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Research Paper

On Some Extremal Results and Bounds of Additively Weighted Edge Mostar Index

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Abstract

The additively weighted edge Mostar index is a topological index(TI) defined as an extension of the edge Mostar index. In this paper, we determine the extrema of the additively weighted edge Mostar index for trees. Additionally, we compute the lower bound and first four upper bounds of additively weighted edge Mostar index of unicyclic graphs and the upper bound for cacti with a fixed number of cycles. All the graphs attaining the bounds are characterized. We also propose two conjectures on additively weighted edge Mostar index of bicyclic graphs.

1 Introduction

Topological indices(TI) are real-valued functions associated with graphs which contain structural information of graphs and preserve graph isomorphisms. The first TI was due to H. Wiener [1], who described it as an estimate of boiling points of conjugated hydrocarbons. Subsequently, a considerable number of TI's were defined and studied. A prominent one among them is the Szeged index (Sz) proposed by I. Gutman [2]. For any simple connected graph $G = (V, E)$

$$Sz(G) = \sum_{e=xy\in E} n_x(e|G)n_y(e|G),$$

where $n_x(e|G)$ represents the number of vertices that are closer to x than to y. Although the Szeged index was defined as an extension of the Wiener index, it has been the subject of numerous studies. For a detailed review of the literature on the Szeged index and other topological indices, see [3–10]. Although the mathematical properties of the Szeged index

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are significant, it does not exhibit a high correlation with the physical properties of chemical compounds compared to other TI. New variants of the Szeged index were proposed to study various physical and chemical properties of compounds. One among them was the Mostar index, $Mo(G)$ proposed in 2018 by T. Došlić *et al.* [11], defined as:

$$Mo(G) = \sum_{e=xy\in E} |n_x(e|G) - n_y(e|G)|,$$

Many more applications and results were obtained for the Mostar index recently, for a detailed literature on the Mostar index, see [12–17]. An analogous edge version of the Mostar index was proposed in 2019 by M. Arockiaraj *et al.* [18]. Muhammad Imran *et al.* [19] determined the edge Mostar index of some nanostructures using graph operations. H. Liu *et al.* [20] determined the extrema of the edge Mostar index for trees and unicyclic graphs and proposed two conjectures on the extrema of bicyclic graphs. Ali Ghalavand *et al.* [21] solved the conjecture for the lower bound of the edge Mostar index for bicyclic graphs. Liju Alex and G. Indulal [22] proposed the correct version of the conjecture for the upper bounds of bicyclic graphs and proved it. Various modified versions of the Mostar index was proposed recently [23], a particular one of interest is the additively weighted edge Mostar index. The additively weighted edge Mostar index of a graph $G = (V, E)$ is defined as:

$$MoA_e(G) = \sum_{e=xy\in E} (d(x) + d(y))|m_x(e|G) - m_y(e|G)|,$$

where $m_x(e|G)$ represents the number of edges closer to x than to y. As it was proposed in 2020, there hasn't been much study done on it. Let $\mathcal{T}_n, \mathcal{U}_n$ represent the collection of all trees, unicyclic graphs of order n respectively and $\mathcal{C}(n, t)$ denotes the collection of all cacti of order n having t cycles. In this paper, we establish bounds of additively weighted edge Mostar index of trees, unicyclic graphs and cacti and characterize the corresponding graphs. Throughout this paper, we consider only simple, connected, finite, undirected graphs.

2 Trees

In Section 2, we obtain the lower bound and upper bound of the additively weighted edge Mostar index of trees. For every edge $e = xy$ of a graph G, let $MoA_e(e|G) = (d(x) + d(y))|m_x(e|G) - m_y(e|G)|$ denotes the contribution of the edge e to the additively weighted edge Mostar index. We tweak the approach in [11] to prove the following results.

Lemma 2.1. *Let G be a graph of order $n > 2$ and size $m \geq 2$. Then for any edge $e = xy$, $|m_x(e|G) - m_y(e|G)| \leq m - 1$. Moreover, $|m_x(e|G) - m_y(e|G)| = m - 1$ if and only if $e = xy$ is a pendant edge.*

Proof. If at least one edge other than $e = xy$ is incident with both the end vertices of e, then $|m_x(e|G) - m_y(e|G)| \leq m - 3$. Thus $|m_x(e|G) - m_y(e|G)|$ is maximum when one among $m_x(e|G), m_y(e|G)$ is zero and other is $m - 1$ which is if and only if e is a pendant edge. ■

A bridge different from a pendant edge is considered as a non-pendant bridge.

Lemma 2.2. *Let $f = pq$ be a non pendant bridge on a graph G and let G_1 be the graph obtained from G by identifying the end vertices p and q to a new vertex r and by adding a new pendant edge rw. Then*

$$MoA_e(G) < MoA_e(G_1).$$

Proof. Let $|E| = m$. For every edge $e = xy$, we have $(d(x) + d(y))|G \leq (d(x) + d(y))|G_1$ with equality holds when $x \neq p, q$ or $y \neq p, q$. For every edge $e = xy \neq rw$, $|m_x(e|G) - m_y(e|G)| = |m_x(e|G_1) - m_y(e|G_1)|$. For the bridge $f = pq$, $(d(p) + d(q))|G = (d(r) + d(w))|G_1$ and $|m_p(f|G) - m_q(f|G)| < |m_r(rw|G_1) - m_w(rw|G_1)| = m - 1$. Thus for any edge e, $MoA_e(e|G) \leq MoA_e(e|G_1)$, hence the claim. ■

Theorem 2.3. *Let $G \in \mathcal{T}_n$, $n \geq 4$. Then*

(a) $MoA_e(G) \geq 2n^2 - 6n + 4$ and the equality holds if and only if $G \cong P_n$.

(b) $MoA_e(G) \leq n^3 - 3n^2 + 2n$ and the equality holds if and only if $G \cong S_n$.

