{v_i v_{i+1}: 1 \leq i \leq k-1\} \bigcup \{v_1 v_k\}$. □

Lemma 9. *Let Γ_k be the graph defined above. If $E_1(\Gamma_k) = \{v_i v_{i+1}: 1 \leq i \leq k-1\} \cup \{v_1 v_k\}$, then $Mo_e(E_1(\Gamma_k)) = Mo(E_1(\Gamma_k))$.*

Proof. Suppose $e = v_{i_1} v_{i_2}$ is an arbitrary edge in $E_1(\Gamma_k)$. Consider the following two cases:

(1) k is even. In this case, there exists a unique edge as $f = v_{j_1} v_{j_2} \in E_1(\Gamma_k) \backslash \{v_{i_1} v_{i_2}\}$ such that $d_{\Gamma_k}(v_{i_1}, v_{j_1}) = d_{\Gamma_k}(v_{i_2}, v_{j_2})$. Therefore, $|n_{v_{i_1}}(e,\Gamma_k) - n_{v_{i_1}}(e,\Gamma_k)| = |n_{v_{i_1}}(e,\Gamma_k - f) - n_{v_{i_1}}(e,\Gamma_k - f)|$ and $|m_{v_{i_1}}(e,\Gamma_k) - m_{v_{i_1}}(e,\Gamma_k)| = |m_{v_{i_1}}(e,\Gamma_k - f) - m_{v_{i_1}}(e,\Gamma_k - f)|$.

(2) k is odd. There exists a unique vertex v_l in $\{v_1, v_2, \ldots, v_k\} \backslash \{v_{i_1}, v_{i_2}\}$ such that $d_{\Gamma_k}(v_{i_1}, v_l) = d_{\Gamma_k}(v_{i_2}, v_l)$. We construct the tree Γ_k^1 from the graph Γ_k by removing the vertices of T_l. Then, $|n_{v_{i_1}}(e,\Gamma_k) - n_{v_{i_1}}(e,\Gamma_k)| = |n_{v_{i_1}}(e,\Gamma_k^1) - n_{v_{i_1}}(e,\Gamma_k^1)|$ and $|m_{v_{i_1}}(e,\Gamma_k) - m_{v_{i_1}}(e,\Gamma_k)| = |m_{v_{i_1}}(e,\Gamma_k^1) - m_{v_{i_1}}(e,\Gamma_k^1)|$.

Now, the proof follows from cases (1), (2), and Proposition 3. □

Theorem 4. *If G is a unicyclic graph, then $Mo(G) \leq Mo_e(G)$ with equality if and only if $G \cong C_n$.*

Proof. The proof follows from Lemmas 8 and 9. □

Proposition 7. *Let $\Theta_{2,2,n-3}$ be an n–vertex bicyclic graph, $n \geq 8$, depicted in Figure 6. Then, $Mo_e(\Theta_{2,2,n-3}) = 2n - 4$.*

Proof. if $e = uv \in \{v_1 v_n, v_1 v_{n-1}, v_{n-2} v_n, v_{n-2} v_{n-1}\}$, then, by the structure of $\Theta_{2,2,n-3}$, $|m_u(e,G) - m_v(e,G)| = ((n-3)/2) - ((n-5)/2) = 1$. We first assume that n is even. If $i = ((n-2)/2)$, then $|m_{v_i}(e,G) - m_{v_{i+1}}(e,G)| = 0$. If $1 \leq i (\neq (n-2)/2) \leq n-3$ and $e = v_i v_{i+1}$, then $|m_{v_i}(e,G) - m_{v_{i+1}}(e,G)| = 5 - 3 = 2$. Next, we assume that n is odd. If $i = ((n-1)/2), ((n+1)/2)$ and $e = v_i v_{i+1}$, then $|m_{v_i}(e,G) - m_{v_{i+1}}(e,G)| = 1$. If $1 \leq i (\neq ((n-1)/2), ((n+1)/2)) \leq n-3$ and $e = v_i v_{i+1}$, then $|m_{v_i}(e,G) - m_{v_{i+1}}(e,G)| = 5 - 3 = 2$. Now, the result follows from above discussions and some easy calculations.

