Research Article

On Mostar and Edge Mostar Indices of Graphs

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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 \( |V[v, G]| \) for the degree of a vertex v and the size of a vertex set 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 pendant path of G if \( \deg_G(v_0) \geq 3 \), \( \deg_G(v_1) = 1 \) and \( \deg_G(v_i) = \deg_G(v_2) = \cdots = \deg_G(v_{r-1}) = 2 \), 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 \( \deg_G(v_0) \), \( \deg_G(v_r) \geq 3 \) and \( \deg_G(v_i) = \deg_G(v_2) = \cdots = \deg_G(v_{s-1}) = 2 \), when \( s \geq 2 \). An edge incident to a pendant vertex is called a pendant 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, Došlić 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 \( M(G) = \sum_{uv \in E(G)} |n_u(uv, G) - n_v(uv, G)| \). 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.
with respect to the Mostar index. Ghorbani et al. [7] proved that a graph $G$ with $\text{Mo}(G) = 1$ 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 a given number of vertices, for which extremal values of the Mostar index are attained.

The characterization of bicyclic graphs with a given number of vertices, maximum Mostar index and gave a sharp upper bound for the extremal hexagonal chains with respect to Mostar index, and Hayat and Zhou [8] determined all $n$-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 Mostar index and fixed the maximum degree, diameter, or number of pendent vertices that are in distance 1 of a vertex $c$.

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 $\text{deg}_G(v) \geq 2$ and $|\{u: uv \in E(G) \text{ and } \text{deg}_G(u) = 1\}| \geq \text{deg}_G(v) - 1$. The set of all such vertices is denoted by $SV(G)$, and we use the name starlike set for $SV(G)$.

\[ T_c = T_c - \{v_1, v_2, \ldots, \text{deg}_{T_c}(v) - 2\} \]

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, $\text{Mo}(T_c) < \text{Mo}(T_c')$.

Proof. We consider two cases as follows:

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

\[ \text{Mo}(T_c) - \text{Mo}(T_c') = n_0(v_1v_{j+1}, T_c) - n_0(v_1v_{j+1}, T_c') - \text{deg}_{T_c}(v) - 2 - \text{deg}_{T_c'}(v) - 2 = 4 - 2\text{deg}_{T_c}(v) < 0. \]

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

\[ \text{Mo}(T_c) - \text{Mo}(T_c') = \sum_{i=1}^{j-1} \left[ (n_0(v_{i+1}v_1, T_c) + (i - l)) - (n_0(v_{i+1}v_1, T_c')) + (i - l) \right] - \sum_{i=1}^{l} \left[ (n_0(v_{i+1}v_1, T_c) + (j - i) + \text{deg}_{T_c}(v) - 2) - (n_0(v_{i+1}v_1, T_c') + (i - l) - \text{deg}_{T_c'}(v) + 2) \right] = \sum_{i=1}^{j-1} \left[ 4 - 2\text{deg}_{T_c}(v) \right] < 0, \]

proving the lemma.
Transformation 3. We assume that $T_c$, $P$, $Q$, and $w_1, w_2, \ldots, w_{\deg(v)}$ are defined in Transformation 2. We also assume that $j \geq l + 2$ and $n_v (v_{i+1}, T_c) < n_v (v_{i+1}, T_c)$. Define
\[ T_c'' = T_c - \{ w_i v_i : i = 1, 2, \ldots, \deg_{T_c} (v_i) - 2 \} + \{ w_i v_{i+1} : i = 1, 2, \ldots, \deg_{T_c} (v_i) - 2 \}. \] (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 $T_c''$,
\[ \Mo(T_c) - \Mo(T_c') = n_{v_{i+1}} (v_{i+1}, T_c) - n_{v_{i+1}} (v_{i+1}, T_c) - [n_{v_{i+1}} (v_{i+1}, T_c) + \deg_{T_c} (v_i) - 2] + [n_{v_{i+1}} (v_{i+1}, T_c) + \deg_{T_c} (v_i) - 2] = 4 - 2 \deg_{T_c} (v_i) < 0, \] (5)
proving the lemma.
Lemma 4. Let \( n, k, \) and \( r \) be three positive integers such that \( k < n \) and \( 1 \leq r \leq n - k \). If \( r < \lfloor (n - k)/2 \rfloor \), then \( Mo(P_{n-k}[r^k]) < Mo(P_{n-k}(r+1)^k)) \).