Proof. $|E| = m = n - 1$. In the case of the upper bound, for each edge $e = xy$, $(d(x)+d(y))|G \leq n$ and $|m_x(e|G)-m_y(e|G)| \leq n-2$, thus the contribution of each edge should be at most $n(n-2)$. Now by Lemma 2.1, $|m_x(e|G) - m_y(e|G)| = n - 2$ if and only if the edge e is a pendant edge. Thus $MoA_e(G)$ is maximum when every edge of G is a pendant edge and hence G must be a star S_n. Now by direct computation, $MoA_e(S_n) = n(n - 1)(n - 2) = n^3 - 3n^2 + 2n$.

Now in the case of lower bound, let $G \in \mathcal{T}_n$ such that $G \ncong P_n$. Then G must have a vertex v with degree $d(v) \geq 3$ such that $G - v$ has at least two components. In each of these components take paths P', P'' of lengths p and q respectively with $p \geq q \geq 1$. Let G' be a graph obtained by removing the pendant edge of the shorter path P'' and adding a pendant edge at a pendant vertex v_p of P'. Let the newly added pendant vertex be v_{p+1}. For every edge e in G which is not incident on the vertices of P' or P'', the contribution of the edge remains unchanged by the transformation. Now consider the following cases,

Case I ($q > 2$) Those edges which lie in the paths P', P'' will contribute in the difference between the additively weighted edge Mostar index of the graphs G and G'. Thus

$$\begin{aligned} MoA_e(G) - MoA_e(G') &= (2 + d(v))(n - 2q) + 4(n - 2q + 2)) + \cdots + 3(n - 2) \\ &\quad + (2 + d(v))(n - 2p) + 4(n - 2p + 2)) + \cdots + 3(n - 2) \\ &\quad - ((2 + d(v))(n - 2q + 2) + 4(n - 2q + 4)) + \cdots + 3(n - 2)) \\ &\quad - ((2 + d(v))(n - 2p - 2) + 4(n - 2p) + \cdots + 3(n - 2)) \\ &= 8(p - q + 1) > 0. \end{aligned}$$

Case II ($q = 2$) When $p > 2$ as in the previous case, $MoA_e(G) - MoA_e(G') = 8(p - 2) > 0$ and when $p = 2$, $MoA_e(G) - MoA_e(G') = 8 > 0$.

Case III ($q = 1$) When $p > 2$ as in the previous case, $MoA_e(G) - MoA_e(G') = n(d(v) - 3) + 8p + 2 > 0$, since $d(v) \geq 3$. When $p = 2$, $MoA_e(G) - MoA_e(G') = n(d(v) - 3) + 18 > 0$, since $d(v) \geq 3$.

In all the cases G cannot attain the minimum value MoA_e. Thus P_n is the graph obtaining the minimum MoA_e. Now by direct computation, $MoA_e(P_n) = 2n^2 - 6n + 4$. ■

3 Unicyclic graphs

In Section 3, we determine the extrema of additively weighted edge Mostar index for unicyclic graphs. We use the results in the previous section to obtain the bounds of MoA_e. Let $C_{r,n-r}$ denotes the unicyclic graph consists of the cycle C_r of length r along with $n - r$ pendant edges incident at a common vertex of C_r.

Lemma 3.1. *Let e be a pendant edge of a graph G of order $n > 2$. Then $MoA_e(e|G) > 0$.*

Proof. Using the definition of MoA_e. ■

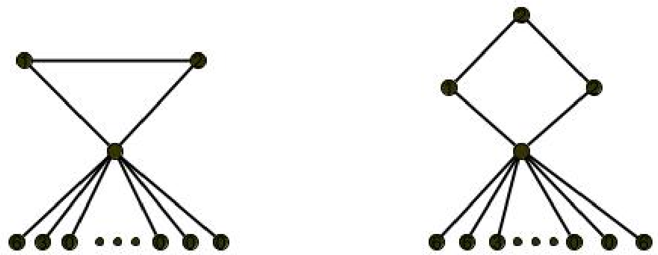

Figure 1: Graphs with largest and second largest additively weighted edge Mostar index among unicyclic graphs.

Proposition 3.2. *Let $n \geq 7$ and $r \geq 3$. Then*

$$MoA_e(C_{r,n-r}) = \begin{cases} n^3 - 2n^2r + 4n^2 + nr^2 - nr - 3n - 3r^2 + 3r, \textit{ if } r \textit{ is even,} \\ n^3 - 2n^2r + 4n^2 + nr^2 - nr - 7n - 3r^2 + 7r, \textit{ if } r \textit{ is odd.} \end{cases}$$

Proof. Let u be the common vertex in $C_{r,n-r}$ with $d(u) > 2$. When r is even, For the $(n-r)$ pendant edges, $MoA_e(e|C_{r,n-r}) = (n-r+3)(n-1)$. For the two edges in the cycle incident on u, $MoA_e(e|C_{r,n-r}) = (n-r+4)(n-r)$ and for the remaining $r-2$ edges, the contribution is $4(n-r)$ each. Thus, $MoA_e(C_{r,n-r}) = (n-r)(n-r+3)(n-1)+2(n-r+4)(n-r)+(r-2)4(n-r) = n^3-2n^2r+4n^2+nr^2-nr-3n-3r^2+3r$. Similarly, when r is odd, except for one edge in the cycle, whose contribution zero, all the other edges have the same contribution as in the previous case. Thus, $MoA_e(C_{r,n-r}) = (n-r)(n-r+3)(n-1)+2(n-r+4)(n-r)+(r-3)4(n-r) = n^3-2n^2r+4n^2+nr^2-nr-7n-3r^2+7r$. ■

Theorem 3.3. *Let $G \in \mathcal{U}_n$. Then*

(a) $MoA_e(G) \geq 0$ and the equality holds if and only if $G \cong C_n$.

(b) $MoA_e(G) \leq n^3 - 2n^2 - n - 6$ and the equality holds if and only if $G \cong C_{3,n-3}$.

Proof. $MoA_e(C_n) = 0$. Now, let $G \in \mathcal{U}_n$ be the graph with minimum additively weighted edge Mostar index. Then G cannot have any bridge, otherwise, if e is a bridge of G. Then e is part of a subtree T of G and T must have a pendant edge $e' = uv$, thus $Mo_A(e'|G) > 0$, impossible. Thus every edge of G should be part of the cycle, thus $G \cong C_n$. Also, if $G \ncong C_n$, then G must have a bridge, hence $MoA_e(G) > 0$.