The following result is an immediate consequence of the pendent path and some easy calculations. □

Proposition 8. *Let $P: = v_1 v_2, \ldots, v_k$ be pendent path in an n–vertex bicyclic graph G. If $k \geq 2$, we choose the edge $e = v_1 v_2$ and if $k \geq 3$, we choose $f = v_2 v_3$. Then, $|m_{v_1}(e,G) - m_{v_2}(e,G)| = n$ and $|m_{v_2}(f,G) - m_{v_3}(f,G)| = n - 2$.*

Corollary 3. *Let G be an n–vertex bicyclic graph. If G has at least two pendent path of order ≥ 2 or one pendent path of order ≥ 3, then $Mo_e(G) \geq 2n - 2$.*

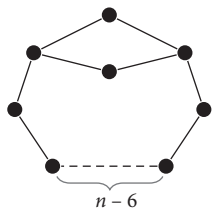

Figure 6: The bicyclic graph $\Theta_{2,2,n-3}$.

Suppose k, l, and r are positive integers. Consider T_i, R_j, and F_t to be trees with these properties that $v_i \in V(T_i)$, $u_j \in V(R_j)$, $w_t \in V(F_t)$, $1 \le i \le k$, $1 \le j \le l$, and $1 \le t \le r$. Define four classes of bicyclic graphs denoted by $\Lambda_{k,l,r}$, $k, l, r \ge 2$, $\Upsilon_{k,l}$, $k \ge 3, l \ge 2$, $\Psi_{k,l}$, $k \ge 3, l \ge 1, k \ge l$, and $\Phi_{k,l,r}$, $l \ge k \ge r$ and $k, r \ge 1, l \ge 2$, with the following vertex and edge sets:

$$\begin{aligned}
V(\Lambda_{k,l,r}) &= \left(\bigcup_{i=1}^{k} V(T_i)\right) \bigcup \left(\bigcup_{i=1}^{l} V(R_i)\right) \bigcup \left(\bigcup_{i=r}^{k} V(F_i)\right),\\
V(\Upsilon_{k,l}) &= \left(\bigcup_{i=1}^{k} V(T_i)\right) \bigcup \left(\bigcup_{i=1}^{l} V(R_i)\right),\\
V(\Psi_{k,l}) &= \left(\bigcup_{i=1}^{k} V(T_i)\right) \bigcup \left(\bigcup_{i=1}^{l} V(R_i)\right),\\
V(\Phi_{k,l,r}) &= \left(\bigcup_{i=1}^{k} V(T_i)\right) \bigcup \left(\bigcup_{i=1}^{l} V(R_i)\right) \bigcup \left(\bigcup_{i=r}^{k} V(F_i)\right),\\
E(\Lambda_{k,l,r}) &= \left(\bigcup_{i=1}^{k} E(T_i)\right) \bigcup \left(\bigcup_{i=l}^{k} E(R_i)\right) \bigcup \left(\bigcup_{i=r}^{k} E(F_i)\right)\\
&\quad \bigcup \{v_i v_{i+1} : 1 \le i \le k-1\} \bigcup \{u_i u_{i+1} : 1 \le i \le l-1\}\\
&\quad \bigcup \{w_i w_{i+1} : 1 \le i \le r-1\} \bigcup \{v_1 w_1, w_1 v_k, u_1 w_r, w_r u_l\},\\
E(\Upsilon_{k,l}) &= \left(\bigcup_{i=1}^{k} E(T_i)\right) \bigcup \left(\bigcup_{i=l}^{k} E(R_i)\right) \bigcup \{v_i v_{i+1} : 1 \le i \le k-1\}\\
&\quad \bigcup \{u_i u_{i+1} : 1 \le i \le l-1\} \bigcup \{v_1 v_k, v_1 u_1, v_1 u_l\},\\
E(\Psi_{k,l}) &= \left(\bigcup_{i=1}^{k} E(T_i)\right) \bigcup \left(\bigcup_{i=l}^{k} E(R_i)\right) \bigcup \{v_i v_{i+1} : 1 \le i \le k-1\}\\
&\quad \bigcup \{u_i u_{i+1} : 1 \le i \le l-1\} \bigcup \{v_1 v_k, v_1 u_1, v_k u_l\},\\
E(\Phi_{k,l,r}) &= \left(\bigcup_{i=1}^{k} E(T_i)\right) \bigcup \left(\bigcup_{i=l}^{k} E(R_i)\right) \bigcup \left(\bigcup_{i=r}^{k} E(F_i)\right)\\
&\quad \bigcup \{v_i v_{i+1} : 1 \le i \le k-1\} \bigcup \{u_i u_{i+1} : 1 \le i \le l-1\}\\
&\quad \bigcup \{w_i w_{i+1} : 1 \le i \le r-1\} \bigcup \{v_1 u_1, u_1 w_1, v_k u_l, u_l w_r\}.
\end{aligned} \tag{22}$$

If, for each T in the set $\{T_i : i = 1, \ldots, k\} \cup \{R_i : i = 1, \ldots, l\} \cup \{F_i : i = 1, \ldots, r\}$, $|V(T)| = 1$, then we use the notation $\Theta_{k,l,r}$ as $\Phi_{k,l,r}$.