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

\[
Mo(T) = \begin{cases} 
  n^2 - 3n - \frac{1}{2}diam(T)^2 + diam(T) + 2, & 2 | diam(T), \\
  n^2 - 3n - \frac{1}{2}diam(T)^2 + diam(T) + \frac{3}{2}, & 2 | diam(T) - 1.
\end{cases}
\]

(6)

Proof. Suppose \( diam(T) = d \). By definition of caterpillar,

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

(7)

and by simple calculations,

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

(8)

with equality if and only if \( T \equiv P_r[s'] \), where \( r = diam(T) + 1, s = \lfloor (diam(T) + 1)/2 \rfloor, \) and \( t = n - r \).

Proof. If \( T \equiv P_r[s'] \), where \( r = diam(T) + 1, s = \lfloor (diam(T) + 1)/2 \rfloor, \) and \( t = n - r \), then Proposition 1 gives the result. Otherwise, we assume that \( P_r = v_1v_2\cdots v_{diam(T)+1} \) is the longest path in \( T \). At first, by repeated applications of Transformation 1 on vertices of \( SV(T) \setminus \{v_1, v_{diam(T)}\} \), we arrive at a caterpillar \( T_c \) with central path \( P \). We now apply Lemma 1 to deduce that \( Mo(T) \leq Mo(T_c) \). Next, by the repeated applications of Transformations 2 and 3 on the internal paths in \( T_c \), we arrive at a caterpillar \( P_r[s'] \), where \( r = diam(T) + 1, 2 \leq s \leq diam(T) \), and \( t = n - r \). Apply Lemmas 2 and 3 to prove that \( Mo(T) \leq Mo(T_c) \leq Mo(P_r[s']) \). Finally, by Lemma 4,

\[
Mo(T) \leq \begin{cases} 
  n^2 - 3n - \frac{1}{2}diam(T)^2 + diam(T) + 2, & 2|diam(T), \\
  n^2 - 3n - \frac{1}{2}diam(T)^2 + diam(T) + \frac{3}{2}, & 2|diam(T) - 1,
\end{cases}
\]

(9)

with equality if and only if \( T \equiv P_r[s'] \), where \( r = diam(T) + 1, s = \lfloor (diam(T) + 1)/2 \rfloor, \) and \( t = n - r \).

Lemma 5. Let \( n \) and \( r \) be two positive integers. If \( 1 \leq r \leq n - r - 4 \), then,
\[ \text{Mo}(P_4[2^{r-1},3^{n-r-3}]) = \text{Mo}(P_4[2^r,3^{n-r-4}]) + 2. \quad (11) \]

**Proof.** By definition, \( \text{Mo}(P_4[2^{r-1},3^{n-r-3}]) - \text{Mo}(P_4[2^r,3^{n-r-4}]) = n - r - 1 - (r + 1) - (n - r - 2 - (r + 2)) = 2. \quad \square \)

**Theorem 2.** Let \( T \) be an \( n \)-vertex tree and

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

**Proof.** By definition,

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

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

**Lemma 6.** Let \( a, b, \) and \( c \) be three positive integers such that \( a < b. \) Then, \( |a + c - b| < |b + c - a| = |c - a| < c + a < 0. \)

**Proof.** Suppose \( i = b - a. \) Then, \( |a + c - b| - |b + c - a| = |c - i| = c + i < 0. \) \quad \square

**Transformation 4.** (see [16]). Suppose that \( w \) is a vertex in a connected graph \( G \) with at least two vertices and \( N[w,G] = \{x_1,x_2,...,x_k[w]\}. \) In addition, we assume that \( P_1, u_1, u_2, u_3, ..., u_k, Q = v_0, v_1, ..., v_i, v_{i+1}, v_{i+2}, ... \) are two paths of lengths \( k \) and \( \ell, \) \( k \geq \ell \geq 1, \) respectively. Let \( G_1 \) be the graph obtained from \( G, P, \) and \( Q \) by attaching edges \( v_0, u_k, \) and \( G_2 = G_1 - \{vx_j: x_j \in N[w,G]\} + \{vy_j: y_j \in N[w,G]\}. \) 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, \( \text{Mo}(G_2) < \text{Mo}(G_1). \)