Now in the case of upper bound, let G be the unicyclic graph with maximum additively weighted edge Mostar index. Then by Lemma 2.2, all the edges of the sub-tree T_i attached at the vertex v_i of the cycle in G should be pendant edges at the vertex v_i for all i. Now we proceed by establishing the following claims on G.

Claim I (All the pendant edges of G should be incident at a single vertex) Let $C_r = v_1v_2v_3\dots v_rv_1$ be the cycle of G with $t_i \geq 0$ pendant edges attached on the vertex v_i for each $i = 1, 2\dots r$ and $\sum_{i=1}^{r} t_i = t$. Let G' be the graph optained by moving all the pendant edges from $v_2, v_3 \dots v_r$ to v_1.

Case I.1 ($r = 2k$) Clearly, $n = 2k + t$. For each pendant edge f incident at v_i, we have $MoA_e(f|G) = (t_i+3)(n-1), i = 1, 2\dots r$ and for the corresponding edge in G', $MoA_e(f|G') = (t+3)(n-1)$. For each edge $f_i = v_iv_{i+1}$ in the cycle C_r, $MoA_e(f|G) = (t_i+t_{i+1}+4)(n-2-m_i)$ where m_i is the dimnishing quantity, $m_i > 0$. For the corresponding edge in G', $MoA_e(f|G') =$

$4(n-2-2(k-1))$ if $i \neq 2, r$, and for v_1v_2 and v_1v_r we have $MoA_e(f|G') = (4+t)(n-2-2(k-1))$. Let $m_0 = \min\{m_1, m_2, \dots, m_r\}$ then clearly, $m_0 \geq 2(k-1)$.

$$\begin{aligned} MoA_e(G') - MoA_e(G) &= t(t+3)(n-1) + (8k-8)(n-2k) + 2(t+4)(n-2k) \\ &\quad - \sum_{i=1}^{r} t_i(t_i+3)(n-1) - \sum_{i=1}^{r}(t_i + t_{i+1} + 4)(n-2-m_i) \\ &\geq \sum_{\substack{i,j=1 \\ i\neq j}}^{r} 2t_it_j(n-1) + 8k(m_0 - 2(k-1)) + 2t(m_0 - 2(k-1)) \\ &\geq 0. \end{aligned}$$

Case I.2 ($r = 2k+1$) Then $n = 2k+1+t$. For $t = 1$, we have nothing to prove. Let $t > 1$, then there exist i, j such that $t_i, t_j \geq 1$. The contribution of pendant edges is as in the previous case. For each edge $f_i = v_iv_{i+1}$ in the cycle C_r, $MoA_e(f|G) = (t_i + t_{i+1} + 4)(n-1-m_i-t_{i+k})$. For the corresponding edge in G', $MoA_e(f|G') = 4(n-1-2k)$ if $i \neq 2, k, r$, and for v_1v_2 and v_1v_r we have $MoA_e(f|G') = (4+t)(n-1-2k)$ and for the remaining one edge the contribution is zero. Let $m_0 = \min\{m_1, m_2, \dots, m_r\}$ then clearly, $m_0 \geq 2k$.

$$\begin{aligned} MoA_e(G') - MoA_e(G) &= t(t+3)(n-1) + (8k-8)(n-1-2k) + (2t+8)(n-1-2k) \\ &\quad - \sum_{i=1}^{r} t_i(t_i+3)(n-1) - \sum_{i=1}^{r}(t_i + t_{i+1} + 4)(n-1-m_i-t_{i+k}) \\ &\geq \sum_{\substack{i,j=1 \\ i\neq j}}^{r} 2t_it_j(n-1) + 8k(m_0 - 2k) - 4(n-1) + 2t(m_0 - 2k) \\ &\geq 0. \end{aligned}$$

Since $\sum_{\substack{i,j=1 \\ i\neq j}}^{r} 2t_it_j \geq 4$. Thus $MoA_e(G') \geq MoA_e(G)$ and all the pendant edges should be attached at a single vertex say v_1.

Claim II (The cycle is of order 3) Let $G \in \mathcal{U}_n$ with cycle $C_r = v_1v_2 \dots v_rv_1$ along with $n-r$ pendant vertices attached to the vertex v_1, $r \geq 5$. Let G' be the graph obtained by the transformation, $G' = G - v_2v_3 - v_{r-1}v_r + v_3v_1 + v_{r-1}v_1$. Then if $r = 2k$ we have

$$\begin{aligned} MoA_e(G') - MoA_e(G) &= (n-r+5)(n-r+2)(n-1) + (2k-4)4(n-2k+2) \\ &\quad + 2(n-r+6)(n-2k+2) \\ &\quad - (n-r+3)(n-r)(n-1) - (2k-2)4(n-2k) \\ &\quad - 2(n-r+4)(n-2k) \\ &= 10(n-1) + 4(n-r)(n-1) + 8(2k-3) \\ &\quad + 4(n-r+4) - 4(n-2-2(k-1)) \\ &\geq 0. \end{aligned}$$

Since $10(n-1) > 4(n-2k)$. When $r = 2k+1$

$$\begin{aligned}
MoA_e(G') - MoA_e(G) &= (n-r+5)(n-r+2)(n-1) + (2k-4)4(n-2k+1) \\
&+ 2(n-r+6)(n-2k+1) \\
&- (n-r+3)(n-r)(n-1) - (2k-2)4(n-(2k+1)) \\
&- 2(n-r+4)(n-(2k+1)) \\
&= 10(n-1) + 4(n-r)(n-1) + 8(2k-3) \\
&+ 4(n-r+4) - 4(n-1-2k) \geq 0.
\end{aligned}$$