Lemma 10. *If $n \ge 9$, then $Mo_e(\Lambda_{k,l,r}) \ge 2n - 3$.*

Proof. Define $A = \{T_i | 1 \le i \le k\} \cup \{R_i | 1 \le i \le l\} \cup \{F_i | 1 \le i \le r\}$. If, for trees $T, T' \in A$, we have $|V(T) \cup V(T')| \ge 4$, then the result follows from Corollary 3. If these exists a tree $T \in A$ such that $E(T) = \{e = uv\}$, then $|m_u(e, \Lambda_{k,l,r}) - m_v(e, \Lambda_{k,l,r})| = n$. On the contrary, there are at most three edges such as $f = xy$ in $E(\Lambda_{k,l,r}) \backslash \{e = uv\}$ such that $|m_x(f, \Lambda_{k,l,r}) - m_y(f, \Lambda_{k,l,r})| = 0$. So, in this case, $Mo_e(\Lambda_{k,l,r}) \ge 2n - 3$. We now assume that, for every $T \in A$, $|V(T)| = 1$. Then, there are at most three edges such as $f_1 = x_1 y_1$ such that $|m_{x_1}(f_1, G) - m_{y_1}(f_1, G)| = 0$, there are at most two edges as $f_2 = x_2 y_2$ with $|m_{x_2}(f_2, \Lambda_{k,l,r}) - m_{y_2}(f_2, \Lambda_{k,l,r})| = 1$, there are at most two edges such as $f_3 = x_3 y_3$ such that $|m_{x_3}(f_3, \Lambda_{k,l,r}) - m_{y_3}(f_3, \Lambda_{k,l,r})| = 2$, there are at most two edges such as $f_4 = x_4 y_4$ such that $|m_{x_4}(f_4, \Lambda_{k,l,r}) - m_{y_4}(f_4, \Lambda_{k,l,r})| = 3$, and for other edges such as $f_5 = x_5 y_5$, $|m_{x_5}(f_5, \Lambda_{k,l,r}) - m_{y_5}(f_5, \Lambda_{k,l,r})| \ge 4$. Therefore, $Mo_e(\Lambda_{k,l,r}) \ge 4n - 20$, proving the lemma. □

Lemma 11. *If $n \ge 9$, then $Mo_e(\Upsilon_{k,l}) \ge 2n - 3$.*

Proof. Suppose $B = \{T_i : i = 1, \ldots, k\} \cup \{R_i : i = 1, \ldots, l\}$. If for two trees T, T' in B, $|V(T) \cup V(T')| \ge 4$, then the result follows from Corollary 3. If there exists a tree T in B such that $E(T) = \{e = uv\}$, then $|m_u(e, \Upsilon_{k,l}) - m_v(e, \Upsilon_{k,l})| = n$. Since there are at most two edges such as $f = xy \in E(\Upsilon_{k,l}) \backslash \{e = uv\}$ such that $|m_x(f, \Upsilon_{k,l}) - m_y(f, \Upsilon_{k,l})| = 0$, $Mo_e(\Upsilon_{k,l}) \ge 2n - 2$. We now assume that, for every $T \in B$, $|V(T)| = 1$. Then, there are at most two edges as $f_1 = x_1 y_1$ such that $|m_{x_1}(f_1, \Upsilon_{k,l}) - m_{y_1}(f_1, \Upsilon_{k,l})| = 0$ and for other edges this value is ≥ 3. Therefore, $Mo_e(\Upsilon_{k,l}) \ge 3n - 3$. □