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

\[ \text{Mo}(G_1) - \text{Mo}(G_2) = |k + c - l| - |l + (c - 1) - (k + 1)| \]
\[ = |k + 1 + (c - 1) - l| \]
\[ - |l + (c - 1) - (k + 1)|, \quad (15) \]

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

**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 \( \text{Mo}(P_{n-3}[2^3]) = (1/2)(n-1)^2 + 6, \)
\( \text{Mo}(P_{n-2}[2^3,3^1]) = (1/2)(n-1)^2 + 8, \) \( \text{Mo}(P_{n-1}[2^3,3^2]) = (1/2)(n-1)^2 + 14, \) \( \text{Mo}(P_{n-2}[3^1,(n-3)^1]) = (1/2)(n-1)^2 + 6, \) \( \text{Mo}(P_{n-1}[3^1]) = (1/2)(n-1)^2 + 4, \) \( \text{Mo}(P_n[4^1]) = (1/2)(n-1)^2 + 6. \)

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

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

\[ T \notin \{P_{n-1}[i^1]|1 \leq i \leq 4| \cup \{P_{n-2}[2^2],P_{n-2}[2^1,(n-3)^1],P_{n-2}[3^1,(n-3)^1]\}, \quad (16) \]
Proof. By Proposition 2,

\[
Mo(P_{n-1}[1^1]) < Mo(P_{n-1}[2^1]) < Mo(P_{n-1}[3^1]) = Mo(P_{n-1}[2^1, (n-3)^1]) < Mo(P_{n-1}[4^1])
\]

\[= Mo(P_{n-2}[3^1, (n-3)^1]) = Mo(P_{n-2}[2^2]) < Mo(T). \quad (17)
\]

then

\[
Mo(P_{n-1}[1^1]) < Mo(P_{n-1}[2^1]) < Mo(P_{n-1}[3^1]) = Mo(P_{n-2}[2^1, (n-3)^1]) < Mo(P_{n-1}[4^1])
\]

\[= Mo(P_{n-2}[3^1, (n-3)^1]) = Mo(P_{n-2}[2^2]). \quad (18)
\]

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) $P_{n-2}[2^1]$. (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) $G_2$. 

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

\[
\text{Figure 5: The graphs } P, Q, G, G_1, \text{ and } G_2 \text{ in Transformation 4. (a) } G_1. \text{ (b) } G_2.
\]

then

\[
Mo(P_{n-1}[1^1]) < Mo(P_{n-1}[2^1]) < Mo(P_{n-1}[3^1]) = Mo(P_{n-2}[2^1, (n-3)^1]) < Mo(P_{n-1}[4^1])
\]

\[= Mo(P_{n-2}[3^1, (n-3)^1]) = Mo(P_{n-2}[2^2]) < Mo(T). \quad (17)
\]

Proof. By Proposition 2,

\[
Mo(P_{n-1}[1^1]) < Mo(P_{n-1}[2^1]) < Mo(P_{n-1}[3^1]) = Mo(P_{n-2}[2^1, (n-3)^1]) < Mo(P_{n-1}[4^1])
\]

\[= Mo(P_{n-2}[3^1, (n-3)^1]) = Mo(P_{n-2}[2^2]). \quad (18)
\]
We now apply repeated applications of Transformation 4 on the pendant paths in $T$ to arrive at a caterpillar $T_\epsilon$ in the

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

and this gives the result. $\square$

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 $E_\epsilon \subseteq E(G)$. Define $Mo(e') = \sum_{e \in E_\epsilon} |m_n(e, G) - n_1(e, G)|$ and $Mo_e(e') = \sum_{e \in E_\epsilon} |m_n(e, G) - m_v(e, G)|$.

**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, $m_n(e, T) = |E(T_u)|$, $m_v(e, T) = |E(T_v)|$, $n_u(e, T) = |V(T_u)|$, and $n_v(e, T) = |V(T_v)|$. The result follows from these facts that $|E(T_u)| = |E(T_v)| - 1$ and $|E(T_u)| = |E(T_v)| - 1$.