Since $10(n-1) > 4(n-(2k+1))$.
Now by the sequential application of the above transformation, G is either of the form $C_{3,n-3}$ or of the form $C_{4,n-4}$. Now by Proposition 3.2, $MoA_e(C_{3,n-3}) = n^3 - 2n^2 - n - 6$ and $MoA_e(C_{4,n-4}) = n^3 - 4n^2 + 9n - 36$. Thus $MoA_e(C_{3,n-3}) > MoA_e(C_{4,n-4})$, the cycle in G should be C_3. Hence the claim. ■

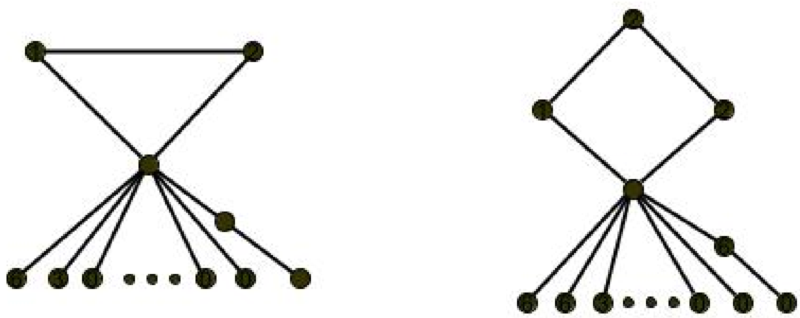

Figure 2: The graphs G_3 and G_4 in Theorem 3.5.

Let G_4 be a graph obtained by attaching $n-6$ pendant edges and a path of length 2 at a vertex to the cycle C_4.

Proposition 3.4. *Let G_3 and G_4 be graphs in $\mathcal{U}_n$ as in Figure 2 Then*

(a) $MoA_e(G_3) = n^3 - 4n^2 + 5n - 8$.

(b) $MoA_e(G_4) = n^3 - 6n^2 + 17n - 36$.

Proof. Let u be the vertex in the graph with $d(u) > 2$. For the $(n-5)$ pendant edges incident on u in G_3, the contribution is $(n-1)^2$ and for the remaining one pendant edge, the contribution is $3(n-1)$. For the 2 edges in the cycle incident on u, the contribution is $n(n-3)$ and for the non pendant bridge, the contribution is $n(n-3)$. Thus $MoA_e(G_3) = (n-5)(n-1)^2 + 3(n-1) + n(n-3) + 2n(n-3) = n^3 - 4n^2 + 5n - 8$. Similarly on G_4, For the $(n-6)$ pendant edges incident on u in G_4, the contribution is $(n-1)(n-2)$ and for the remaining one pendant edge, the contribution is $3(n-1)$. For the 2 edges in the cycle incident on u, the contribution is $(n-1)(n-4)$ and for the remaining two edges in the cycle, $MoA_e(e|G_4) = 4(n-4)$. For the non pendant bridge the contribution is $(n-1)(n-3)$. Thus, $MoA_e(G_4) = (n-6)(n-1)(n-2) + 3(n-1) + (n-1)(n-3) + 2(n-1)(n-4) + 8(n-4) = n^3 - 6n^2 + 17n - 36$. ■

Now we establish the second largest upper bound of additively weighted edge Mostar index of unicyclic graphs. Let $\mathcal{U}_n|\{H\}$ denote the collection of all unicyclic graphs of order n without the graph H.

Theorem 3.5. *Let $G \in \mathcal{U}_n|\{C_{3,n-3}\}$, $n \geq 8$. Then $MoA_e(G) \leq n^3 - 4n^2 + 9n - 36$. Moreover, equality holds if and only if $G \cong C_{4,n-4}$.*

Proof. Let $G \in \mathcal{U}_n|\{C_{3,n-3}\}$ attain the upper bound of additively weighted edge Mostar index. Then by Lemma 2.2, all the tree edges should be pendant edges and by the claims in Theorem 3.3, all the pendant edges of G should be in a single vertex and the cycle of G cannot be of length more than 5. Thus G must be one among the three graphs $G_1 = C_{4,n-4}$ or $G_2 = C_{5,n-5}$ or G_3, a graph obtained by inserting $n-5$ pendant edges and a path of length 2 at a vertex of the cycle C_3. Now by Proposition 3.2 and Proposition 3.4, $MoA_e(G_1) = n^3 - 4n^2 + 9n - 36$ and $MoA_e(G_2) = n^3 - 6n^2 + 13n - 40$ and $MoA_e(G_3) = n^3 - 4n^2 + 5n - 8$. $MoA_e(G_1) - MoA_e(G_2) = 2n^2 - 4n + 4 > 0$ and $MoA_e(G_1) - MoA_e(G_3) = 4n - 28 > 0$ and $MoA_e(G_3) - MoA_e(G_2) = 2n^2 - 8n + 32 > 0$ as $n \geq 8$. Thus $Mo_A(G) \leq n^3 - 4n^2 + 9n - 36$, with equality if and only if $G \cong C_{4,n-4}$. ∎

Using the method described in Theorem 3.5 the third and fourth largest upper bounds of additively weighted edge Mostar index of unicyclic graphs can be obtained.

Corollary 3.6. *Let $G \in \mathcal{U}_n|\{C_{3,n-3}, C_{4,n-4}\}$. Then $MoA_e(G) \leq n^3 - 4n^2 + 5n - 8$ with equality holds if and only if $G \cong G_3$.*

Corollary 3.7. *Let $G \in \mathcal{U}_n|\{C_{3,n-3}, C_{4,n-4}, G_3\}$ with $n \geq 9$. Then $MoA_e(G) \leq n^3 - 6n^2 + 17n - 36$ with equality holds if and only if $G \cong G_4$.*

4 Cacti

In Section 4, we establish the maximum value of additively weighted edge Mostar index for Cacti. Let $C_0(n,t)$ denotes the cacti bundle with t triangles and $n - 2t - 1$ pendant edges incident on a single vertex.