Lemma 12. *If $n \ge 9$, then $Mo_e(\Psi_{k,l}) \ge 2n - 3$.*

Proof. Suppose $B = \{T_i : i = 1, \ldots, k\} \cup \{R_i : i = 1, \ldots, l\}$. If, for trees $T, T' \in B$, $|V(T) \cup V(T')| \ge 4$, then the result follows from Corollary 3. If there exists a tree $T \in B$ such that $E(T) = \{e = uv\}$, then $|m_u(e, \Psi_{k,l}) - m_v(e, \Psi_{k,l})| = n$. Also, for $e_1 = v_1 u_1$ and $f = v_k u_k$, we have $|m_{v_1}(e_1, \Psi_{k,l}) - m_{u_1}(e_1, \Psi_{k,l})| \ge 2$ and $|m_{v_k}(f, \Psi_{k,l}) - m_{u_k}(f, \Psi_{k,l})| \ge 2$. Since there are at most three edges as $f_1 = xy \in E(\Psi_{k,l}) \backslash \{e, e_1, f\}$ such that $|m_x(f_1, \Psi_{k,l}) - m_y(f_1, \Psi_{k,l})| = 0$, $Mo_e(G) \ge 2n - 1$.

We now assume that, for each $T \in B$, $|V(T)| = 1$. If $l = 1$, then

$$Mo_e(G) = \begin{cases} 3n - 8, & 2|n, \\ 3n - 7, & 2|n - 1, \end{cases} \tag{23}$$

as desired. Suppose $l \ge 2$. We consider two cases as follows:

(1) n is even. Since $n \ge 9$, $|m_{v_1}(e, G) - m_{u_1}(e, G)| = k - 1 \ge 5$ and $|m_{v_k}(f, G) - m_{u_k}(f, G)| = k - 1 \ge 5$. Again, there are at most three edges such as $f_2 = x_2 y_2$ such that $|m_{x_2}(f_2, G) - m_{y_2}(f_2, G)| = 0$, there are at most four edges $f_3 = x_3 y_3$ such that $|m_{x_3}(f_3, G) - m_{y_3}(f_3, G)| = 1$, and, for other edges, this quantity is at most 2. Thus, $Mo_e(G) \ge 2n - 2$.

(2) n is odd. Since $n \ge 9$, $|m_{v_1}(e, G) - m_{u_1}(e, G)| = k - 1 \ge 4$ and $|m_{v_k}(f, G) - m_{u_k}(f, G)| = k - 1 \ge 4$. There are two edges such as $f_2 = x_2 y_2$ such that $|m_{x_2}(f_2, G) - m_{y_2}(f_2, G)| = 0$, there are at most two edges as $f_3 = x_3 y_3$ such that $|m_{x_3}(f_3, G) - m_{y_3}(f_3, G)| = 1$, and, for other edges, this value is at most 2. Hence, $Mo_e(G) \ge 2n$.

Hence, the result. □

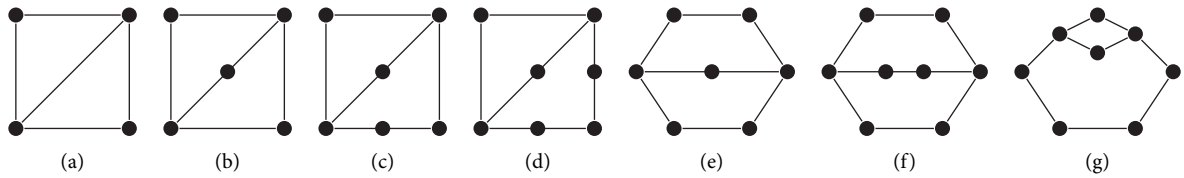

Figure 7: Bicyclic graphs with minimum edge Mostar index of order $4 \le n \le 8$. (a) G_4. (b) G_5. (c) G_6. (d) G_7^1. (e) G_7^2. (f) G_8^1. (g) G_8^2.

Table 1: The edge Mostar index of graphs in Figure 7.

Graphs	Mo_e	
G_4	4	
G_5	6	
G_6	8	
G_7^i	10	$i = 1, 2$
G_8^i	12	$i = 1, 2$

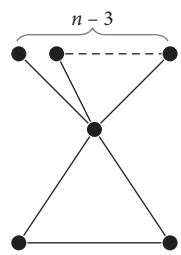

Figure 8: The unicyclic graph S_n^1.