**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 $CT^1(G)$ and $CT^2(G)$, respectively.

**Proposition 4.** If $G$ is not acyclic graph, $e_1 = x_1y_1$ and $e_2 = x_2y_2 \in CT^1(G)$, then $w(e_1) < w(e_2)$

**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

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, $Mo(T_\epsilon) < Mo(T)$. Therefore, by Proposition 2, $e_1, e_2 \in CT^1(G)$, $G_{y_1}$ is a subgraph of $G_{y_2}$ or $G_{y_2}$ is a subgraph of $G_{y_1}$, as desired. $\square$

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

**Proof.** Suppose $CT^1(G) = \{e_1, e_2, \ldots, e_k = x_k y_k\}$ and $w(e_1) > w(e_2) > \cdots > w(e_k)$. We also assume that $G_{x_1}$ and $G_{y_k}$ are two components of $G - e_k$. Without loss of generality, we can assume that $G_{y_k}$ is a tree. Since all edges of a tree is a cut edge, $e_2 \in CT^1(G)$ and $w(e_2) = \max\{w(e_1), w(e_2), \ldots, w(e_k)\}$, it can be proved that $x_2 = y_1$ or $y_1 = y_2$. Choose the edge $e_2$ and repeat this process to complete the proof.

**Proposition 6.** If $G$ is not acyclic, then $|CT^2(G) = |CT^1(G)| \leq |CT^2(G)|$.

**Proof.** Suppose $CT^2(G) = \{e_1, \ldots, e_k = x_k y_k\}$ and $w(e_1) > w(e_2) > \cdots > w(e_k)$. We also assume that $G_{x_1}$ 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 $e_k \in CT^2(G)$, $|V(G_{x_1})| < |V(G_{y_k})|$. On the contrary, $w(e_k) = \min\{w(e_1), w(e_2), \ldots, w(e_k)\}$ and $e \in E(G_{y_k})$ implies that $e \in CT^1(G)$. Apply Proposition 5 and the fact that a cut edge cannot be on a cycle to complete our argument.

**Corollary 2.** Suppose $G$ is the cyclomatic number of a connected graph $G$ with $|CT^1(G)| \equiv 1$; then,

1. If $\gamma = 1$, then $|CT^1(G)| \equiv |CT^2(G)| - 2$.
2. If $\gamma = 2$, then $|CT^1(G)| \equiv |CT^2(G)| - 3$.

**Lemma 8.** Let $G$ be $\gamma$-cyclic graph such that $|CT(G)| \equiv 1$; then,

1. If $\gamma = 1$, then $Mo_e(CT(G)) \equiv Mo(CT(G)) + 1$.
2. If $\gamma = 2$, then $Mo_e(CT(G)) \equiv Mo(CT(G)) + 2$.

**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 $G_e$ is a tree. By definition, $m_v(e, T) = |E(G_u)|$, $m_u(e, G) = |E(G_v)|$, $n_u(e, G) = |V(G_v)|$, and $n_v(e, G) = |V(G_u)|$. Our main proof will consider two cases as follows:

1. $\gamma = 1$. In this case, $|E(G_u)| = |V(G_v)| - 1$ and $|E(G_v)| = |V(T_v)|$. Thus,
Consider the following two cases:

Suppose \( k \) is even. In this case, there exists a unique edge as

\[
\Gamma_k = E(T_i) \cup \{v_i, v_i+1\} \quad \text{for } 1 \leq i \leq k-1 \text{ and } \{v_1, v_k\}.
\]

Again by Corollary 2, \( M_{\phi}(C T(G)) \geq M_{\phi}(C T(G)) + 2 \).

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 \( \Gamma_k \) with vertex set \( V(\Gamma_k) = \cup_{i=1}^{k} V(T_i) \) and edge set \( E(\Gamma_k) = \cup_{i=1}^{k} E(T_i) \cup \{v_i, v_{i+1}\} \quad \text{for } 1 \leq i \leq k-1 \text{ and } \{v_1, v_k\} \).

Lemma 9. Let \( \Gamma_k \) be the graph defined above. If \( E(\Gamma_k) = \{v_i, v_{i+1}\} \quad \text{for } 1 \leq i \leq k-1 \text{ and } \{v_1, v_k\} \), then \( M_{\phi}(E(\Gamma_k)) = M_{\phi}(E(\Gamma_k)) \).