Lemma 4.1. *Let $G = (V, E)$ be a cacti and $C_r = v_1 v_2 ... v_r v_1$ be a cycle in G with components of $G - E(Cr)$, $G_i = (V_i, E_i)$ attached on each $v_i, i = 1, \ldots, r$. Let*

$$G' = G - \bigcup_{i=2}^{r} \bigcup_{x \in A_i} xv_i + \bigcup_{i=2}^{r} \bigcup_{x \in A_i} xv_1,$$

where $A_i = \{u \in G_i : uv_i \in E_i\}, i = 1, \ldots, r$. Then $MoA_e(G') \geq MoA_e(G)$. Moreover, equality holds if and only if $G \cong G'$.

Proof. Let $|E_i| = m_i, i = 1, 2, ..., r$ and $\sum_{i=1}^{r} m_i + r = m$. Let t_i denotes the number of edges in G_i incident to the vertex v_i and $\sum_{i=1}^{r} t_i = t$. For each edge $e = xy \in G_i, i = 1, 2, 3..., r$, every edge which is closer to x or y in G should be closer to the same vertex x or y in G' and every edge which is of equidistant from both x and y in G should be equidistant from both x and y in G'. Thus for $e = xy \in G_i$, $|m_x(e|G) - m_y(e|G)| = |m_x(e|G') - m_y(e|G')|$, $i = 1, \ldots, r$. For each edge $e = xy \in G_i$ such that $x, y \neq v_i, i = 1, \ldots, r$, $(d(x) + d(y))|G = (d(x) + d(y))|G'$. For the edges $xv_i \in G_i$, $i = 1, \ldots, r$, $(d(x) + d(v_i))|G = d(x) + t_i + 2$ and for the corresponding transformed edge in G' $(d(x) + d(v_i))|G' = d(x) + t + 2$. Then

$$\sum_{i=1}^{r} \sum_{e=xy \in G_i} (MoA_e(e|G') - MoA_e(e|G)) = \sum_{i=1}^{r} \sum_{e=xv_i \in G_i} (t - t_i)|m_{v_i}(e|G) - m_u(e|G)| > 0. \quad (1)$$

Now, for the edges $v_iv_{i+1} \in C_r$, we consider the following subcases.

Case I (r is even, $r = 2k$**)** For each edge $e_i = v_iv_{i+1} \in C_{2k}$, $i = 1, 2, ..., 2k-1$ and $e_{2k} = v_{2k}v_1$ we have $|m_{v_i}(e|G') - m_{v_{i+1}}(e|G')| = m - 2k$ and

$$\begin{aligned}&|m_{v_i}(e|G) - m_{v_{i+1}}(e|G)|\\&= ((m_i + m_{i-1} + ... + m_{i-k+1}) - (m_{i+1} + m_{i+2} + ... + m_{i+k})) = (m - a_i) \leq (m - 2k),\end{aligned}$$

where $a_i \geq 2k$. For the edge $e_i = v_iv_{i+1} \in C_{2k}, i \neq 1, 2k$, $(d(v_i) + d(v_{i+1}))|G = t_i + t_{i+1} + 4$ and $(d(v_i) + d(v_{i+1}))|G' = 4$. For the remaining two edges in C_{2k}, $(d(v_i) + d(v_{i+1}))|G = t_i + t_{i+1} + 4$ and $(d(v_i) + d(v_{i+1}))|G' = 4 + t$. Thus,

$$\begin{aligned}&\sum_{i=1}^{2k} \sum_{e=v_iv_{i+1} \in C_{2k}} (MoA_e(e|G') - MoA_e(e|G))\\&\quad = (8k + 2t)(m - 2k) - \sum_{i=1}^{2k} (t_i + t_{i+1} + 4)(m - a_i)\\&\quad \geq (8k + 2t)(m - 2k) - (8k + 2t)(m - 2k) \geq 0. \qquad (2)\end{aligned}$$

From Equations (1) and (2), $MoA_e(G') - MoA_e(G) \geq 0$ with equality if and only if there exist a j, $1 \leq j \leq 2k$ such that $m_j = m - 2k$ and $m_i = 0, \quad \forall i \neq j$. Thus, $Mo_A(G') - Mo_A(G) \geq 0$ where the equality holds whenever $G \cong G'$.

Case II (r is odd, $r = 2k+1$**)** For each edge $e_i = v_iv_{i+1} \in C_{2k+1}$, $i \neq k$ we have $|m_{v_i}(e|G') - m_{v_{i+1}}(e|G')| = m - 2k - 1$ and for $e = v_kv_{k+1}$ $|m_{v_k}(e|G') - m_{v_{k+1}}(e|G')| = 0$ and

$$\begin{aligned}|m_{v_i}(e|G) - m_{v_{i+1}}(e|G)| &= ((m_i + m_{i-1} + ... + m_{i-k+1}) - (m_{i+1} + m_{i+2} + ... + m_{i+k}))\\&= (m - b_i) \leq (m - 2k - 1 - m_{i-k}),\end{aligned}$$

where $b_i \geq 2k + 1$. For the edge $e_i = v_iv_{i+1} \in C_{2k+1}, i \neq 1, 2k+1$, $(d(v_i) + d(v_{i+1}))|G = t_i + t_{i+1} + 4$ and $(d(v_i) + d(v_{i+1}))|G' = 4$. For the remaining two edges in C_{2k+1}, $(d(v_i) + d(v_{i+1}))|G = t_i + t_{i+1} + 4$ and $(d(v_i) + d(v_{i+1}))|G' = 4 + t$. Thus,

$$\begin{aligned}&\sum_{i=1}^{2k+1} \sum_{e=v_iv_{i+1} \in C_{2k}} (MoA_e(e|G') - MoA_e(e|G))\\&= (8k + 2t)(m - 2k - 1) - \sum_{i=1}^{2k+1} (t_i + t_{i+1} + 4)(m - b_i)\\&\geq (8k + 2t)(m - 2k - 1) - \sum_{i=1}^{2k+1} (t_i + t_{i+1} + 4)(m - 2k - 1 - m_{i-k})\\&\geq -4(m - 2k - 1) + \sum_{i=1}^{2k+1} (t_i + t_{i+1} + 4)(m_{i-k})\\&\geq \sum_{i=1}^{2k+1} (t_i + t_{i+1})(m_{i-k}) \geq 0. \qquad (3)\end{aligned}$$