Lemma 13. *If $n \ge 9$, then $Mo_e(\Phi_{k,l,r}) \ge 2n - 4$, with equality if and only if $G \cong \Theta_{2,2,n-3}$.*

Proof. Suppose that $A = \{T_i: i = 1, \ldots, k\} \cup \{R_i: i = 1, \ldots, l\} \cup \{F_i: i = 1, \ldots, r\}$. If, for trees $T, T' \in A$, $|V(T) \cup V(T')| \ge 4$, the proof follows from Corollary 3. If there exists a tree $T \in A$ with $E(T) = \{e = uv\}$, then $|m_u(e, G) - m_v(e, G)| = n$. On the contrary, there are at most three edges $f = xy \in E(G) \backslash \{e = uv\}$ such that $|m_x(f, G) - m_y(f, G)| = 0$. Thus, $Mo_e(G) \ge 2n - 3$. Next, we assume that, for each $T \in A$, $|V(T)| = 1$. Suppose $0 \le \varepsilon_0 \le 3$ are the number of distinct edges as $f_1 = x_1 y_1$ such that $|m_{x_1}(f_1, G) - m_{y_1}(f_1, G)| = 0$. Then, there are exactly $2(3 - \varepsilon_0)$ edges such as $f_2 = x_2 y_2$ such that $|m_{x_2}(f_2, G) - m_{y_2}(f_2, G)| = 1$. Also, for $e' = x' y' \in \{e_1 = u_1 u_2, e_2 = u_{l-1} u_l\}$, we have $|m_{x'}(e', G) - m_{y'}(e', G)| \ge 3$ and for other edges, this quantity is ≥ 2. Therefore, $Mo_e(G) \ge 2(n - 2 - \varepsilon_0 - 2(3 - \varepsilon_0)) + 2(3 - \varepsilon_0) + 6 = 2n - 4$, with equality if and only if $G \cong \Theta_{2,2,n-3}$.

We are now ready to prove Conjecture 5.5 in [17], see Figure 6. □

Theorem 5. *If G is a bicyclic graph of order $n \ge 9$, then $Mo_e(G) \ge 2n - 4$ and equality is occurred if and only if $G \cong \Theta_{2,2,n-3}$.*

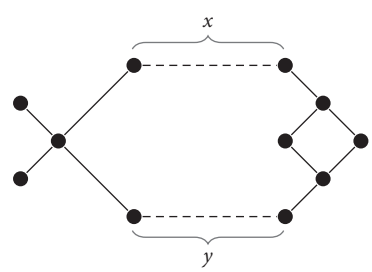

Figure 9: The bicyclic graph $G_{x,y}$.

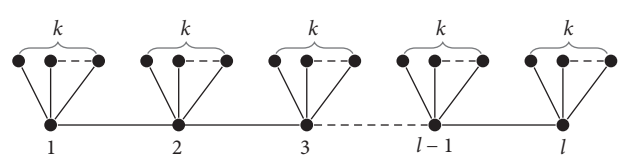

Figure 10: The caterpillar tree T_l^k.

Proof. The proof follows from Lemmas 10–13.

In Figure 7 and Table 1, the data of the bicyclic graphs with minimum edge Mostar index of order $4 \le n \le 8$ are given. □

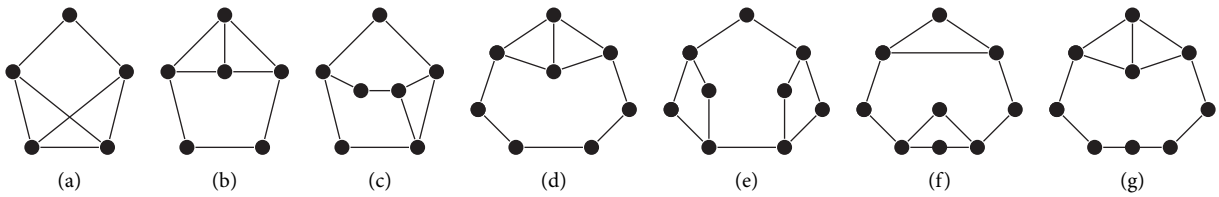

Figure 11: Tricyclic graphs with minimum edge Mostar index of order n, $5 \leq n \leq 9$. (a) G_5. (b) G_6. (c) G_7. (d) G_8. (e) G_9^1. (f) G_9^2. (g) G_9^3.

Table 2: The edge Mostar index of graphs in Figure 11.