Proof. Suppose \( e = v_i v_j \) is an arbitrary edge in \( E(\Gamma_k) \). Consider the following two cases:

1. \( k \) is even. In this case, there exists a unique edge as \( f = v_i v_j \in E(\Gamma_k) \setminus \{v_i, v_j\} \) such that \( d_{\Gamma_k}(v_i, v_j) = d_{\Gamma_k}(v_i, v_j) \). Therefore, \( |u(e, \Gamma_k) - n_{\phi}(e, \Gamma_k)| = |u(e, \Gamma_k) - n_{\phi}(e, \Gamma_k)| \) and \( |u(e, \Gamma_k) - n_{\phi}(e, \Gamma_k)| = |u(e, \Gamma_k) - n_{\phi}(e, \Gamma_k)| \).

2. \( k \) is odd. There exists a unique vertex \( v_{i+1} \) in \( \{v_1, v_2, \ldots, v_k\} \) such that \( d_{\Gamma_k}(v_i, v_{i+1}) = d_{\Gamma_k}(v_i, v_{i+1}) \). We construct the tree \( \Gamma_k \) from the vertices of \( T_i \) by removing the pendent vertices of \( T_i \). Then, \( |u(e, \Gamma_k) - n_{\phi}(e, \Gamma_k)| = |u(e, \Gamma_k) - n_{\phi}(e, \Gamma_k)| \) and \( |u(e, \Gamma_k) - n_{\phi}(e, \Gamma_k)| = |u(e, \Gamma_k) - n_{\phi}(e, \Gamma_k)| \).

Now, the proof follows from cases (1), (2), and Proposition 3.
Figure 6: The bicyclic graph $\Theta_{2,n-3}$.

Suppose $k,l$, and $r$ are positive integers. Consider $T_j$, $R_j$, and $F_i$ to be trees with these properties that $v_j \in V(T_j)$, $u_i \in V(R_j)$, $1 \leq i \leq k$, $1 \leq j \leq l$, and $1 \leq t \leq r$. Define four classes of bicyclic graphs denoted by $\Lambda_{k,l,r}$, $k,l,r \geq 2$, $\Phi_{k,l}$, $k \geq 3$, $l \geq 1$, $k \geq 1$, and $\Phi_{k,l,r}$, $l \geq r$ and $k,l \geq 1$, with the following vertex and edge sets:

\[
V(\Lambda_{k,l,r}) = \left( \bigcup_{i=1}^k V(T_i) \right) \bigcup \left( \bigcup_{i=1}^l V(R_i) \right) \bigcup \left( \bigcup_{j=r}^k V(F_j) \right),
\]

\[
V(\Phi_{k,l}) = \left( \bigcup_{i=1}^k V(T_i) \right) \bigcup \left( \bigcup_{i=1}^l V(R_i) \right),
\]

\[
V(\Psi_{k,l}) = \left( \bigcup_{i=1}^k V(T_i) \right) \bigcup \left( \bigcup_{i=1}^l V(R_i) \right) \bigcup \left( \bigcup_{i=r}^k V(F_i) \right),
\]

\[
E(\Lambda_{k,l,r}) = \left( \bigcup_{i=1}^k E(T_i) \right) \bigcup \left( \bigcup_{i=1}^l E(R_i) \right) \bigcup \left( \bigcup_{j=r}^k E(F_j) \right)
\]

\[
\bigcup \left\{ v_iu_{i+1} : 1 \leq i \leq k-1 \right\} \bigcup \left\{ w_iu_{i+1} : 1 \leq i \leq l-1 \right\} \bigcup \left\{ u_iu_{i+1} : 1 \leq i \leq r-1 \right\},
\]

\[
E(\Phi_{k,l}) = \left( \bigcup_{i=1}^k E(T_i) \right) \bigcup \left( \bigcup_{i=1}^l E(R_i) \right) \bigcup \left( \bigcup_{i=r}^k E(F_i) \right)
\]

\[
\bigcup \left\{ u_iu_{i+1} : 1 \leq i \leq l-1 \right\} \bigcup \left\{ v_iu_{i+1} : 1 \leq i \leq k-1 \right\} \bigcup \left\{ w_iu_{i+1} : 1 \leq i \leq r-1 \right\},
\]

\[
E(\Psi_{k,l}) = \left( \bigcup_{i=1}^k E(T_i) \right) \bigcup \left( \bigcup_{i=1}^l E(R_i) \right) \bigcup \left( \bigcup_{i=r}^k E(F_i) \right)
\]

