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# On weighted vertex and edge Mostar index for trees and cacti with fixed parameter

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**Abstract.** It was introduced by Došlić and Ivica et al. (*Journal of Mathematical chemistry*, 56(10) (2018): 2995–3013), as an innovative graph-theoretic topological identifier, the Mostar index is significant in simulating compounds thermodynamic properties in simulations, which is defined as sum of absolute values of the differences among $n_u(\mathrm{e}|\Omega)$ and $n_v(\mathrm{e}|\Omega)$ over all lines $\mathrm{e} = uv \in \Omega$, where $n_u(\mathrm{e}|\Omega)$ (resp. $n_v(\mathrm{e}|\Omega)$) is the collection of vertices of $\Omega$ closer to vertex $u$ (resp. $v$) than to vertex $v$ (resp. $u$). Let $\mathbb{C}(n,k)$ be the set of all $n$-vertex cactus graphs with exactly $k$ cycles and $T(n,d)$ be the set of all $n$-vertex tree graphs with diameter $d$.
It is said that a cactus is a connected graph with blocks that comprise of either cycles or edges. Beginning with the weighted Mostar index of graphs, we developed certain transformations that either increase or decrease the index. To advance this analysis, we determine the extreme graphs where the maximum and minimum values of the weighted edge Mostar index are accomplished. Moreover, we compute the maximum weighted vertex Mostar invariant for trees with order $n$ and fixed diameter $d$.

**2020 Mathematics Subject Classifications**: 05C05, 05C35, 05C12, 05C92

**Key Words and Phrases**: Weighted Mostar index, Trees, Diameter, Extremal values, Cactus graphs

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## 1. Introduction

Graph theory is a subfield of mathematics that studies the properties of graphs. It is currently being applied in a variety of scientific disciplines including chemistry, engineering, and physics. Graph theory can be used to model and study various problems and phenomena in mathematics, computer science, biology, sociology, and operations research. One of the tools that graph theory provides is the concept of topological descriptors, which are numerical values that capture some aspects of the structure and properties of graphs.

Quantitative structure-property/ quantitative structure-activity relationship (QSPR/QSAR) schemes are utilized as regression models in reticular chemistry to correlate with various of biological and physicochemical activities. Harold Wiener [31] pioneered a novel way to estimate the boiling point of alkanes from their molecular shape. He converted the chemical structure into a single number that reflected its characteristics. This number, called a topological descriptor or index, was obtained from a chemical graph, a simplified representation of an organic molecule as a network of atoms and bonds. This technique also enables us to model many other properties of molecules, such as their behavior under extreme conditions, their energy release or absorption, and their interaction with living systems [4, 35]. In this study, we apply topological descriptors to develop robust regression models for these properties.

Topological descriptors play a crucial role in the definitional work done in the chemical sciences, mathematical chemistry, chemical graph theory, and pharmaceutical science; for example, topological indices for bond connectivity are used to quantify properties like branching, compactness, centrality, regularity, variability, bioactivity, etc [27]. There are remarkable subclasses of indices known as vertex and edge bond-additive indices or degree based indices that attempt to capture some valuable aspects of complete graphs by adding up the contributions of individual vertices and/or edges. It garnered a lot of interest in the context of complex networks and in more traditional chemical graph theory applications. A distance based index is a invariant based on the distance between the vertices or edges of any graph [20].

Wiener [32] introduced the first graph index based on distance between vertices of a graph, which is described as

$$W(\Omega) = \sum_{u,v \in V(\Omega)} d_{\Omega}(u, v),$$

where $d_{\Omega}(u, v)$ represents the shortest distance between $u$ and $v$. Many researchers have been exclusively studied the Wiener index and mostly characterize the sharp lower and upper bounds for different graph families which can be read in [5, 8, 10, 33] and then research extend to discover the new form of Wiener index named polarity index $W_P(\Omega)$, which is restricted to distance 3 among all unordered pairs of vertices in $\Omega$. The applications and detailed classification of Wiener polarity index have been discussed in [18, 22].

Consider an edge $\mathrm{e} = uv \in \Omega$ and the following three sets defined as $N_u(\mathrm{e}) = \{k \in V_{\Omega} : d(u, k) < d(v, k)\}$, $N_v(\mathrm{e}) = \{k \in V_{\Omega} : d(v, k) < d(u, k)\}$, $N_o(\mathrm{e}) = \{k \in V_{\Omega} : d(u, k) = d(v, k)\}$. Thus, the divisions of nodes in $\Omega$ with respect to edge e are represented by