Graphs	Mo_e	
G_5	4	
G_6	6	
G_7	9	
G_8	12	
G_9^i	16	$1 \leq i \leq 3$

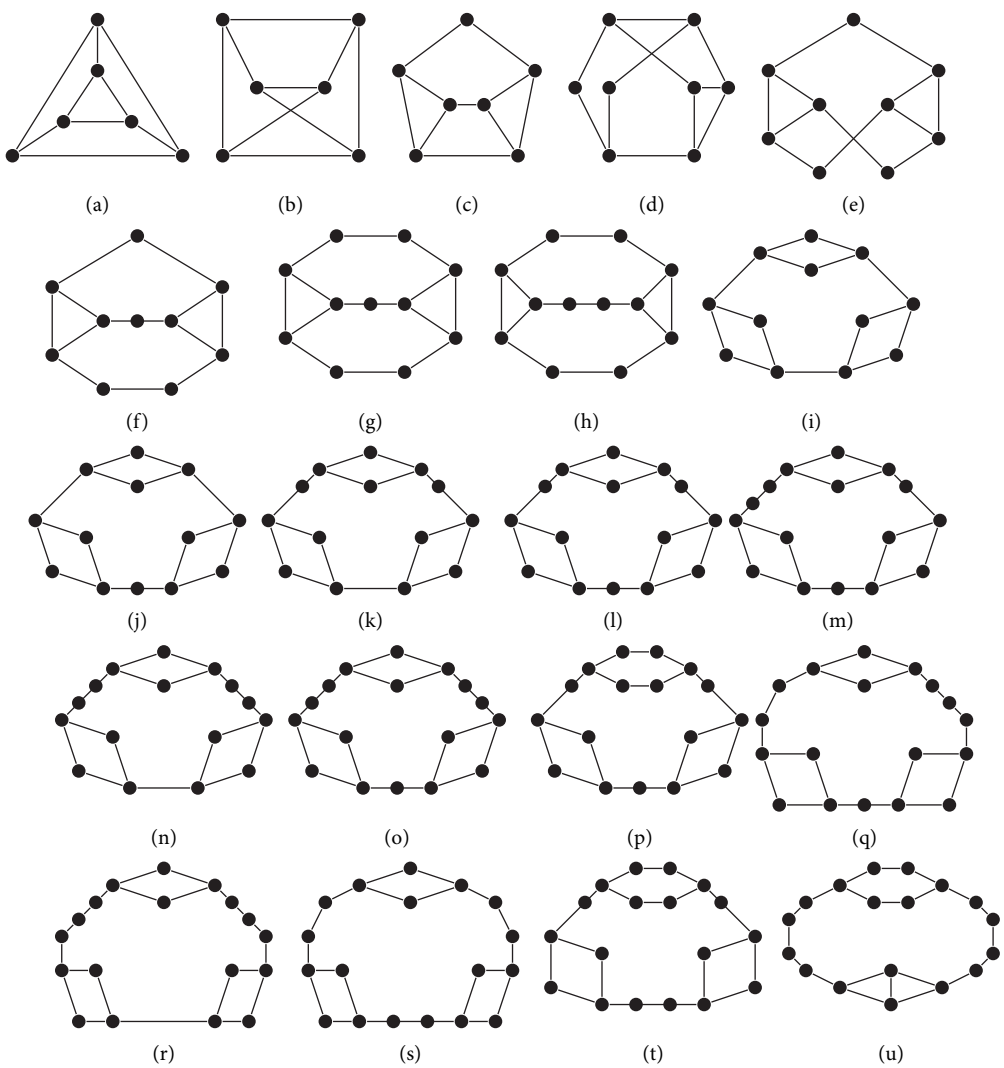

Figure 12: Tetracyclic graphs with minimum edge Mostar index of order n, $6 \leq n \leq 18$. (a) G_6^1. (b) G_6^2. (c) G_7. (d) G_8. (e) G_9. (f) G_{10}. (g) G_{11}. (h) G_{12}^1. (i) G_{12}^2. (j) G_{13}. (k) G_{14}. (l) G_{15}. (m) G_{16}^1. (n) G_{16}^2. (o) G_{17}^1. (p) G_{17}^2. (q) G_{18}^1. (r) G_{18}^2. (s) G_{18}^3. (t) G_{18}^4. (u) G_{18}^5.

Table 3: The edge Mostar index of graphs in Figure 12.