\[
\bigcup \left\{ u_iu_{i+1} : 1 \leq i \leq l-1 \right\} \bigcup \left\{ v_iu_{i+1} : 1 \leq i \leq k-1 \right\} \bigcup \left\{ w_iu_{i+1} : 1 \leq i \leq r-1 \right\},
\]

\[
E(\Phi_{k,l,r}) = \left( \bigcup_{i=1}^k E(T_i) \right) \bigcup \left( \bigcup_{i=1}^l E(R_i) \right) \bigcup \left( \bigcup_{j=r}^k E(F_j) \right)
\]

\[
\bigcup \left\{ v_iu_{i+1} : 1 \leq i \leq k-2 \right\} \bigcup \left\{ u_iu_{i+1} : 1 \leq i \leq l-1 \right\} \bigcup \left\{ w_iu_{i+1} : 1 \leq i \leq r-1 \right\}.
\]

(22)

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

Lemma 10. If $n \geq 9$, then $M_0(\Lambda_{k,l,r}) \geq 2n - 3$.

Proof. Define $A = \{ T_i : 1 \leq i \leq k \} \cup \{ R_i : 1 \leq i \leq l \} \cup \{ F_i : 1 \leq i \leq r \}$. If, for trees $T, T' \in A$, we have $|V(T)| = 4$, then the result follows from Corollary 3. If these exists a tree $T \in A$ such that $E(T) = \{ e = uv \}$, then $m_{\Lambda}(\Lambda_{k,l,r}) = n$. On the contrary, there are at most three edges such as $f = xy$ in $E(\Lambda_{k,l,r}) \{ e = uv \}$ such that $m_{\Lambda}(\Lambda_{k,l,r}) = 0$. So, in this case, $M_0(\Lambda_{k,l,r}) \geq 2n - 3$. We now assume that, for every $T \in A$, $|V(T)| = 1$. Then, there are at most three edges such as $f_1 = x_1y_1$ such that $m_{\Lambda}(f_1, G) = m_{\Lambda}(f, G) = 0$, there are at most two edges as $f_2 = x_2y_2$ with $m_{\Lambda}(f_2, \Lambda_{k,l,r}) = 1$, there are at most two edges such as $f_3 = x_3y_3$ such that $m_{\Lambda}(f_3, \Lambda_{k,l,r}) = 2$, and for other edges such as $f_4 = x_4y_4$ such that $m_{\Lambda}(f_4, \Lambda_{k,l,r}) = 3$, and for other edges $\geq 4$. Therefore, $M_0(\Lambda_{k,l,r}) \geq 4n - 20$, proving the lemma.

Lemma 11. If $n \geq 9$, then $M_0(\Phi_{k,l}) \geq 2n - 3$.

Proof. Suppose $B = \{ T_i : i = 1, \ldots, k \} \cup \{ R_i : i = 1, \ldots, l \}$. If, for two trees $T, T' \in B$, $|V(T) \cup V(T')| \geq 4$, then the result follows from Corollary 3. If there exists a tree $T \in B$ such that $E(T) = \{ e = uv \}$, then $m_{\Phi}(\Phi_{k,l}) = n$. Also, since there are at most two edges as $f = xy \in E(\Phi_{k,l}) \{ e = uv \}$ such that $m_{\Phi}(f, \Phi_{k,l}) = 0$, $M_0(\Phi_{k,l}) \geq 2n - 2$. We now assume that, for every $T \in B$, $|V(T)| = 1$. Then, there are at most two edges as $f_1 = x_1y_1$ such that $m_{\Phi}(f_1, \Phi_{k,l}) = 0$ and for other edges this value is $\geq 3$. Therefore, $M_0(\Phi_{k,l}) \geq 3n - 3$.

Lemma 12. If $n \geq 9$, then $M_0(\Psi_{k,l}) \geq 2n - 3$.