Since $\sum_{i=1}^{2k+1}(m_{i-k}) = (m - 2k - 1)$. From Equations (1) and (3) we have $MoA_e(G') - MoA_e(G) \geq 0$ with equality if and only if there exists a j, $1 \leq j \leq 2k + 1$ such that

$m_j = m - 2k - 1$ and $m_i = 0$, $\forall i \neq j$. Thus, $MoA_A(G') - MoA_A(G) \geq 0$ where the equality holds whenever $G \cong G'$. ■

Proposition 4.2. *Let $n \geq 7$. Then $MoA_e(C_0(n,t)) = n^3 + n^2t - 3n^2 - 3nt + 2n + 2t^2 - 8t$.*

Proof. Let u be the vertex in $C_0(n,t)$ with $d(u) > 2$. For the $(n - 2t - 1)$ pendant edges, the contribution $MoA_e(e|C_0(n,t)) = n(n + t - 2)$. For the $2t$ edges on the cycle incident on u, $MoA_e(e|C_0(n,t)) = (n + 1)(n + t - 4)$ and for the rest of the edges, the contribution is zero. Thus $MoA_e(C_0(n,t)) = (n-2t-1)n(n+t-2)+2t(n+1)(n+t-4) = n^3+n^2t-3n^2-3nt+2n+2t^2-8t$. ■

Theorem 4.3. *Let $G \in \mathcal{C}(n,t)$. Then $MoA_e(G) \leq n^3 + n^2t - 3n^2 - 3nt + 2n + 2t^2 - 8t$. Moreover, equality holds if and only if $G \cong C_0(n,t)$.*

Proof. Let $G = (V,E) \in \mathcal{C}(n,t)$ is the graph with maximum additively weighted edge Mostar index. By Lemma 2.2, all the bridges of G should be pendant edges and by Lemma 4.1 all the cycles and pendant edges should be attached to a single vertex. Now we prove that all the cycles should be of length 3.

Claim (All the cycles of G should be of length 3) Assume that $|E| = m$. Let $C_r = v_1v_2....v_rv_1$ be a cycle of G with $d(v_1) > 2$. Let G' be the graph obtained from G by the following transformation $G' = G - v_2v_3 - v_{r-1}v_r + v_3v_1 + v_{r-1}v_1$. In G' the degree of the vertex v_1 is increased by 2 and degrees of v_2 and v_r are decreased by 1. Except for v_1, v_2, v_r, the degrees of every other vertex remains the same. Also for the edge $e = uv_1$ and $u \notin C_r$, $|m_u(e|G) - m_{v_1}(e|G)| = |m_u(e|G') - m_{v_1}(e|G')|$. For the edge v_1v_2 and v_1v_r, $|m_{v_j}(e|G) - m_{v_1}(e|G)| = (m - r)$ and $|m_{v_j}(e|G') - m_{v_1}(e|G')| = (m - 1)$ for $j = 2, r$. For the edge v_1v_3 and v_1v_{r-1} in G', $|m_{v_1}(e|G') - m_{v_j}(e|G')| = (m - (r-2))$, $j = 2, r-1$. For the other edges $xy \in C_r$, $|m_x(e|G) - m_y(e|G)| = (m - r)$, $|m_x(e|G') - m_y(e|G')| = (m - (r - 2))$ when r is even. When r is odd, the contribution of $r - 1$ edges is the same as in the previous case. For the remaining one edge, $|m_x(e|G') - m_y(e|G')| = |m_x(e|G) - m_y(e|G)| = 0$. Thus

$$\begin{aligned} MoA_e(G') - MoA_e(G) = &\sum_{\substack{uv_1 \\ u \notin C_r}} 2(|m_u(e|G) - m_{v_1}(e|G)|) + 8r_0 + 4d(v_1) \\ &+ 2(d(v_1) + 3)(m - 1) - 4(m - r) > 0, \end{aligned}$$

where $r_0 = \begin{cases} r - 2, & \text{when } r \text{ is even} \\ r - 3, & \text{when } r \text{ is odd} \end{cases}$, and since $m - 1 > m - r$ and all other quantitites are positive. Thus by applying the transformation repeatedly, we conclude that every cycle of G is either of order 3 or 4. Now we will prove that the cycle should be a 3 cycle. Let $C_4 = v_1v_2v_3v_4v_1$ be the 4 cycle in G. Let $G' = G - v_2v_3 + v_1v_3$, as in the previous case for every edge $e = xy$ which is not in C_4, $|m_x(e|G') - m_y(e|G')| = |m_x(e|G) - m_y(e|G)|$. In G' degree of v_1 is increased by 1 and degree of v_2 is decreased by 1 and for all the other vertices the degree remains same. Thus:

$$\begin{aligned} MoA_e(G') - MoA_e(G) = &\sum_{\substack{uv_1 \\ u \notin C_4}} (|m_u(e|G) - m_{v_1}(e|G)|) \\ &+ 4(d(v_1) + 2) + (d(v_1) + 4)(m - 3) - 8(m - 4) > 0, \end{aligned}$$

since there is at least two cycles incidenting on v_1. i.e, $d(v_1) \geq 4$. If there is exactly one cycle at v_1, by direct calculation $MoA_e(G') - MoA_e(G) > 0$. Thus G cannot have a cycle of length

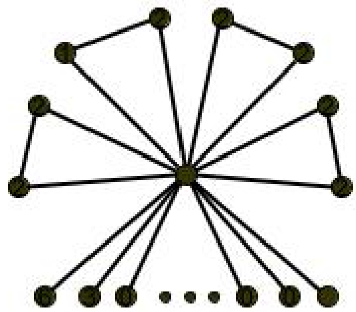

Figure 3: Graph with largest additively weighted edge Mostar index among cacti.

more than 3. Thus $G \cong C_0(n,t)$. By Proposition 4.2, $MoA_e(C_0(n,t)) = n^3 + n^2t - 3n^2 - 3nt + 2n + 2t^2 - 8t$. ■