Graphs	Mo_e	
G_6^i	0	$i = 1, 2$
G_7	8	
G_8	11	
G_9	6	
G_{10}	14	
G_{11}	18	
G_{12}^i	12	$i = 1, 2$
G_{13}	20	
G_{14}	16	
G_{15}	18	
G_{16}^i	20	$i = 1, 2$
G_{17}^i	22	$i = 1, 2$
G_{18}^i	24	$i = 1, 2, 3, 4, 5$

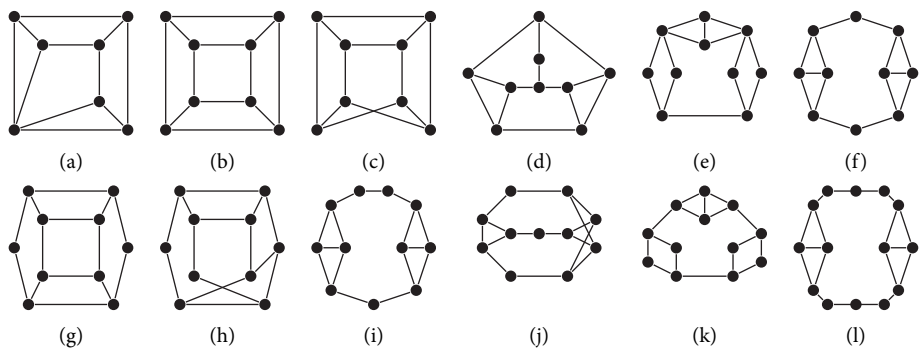

Figure 13: Pentacyclic graphs with minimum edge Mostar index of order n, $7 \leq n \leq 13$. (a) G_7. (b) G_8^1. (c) G_8^2. (d) G_9. (e) G_{10}^1. (f) G_{10}^2. (g) G_{10}^3. (h) G_{10}^4. (i) G_{11}^1. (j) G_{11}^2. (k) G_{12}. (l) G_{13}.

Table 4: The edge Mostar index of graphs in Figure 13.

Graphs	Mo_e	
G_7	8	
G_8^i	0	$i = 1, 2$
G_9	8	
G_{10}^i	16	$1 \leq i \leq 4$
G_{11}^i	12	$i = 1, 2$
G_{12}	10	
G_{13}	12	

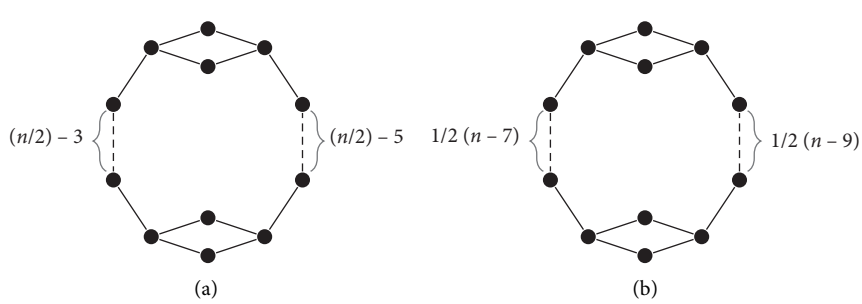

Figure 14: Tricyclic graphs with minimum edge Mostar index of order n, $n(\geq 10)$. (a) G_{even}. (b) G_{odd}.

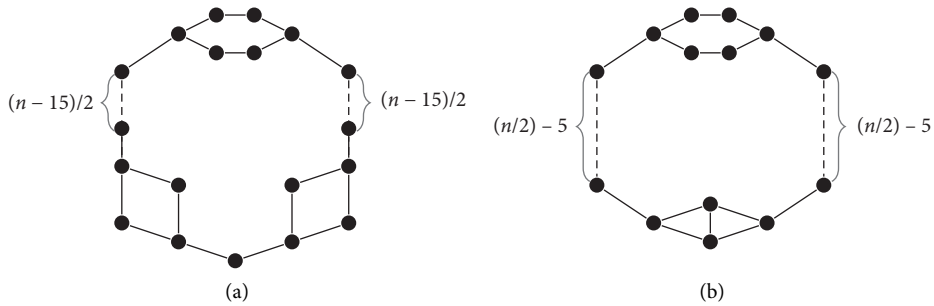

Figure 15: Tetracyclic graphs with minimum edge Mostar index of order $n(\geq 19)$. (a) G_{odd}. (b) G_{even}.