Proof. Suppose $B = \{ T_i : i = 1, \ldots, k \} \cup \{ R_i : i = 1, \ldots, l \}$. If, for trees $T, T' \in B$, $|V(T) \cup V(T')| \geq 4$, then the result follows from Corollary 3. If there exists a tree $T \in B$ such that $E(T) = \{ e = uv \}$, then $m_{\Psi}(\Psi_{k,l}) = n$. Also, for $e_1 = v_1u_1$ and $f = v_1u_2$, we have $m_{\Psi}(e_1, \Psi_{k,l}) = 2$ and $m_{\Psi}(f, \Psi_{k,l}) = 2$. Since there are at most three edges as $f_1 = xy \in E(\Psi_{k,l}) \{ e_1, f \}$ such that $m_{\Psi}(f_1, \Psi_{k,l}) = 0$, $M_0(\Psi_{k,l}) \geq 2n - 1$. We now assume that, for each $T \in B$, $|V(T)| = 1$. If $l = 1$, $M_0(\Psi_{k,l}) = \left\{ \begin{array}{ll} 3n - 8, & 2n, \\ 3n - 7, & 2n - 1, \end{array} \right.$

(23)
as desired. Suppose $l \geq 2$. We consider two cases as follows:

(1) $n$ is even. Since $n \geq 9$, $m_{\Psi}(\Psi_{k,l}) = m_{\Psi}(\Psi_{k,l}) = k - 1 \geq 5$ and $m_{\Psi}(\Psi_{k,l}) = \frac{n}{2} - 5$. Again, there are at most three edges such as $f_2 = x_2y_2$ such that $m_{\Psi}(f_2, G) = 0$, are at most four edges $f_3, f_4 = x_3y_4$ such that $m_{\Psi}(f_3, G) = f_4, G = 0$, and, for other edges, this quantity is at most 2. Thus, $M_0(\Psi_{k,l}) \geq 2n - 2$.

(2) $n$ is odd. Since $n \geq 9$, $m_{\Psi}(\Psi_{k,l}) = m_{\Psi}(\Psi_{k,l}) = k - 1 \geq 4$ and $m_{\Psi}(\Psi_{k,l}) = \frac{n}{2} - 4$. There are at most two edges as $f_2 = x_2y_2$ such that $m_{\Psi}(f_2, G) = 0$, are at most two edges as $f_3, f_4 = x_3y_4$ such that $m_{\Psi}(f_3, G) = f_4, G = 0$, and, for other edges, this value is at most 2. Hence, $M_0(\Psi_{k,l}) \geq 2n$.

Hence, the result.
Lemma 13. If \( n \geq 9 \), then \( M_{\text{e}}(\Phi_{k,l,r}) \geq 2n - 4 \), 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 \( T, T' \in A \), \( |V(T) \cup V(T')| \geq 4 \), the proof follows from Corollary 3. If there exists a tree \( T \in A \) with \( E(T) = \{e = uv\} \), then \( |m_x(f, G) - m_y(e, G)| = n \). On the contrary, there are at most three edges \( f = xy \in E(G) \setminus \{e = uv\} \) such that \( |m_x(f, G) - m_y(f, G)| = 0 \). Thus, \( M_{\text{e}}(G) \geq 2n - 3 \). Next, we assume that, for each \( T \in A \), \( |V(T)| = 1 \). Suppose \( 0 \leq \varepsilon_0 \leq 3 \) are the number of distinct edges as \( f_1 = x_1y_1 \) 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 \( f_2 = x_2y_2 \) such that \( |m_{x_2}(f_2, G) - m_{y_2}(f_2, G)| = 1 \). Also, for \( e' = x'y' \in \{e_1 = u_1u_2, e_2 = u_2u_3, \ldots, u_{k-1}u_k\} \), we have \( |m_{x'}(e', G) - m_{y'}(e', G)| \geq 3 \) and for other edges, this quantity is \( \geq 2 \). Therefore, \( M_{\text{e}}(G) \geq 2(n - 2 - \varepsilon_0 - 2(3 - \varepsilon_0)) + 2(3 - \varepsilon_0) + 6 = 2n - 4 \), 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 \( n \geq 9 \), then \( M_{\text{e}}(G) \geq 2n - 4 \) and equality is occurred if and only if \( G \cong \Theta_{2,2,n-3} \).

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 \( 4 \leq n \leq 8 \) 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.