5 Application of additively weighted edge Mostar index

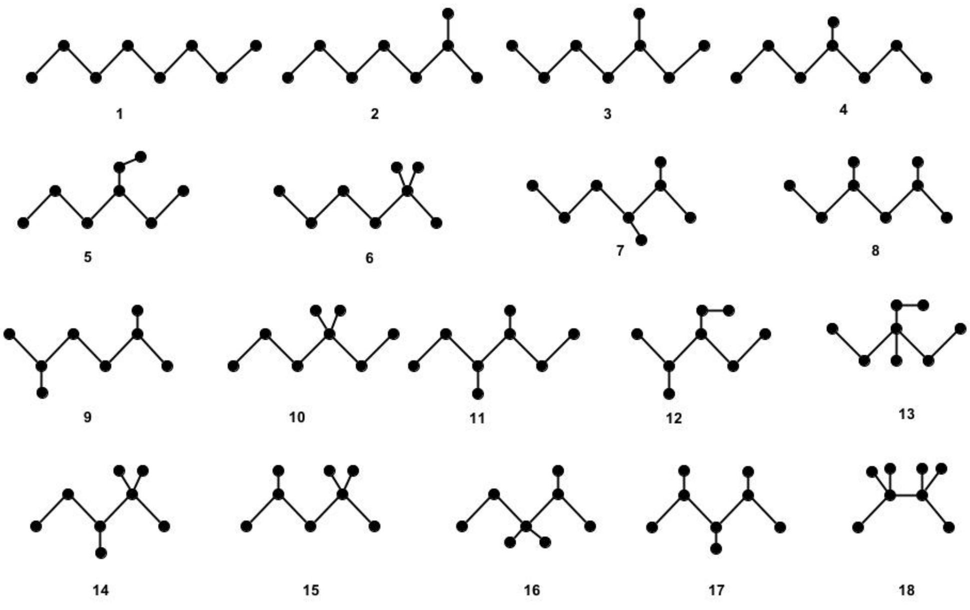

Figure 4: Octane isomers.

In this section, we examine the correlation between the additively weighted edge Mostar index and some chemical properties of octane isomers. All the experimental values of the chemical compounds are taken from [24]. The correlation between additively weighted edge Mostar index and acentric factor is about -0.9835 and the correlation between additively weighted edge

Mostar index and entropy is -0.9174. This indicates a strong linear relationship among additively weighted edge Mostar index and acentric factor, the entropy of the octane isomers. We also present a comparative study of the additively weighted edge Mostar index with some other topological indices such as Szeged index (Sz), Mostar index (Mo), edge Mostar index (Mo_e), the first eccentric connectivity index (S_1), second eccentric connectivity index (S_2), the first status connectivity index (ζ_1), second status connectivity index (ζ_2), weighted Szeged index (wSz), weighted edge Szeged index (wSz_e) and weighted PI index (wPI). We found that the additively weighted edge Mostar index is a better predictor of the acentric factor and entropy of octane isomers compared to almost all other topological indices; see Table 2.

Table 1: Acentric factor and entropy of additively weighted edge Mostar index and other topological indices of the octane isomers.

No	Acent Factor	Entropy	MoA_e	Sz	Mo	Mo_e	S_1	S_2	ζ_1	ζ_2	wSz	wSz_e	wPI
1	0.4	111.67	84	84	24	24	280	2856	74	200	322	140	196
2	0.38	109.84	100	79	26	26	260	2441	65	154	324	128	224
3	0.37	111.26	104	76	28	28	248	2224	63	144	318	122	224
4	0.37	109.32	112	75	30	30	244	2157	61	136	316	120	224
5	0.36	109.43	120	72	32	32	228	1865	56	113	306	110	224
6	0.34	103.42	132	71	30	30	224	1796	54	105	330	106	256
7	0.35	108.02	128	70	32	32	228	1853	54	105	318	108	240
8	0.34	106.98	120	71	30	30	240	2052	56	113	320	110	240
9	0.36	105.72	116	74	28	28	212	1609	52	97	326	116	240
10	0.32	104.74	148	67	34	34	216	1664	52	97	322	98	256
11	0.34	106.59	124	68	32	32	232	1940	54	105	314	104	240
12	0.33	106.06	136	67	34	34	196	1349	43	66	308	98	240
13	0.31	101.48	156	64	36	36	208	1520	45	72	314	90	256
14	0.30	101.31	152	63	34	34	192	1292	41	60	326	88	272
15	0.31	104.09	148	66	32	32	204	1461	43	66	332	94	272
16	0.29	102.06	164	62	36	36	212	1597	43	66	324	86	272
17	0.32	102.39	144	65	34	34	200	1420	41	60	320	96	256
18	0.26	93.06	180	58	36	36	176	1060	34	40	338	72	304

Table 2: Correlation coefficient (R), coefficient of determination(R^2) and standard error of estimates (SEE) between chemical properties of octane isomers and topological indices.

	Acentric Factor			Entropy		
	R	R^2	SEE	R	R^2	SEE
MoA_e	-0.9835	0.9674	0.0065	-0.9174	0.8415	1.8537
Sz	0.9732	0.9471	0.0083	0.8778	0.7705	2.2308
Mo	-0.8874	0.7874	0.0166	-0.7549	0.5699	3.0539
Mo_e	-0.8874	0.7874	0.0166	-0.7549	0.5699	3.0539
S_1	0.8823	0.7785	0.0170	0.8545	0.7301	2.4193
S_2	0.8787	0.7721	0.0172	0.8382	0.7026	2.5395
ζ_1	0.9328	0.8701	0.0130	0.8779	0.7707	2.2300
ζ_2	0.9157	0.8384	0.0145	0.8458	0.7153	2.4845
wSz	-0.4161	0.1732	0.0328	-0.5597	0.3133	3.8588
wSz_e	0.9845	0.9693	0.0063	0.9046	0.8184	1.9844
wPI	-0.9629	0.9271	0.0097	-0.9543	0.9107	1.3917

Figure 5: Graphs with smallest and largest additively weighted edge Mostar index among bicyclic graphs.