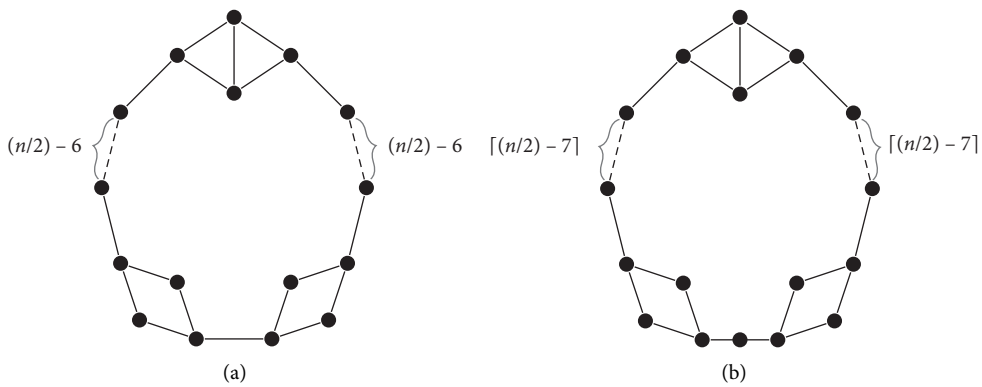

Figure 16: Pentacyclic graphs with minimum edge Mostar index of oder $n(\geq 14)$. (a) G_{even}. (b) G_{odd}.

4. Concluding remarks

The aim of this section is to compute some examples about invariants presented in Sections 1–3 and then suggest some conjectures.

Example 1. Let S_n^1, $G_{x,y}$, and T_l^k be three graphs depicted in Figures 8–10, such that $n \geq 3$, $x, y \geq 1$, $k \geq 0$, and $l \geq 2$. Then,

$$
\begin{aligned}
Mo\left(S_n^1\right) &= n^2 - 3n,\\
Mo_e\left(S_n^1\right) &= n^2 - 2n - 3,\\
Mo\left(G_{x,y}\right) &= \begin{cases} 3(x+y+7)+3, & |x-y| = 0,\\ 3(x+y+7), & |x-y| = 1,\\ 3(x+y+7)+1, & |x-y| = 2,\\ 3(x+y+7)+2, & |x-y| = 3,\end{cases}\\
Mo_e\left(G_{x,y}\right) &= \begin{cases} 2(x+y+7)+14, & |x-y| = 0,\\ 2(x+y+7)+10, & |x-y| = 1,\\ 2(x+y+7)+12, & |x-y| = 2,\\ 2(x+y+7)+16, & |x-y| = 3,\end{cases}\\
Mo\left(T_l^k\right) = Mo_e\left(T_l^k\right) &= \begin{cases} \frac{1}{2}l\left(2k^2l + 3kl - 6k + l - 2\right), & 2|l,\\ \frac{3}{2}kl^2 - 3kl + \frac{1}{2}k + \frac{1}{2}l^2 - l + k^2l^2 + \frac{1}{2}, & 2\nmid l.\end{cases}
\end{aligned}
\tag{24}
$$

By Example 1, $Mo_e(S_n^1) - Mo(S_n^1) = n - 3$ and

$$Mo\left(G_{x,y}\right) - Mo_e\left(G_{x,y}\right) = \begin{cases} x + y - 4, & |x - y| = 0 \text{ or } 2, \\ x + y - 3, & |x - y| = 1, \\ x + y - 7, & |x - y| = 3. \end{cases} \tag{25}$$

Remark 3. Let n be a positive integer.

(1) If $5 \le n \le 9$, then, in Figure 11 and Table 2, all tricyclic graphs with minimum edge Mostar index are given.

(2) If $6 \le n \le 18$, then, in Figure 12 and Table 3, all tetracyclic graphs with minimum edge Mostar index are given.

(3) If $7 \le n \le 13$, then, in Figure 13 and Table 4, all pentacyclic graphs with minimum edge Mostar index are given.

Our calculations with Nauty [13] on graphs with at most 22 vertices suggest the following conjecture.

Conjecture 1. *Suppose G is a graph with n vertices.*

(1) Suppose G is a tricyclic graph and $n \ge 10$. If n is odd, then $Mo_e(G) \ge 16$, and the equality holds if and only if $G \cong G_{odd}$, see Figure 14. If n is even, then $Mo_e(G) \ge 14$, and the equality holds if and only if $G \cong G_{even}$, see Figure 14, for details.

(2) Suppose G is an n–vertex tetracyclic graph, $n \ge 19$. If n is odd, then $Mo_e(G) \ge n + 5$, and the equality holds if and only if $G \cong G_{odd}$, see Figure 15. If n is even, then $Mo_e(G) \ge 24$, and the equality holds if and only if $G \cong G_{even}$, see Figure 15, for details.

(3) Suppose G is a pentacyclic graph and $n \ge 14$. If n is odd, then $Mo_e(G) \ge n + 1$, and the equality if and only if $G \cong G_{odd}$, see Figure 16. If n is even, then $Mo_e(G) \ge n - 2$, with equality if and only if $G \cong G_{even}$, see Figure 16, for details.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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