<table>
<thead>
<tr>
<th>Graphs</th>
<th>$M_{te}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_5$</td>
<td>4</td>
</tr>
<tr>
<td>$G_6$</td>
<td>6</td>
</tr>
<tr>
<td>$G_7$</td>
<td>9</td>
</tr>
<tr>
<td>$G_8$</td>
<td>12</td>
</tr>
<tr>
<td>$G_9^{1i}$</td>
<td>16</td>
</tr>
</tbody>
</table>

$1 \leq i \leq 3$

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) $G_9^{1}$, (f) $G_{10}$, (g) $G_{11}$, (h) $G_{12}$, (i) $G_{12}^{1}$, (j) $G_{13}$, (k) $G_{14}$, (l) $G_{15}$, (m) $G_{16}$, (n) $G_{17}$, (o) $G_{17}^{1}$, (p) $G_{18}$, (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.

<table>
<thead>
<tr>
<th>Graphs</th>
<th>$Mo_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_6$</td>
<td>0</td>
</tr>
<tr>
<td>$G_7$</td>
<td>8</td>
</tr>
<tr>
<td>$G_8$</td>
<td>11</td>
</tr>
<tr>
<td>$G_9$</td>
<td>6</td>
</tr>
<tr>
<td>$G_{10}$</td>
<td>14</td>
</tr>
<tr>
<td>$G_{11}$</td>
<td>18</td>
</tr>
<tr>
<td>$G_{12}$</td>
<td>12</td>
</tr>
<tr>
<td>$G_{13}$</td>
<td>20</td>
</tr>
<tr>
<td>$G_{14}$</td>
<td>16</td>
</tr>
<tr>
<td>$G_{15}$</td>
<td>12</td>
</tr>
<tr>
<td>$G_{16}$</td>
<td>20</td>
</tr>
<tr>
<td>$G_{17}$</td>
<td>22</td>
</tr>
<tr>
<td>$G_{18}$</td>
<td>24</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Graphs</th>
<th>$Mo_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_7$</td>
<td>8</td>
</tr>
<tr>
<td>$G_8$</td>
<td>0</td>
</tr>
<tr>
<td>$G_9$</td>
<td>8</td>
</tr>
<tr>
<td>$G_{10}$</td>
<td>16</td>
</tr>
<tr>
<td>$G_{11}$</td>
<td>12</td>
</tr>
<tr>
<td>$G_{12}$</td>
<td>10</td>
</tr>
<tr>
<td>$G_{13}$</td>
<td>12</td>
</tr>
</tbody>
</table>

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

Figure 14: Tricyclic graphs with minimum edge Mostar index of order $n$, $n \geq 10$. (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,

\[
Mo(S_n^1) = n^2 - 3n,
\]

\[
Mo(G_{x,y}) = \begin{cases} 
3(x + y + 7) + 3, & |x - y| = 0, \\
3(x + y + 7), & |x - y| = 1, \\
3(x + y + 7) + 1, & |x - y| = 2, \\
3(x + y + 7) + 2, & |x - y| = 3,
\end{cases}
\]

\[
Mo(G_{x,y}) = \begin{cases} 
2(x + y + 7) + 14, & |x - y| = 0, \\
2(x + y + 7) + 10, & |x - y| = 1, \\
2(x + y + 7) + 12, & |x - y| = 2, \\
2(x + y + 7) + 16, & |x - y| = 3,
\end{cases}
\]

\[
Mo(T_l^k) = Mo(T_l^k) = \begin{cases} 
\frac{1}{2}(2k^2l + 3kl - 6k + l - 2), & 2|l|, \\
\frac{3}{2}kl^2 - 3kl + \frac{1}{2}k + \frac{1}{2}l^2 - l + k^2l^2 + \frac{1}{2}, & 2|l|.
\end{cases}
\]
Remark 3. Let $n$ be a positive integer.

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

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

(3) If $7 \leq n \leq 13$, 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 $n \geq 10$. If $n$ is odd, then $M_o(G) \geq 4$, and the equality holds if and only if $G \cong G_{odd}$, see Figure 14. If $n$ is even, then $M_o(G) \geq 14$, 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, $n \geq 19$. If $n$ is odd, then $M_o(G) \geq n + 5$, and the equality holds if and only if $G \cong G_{odd}$, see Figure 15. If $n$ is even, then $M_o(G) \geq 24$, 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 $n \geq 14$. If $n$ is odd, then $M_o(G) \geq n + 1$, and the equality if and only if $G \cong G_{odd}$, see Figure 16. If $n$ is even, then $M_o(G) \geq n - 2$, 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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**References**