6 Conclusion

The additively weighted edge Mostar index is a recently defined topological index, and as a result, only a few studies are available in the literature. In this paper, we have computed the extrema of additively weighted edge Mostar index for trees and unicyclic graphs. We also found the upper bound of the additively weighted edge Mostar index for cacti of a given order. We propose the following problems for further studies:

Let $\Theta_{a,b,c}$ be the bicyclic graph with two vertices x and y of degree 3 having three paths of lengths a, b, c respectively connecting x and y. Let $\phi_{a,b,c}$ is a bicyclic graph with two cycles of lengths a and b incident on a vertex x along with c pendant edges attached at x. We propose the following conjectures on additively weighted edge Mostar index of bicyclic graphs.

Conjecture 6.1. *Let G be a bicyclic graph of order $n \geq 5$. Then $MoA_e(G) \geq 8n - 8$, equality holds if and only if $G \cong \Theta_{n-3,2,2}$.*

Conjecture 6.2. *Let G be a bicyclic graph of order $n \geq 5$. Then $MoA_e(G) \leq n^3 - n^2 - 4n - 8$, equality holds if and only if $G \cong \phi_{3,3,n-5}$.*

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

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References

[1] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20, https://doi.org/10.1021/ja01193a005.

[2] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes NY*, **27** (1994) 9–15.

[3] G. Indulal, L. Alex and I. Gutman, On graphs preserving PI index upon edge removal, *J. Math. Chem.* **59** (2021) 1603–1609, https://doi.org/10.1007/s10910-021-01255-1.

[4] P. V. Khadikar, N. V. Deshpande, P. P. Kale, A. Dobrynin, I. Gutman and G. Domotor, The Szeged index and an analogy with the Wiener index, *J. Chem. Inf. Comput. Sci.* **35** (1995) 547–550, https://doi.org/10.1021/ci00025a024.

[5] S. Klavžar, A. Rajapakse and I. Gutman, The Szeged and the Wiener index of graphs, *Appl. Math. Lett.* **9** (1996) 45–49, https://doi.org/10.1016/0893-9659(96)00071-7.

[6] F. Movahedi, M. H. Akhbari and H. Kamarulhaili, On the hosoya index of some families of graph, *Math. Interdisc. Res.* **6** (2021) 225–234, https://doi.org/10.22052/MIR.2021.240266.1238.

[7] I. Rezaee Abdolhosseinzadeh, F. Rahbarnia and M. Tavakoli, Sombor index under some graph products, *Math. Interdisc. Res.* **7** (2022) 331–342, https://doi.org/10.22052/MIR.2022.246533.1362.

[8] R. Sharafdini, M. Azadimotlagh, V. Hashemi and F. Parsanejad, On eccentric adjacency index of graphs and trees, *Math. Interdisc. Res.* **8** (2023) 1–17, https://doi.org/10.22052/MIR.2023.246384.1391.

[9] S. Simić, I. Gutman and V. Baltić, Some graphs with extremal Szeged index, *Math. Slovaca* **50** (2000) 1–15.

[10] B. Zhou, X. Cai and Z. Du, On Szeged indices of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 113–132.

[11] T. Došlić, I. Martinjak, R. Škrekovski, S. Tipurić Spužević and I. Zubac, Mostar index, *J. Math. Chem.* **56** (2018) 2995–3013, https://doi.org/10.1007/s10910-018-0928-z.

[12] A. Ali and T. Došlić, Mostar index: results and perspectives, *Appl. Math. Comput.* **404** (2021) #126245, https://doi.org/10.1016/j.amc.2021.126245.

[13] N. Ghanbari and S. Alikhani, Mostar index and edge Mostar index of polymers, *Comp. Appl. Math.* **40** (2021) 1–21, https://doi.org/10.1007/s40314-021-01652-x.

[14] L. Alex and G. Indulal, Sharp bounds on additively weighted Mostar index of cacti, *Commun. Comb. Optim.* In press, https://doi.org/10.22049/CCO.2024.28757.1702.

[15] L. Alex and I. Gutman, On the inverse Mostar index problem for molecular graphs, *Trans. Comb.* **14** (2025) 66–77.

[16] F. Hayat and B. Zhou, On cacti with large Mostar index, *Filomat* **33** (2019) 4865–4873, https://doi.org/10.2298/FIL1915865H.

[17] A. Tepeh, Extremal bicyclic graphs with respect to Mostar index, *Appl. Math. Comput.* **355** (2019) 319–324, https://doi.org/10.1016/j.amc.2019.03.014.

[18] M. Arockiaraj, J. Clement and N. Tratnik, Mostar indices of carbon nanostructures and circumscribed donut benzenoid systems, *Int. J. Quantum Chem.* **119** (2019) #e26043, https://doi.org/10.1002/qua.26043.

[19] M. Imran, S. Akhter and Z. Iqbal, Edge Mostar index of chemical structures and nanostructures using graph operations, *Int. J. Quantum Chem.* **120** (2020) #e26259, https://doi.org/10.1002/qua.26259.

[20] H. Liu, L. Song, Q. Xiao and Z. Tang, On edge Mostar index of graphs, *Iranian J. Math. Chem.* **11** (2020) 95–106, https://doi.org/10.22052/IJMC.2020.221320.1489.

[21] A. Ghalavand, A. R. Ashrafi and M. Hakimi-Nezhaad, On Mostar and edge Mostar indices of graphs, *J. Math.* (2021) #6651220, https://doi.org/10.1155/2021/6651220.

[22] L. Alex and G. Indulal, On a conjecture on edge Mostar index of bicyclic graphs, *Iranian J. Math. Chem.* **14** (2023) 97–108, https://doi.org/ 10.22052/IJMC.2023.248632.1680.

[23] S. Brezovnik and N. Tratnik, General cut method for computing Szeged-like topological indices with applications to molecular graphs, *Int. J. Quantum Chem.* **121** (2021) #e26530, https://doi.org/10.1002/qua.26530.

[24] K. Deng and S. Li, On the extremal values for the Mostar index of trees with given degree sequence, *Appl. Math. Comput.* **390** (2021) #125598, https://doi.org/10.1016/j.amc.2020.125598.