$[N_u(\mathrm{e}), N_v(\mathrm{e}), N_o(\mathrm{e})]$. The collection of vertices in $N_u(\mathrm{e})$, $N_v(\mathrm{e})$ and $N_o(\mathrm{e})$ are symbolized by $n_u(\mathrm{e}|\Omega)$, $n_v(\mathrm{e}|\Omega)$, and $n_o(\mathrm{e}|\Omega)$, respectively. The mathematical term of Wiener index is explained as follows [3],

$$W_{\mathrm{e}}(\Omega) = \sum_{uv \in E(\Omega)} n_u(\mathrm{e}|\Omega) n_v(\mathrm{e}|\Omega),$$

where all right-hand side sums have $n-1$, and their individual values can be roughly estimated. Mostar index was recently introduced by Doslić et al. (*Journal of Mathematical chemistry*, 56(10) (2018): 2995–3013), which is defined as

$$Mo_v(\Omega) = \sum_{uv \in E(\Omega)} |n_u(\mathrm{e}|\Omega) - n_v(\mathrm{e}|\Omega)|,$$

where $n_u(\mathrm{e}|\Omega)$ (resp. $n_v(\mathrm{e}|\Omega)$) is the collection of vertices of $\Omega$ closer to vertex $u$ (resp. $v$) than to vertex $v$ (resp. $u$).

Arockiaraj and Clement, et al. (*SAR and QSAR in Environmental Research*, 31(3) (2020): 187–208) have recently proposed two new topological indices in this vein, the weighted edge Mostar index and the weighted vertex Mostar index, which are defined as

$$Mo_v^w(\Omega) = \sum_{uv \in E(\Omega)} (d_\Omega(u) + d_\Omega(v)) |n_u(\mathrm{e}|\Omega) - n_v(\mathrm{e}|\Omega)|,$$

$$Mo_{\mathrm{e}}^w(\Omega) = \sum_{uv \in E(\Omega)} (d_\Omega(u) + d_\Omega(v)) |m_u(\mathrm{e}|\Omega) - m_v(\mathrm{e}|\Omega)|,$$

where $m_u(\mathrm{e}|\Omega)$ (resp. $m_v(\mathrm{e}|\Omega)$) is the collection of edges of $\Omega$ closer to vertex $u$ (resp. $v$) than to vertex $v$ (resp. $u$). Many researchers have been extensively worked on different distance based indices, see [1, 6, 11, 16, 17, 36]. Motivated by the success of previous research, Došlić and Ivica et al. recently introduced Mostar invariant (*Journal of Mathematical chemistry*, 56(10) (2018): 2995–3013), which belongs to bond-additive indices as they capture the relevant properties of a graph. Many research works have been done on Mostar index, read [13, 14, 23, 25].

A graph is said to be cactus if all of its vertices must be either edges or cycles, and no two cycles can share more than one vertex. Readers can read many works on cactus graph herein [9, 21, 28–30]. Extremal bicyclic graphs were obtained by Tepeh with respect to the Mostar index [26], while extremal catacondensed benzenoids were established by Deng [12]. There are a number of different conclusions and points of view that can be drawn from the Mostar index, which are all explained by Ali [2]. Imran et al., [19] computed Weighted Mostar Invariants of Phthalocyanines, Triazine-Based and Nanostar Dendrimers. Brezovnik [7] studied Szeged and Mostar root-indices of graphs.

Consider $\mathbb{C}(n, k)$, the collection of all cactus graphs with $n$ vertices and $k$ cycles. Inspired by the existing literature on cactus graphs and weighted edge Mostar index, we extend the previous results to a more general setting by using the extremal graphs as an illustrative example. We then establish an upper bound for the weighted edge Mostar index and identify the extremal graph among all the graphs in $\mathbb{C}(n,k)$. Let $T(n,d)$ denote the set of tree graphs with $n$ vertices and diameter $d$. Let $\widehat{T(n,d)} \in T(n,d)$ be the special tree graph with diameter $d$ and $n-d-1$ pendent vertices attached to a fixed vertex. Finally, we determine the maximum value of the weighted vertex Mostar index over all the tree graphs.

## 2. Preliminaries results and Notations

Here, we only deal with simple finite connected graphs. Other notations can be studied in [15]. Let $\Omega$ be a connected graph comprises vertex set $V(\Omega)$ and edge set $E(\Omega)$. For an edge $uv \in E(\Omega)$, the graph $\Omega - uv$ is obtained by removing $uv \in E(\Omega)$ from $\Omega$. For any vertex $u \in V(\Omega)$, let $N_u(\Omega)$ represents the number of edges incidents to $u$ in $\Omega$ and $d_\Omega(u) = |N_u(\Omega)|$ represents the degree of $u$. A vertex with exactly one degree is called pendant. A cut vertex of a graph is any vertex that when it removed the number of connected components of this graph increases. Similarly, An edge is called cut edge if, by deleting that edge, the graph is converted into exactly two components. Consider that $\mathbb{P}_n$, $\mathbb{S}_n$, $\mathbb{C}_n$ and $\mathbb{K}_n$ the path, star, cycle, and complete graph with $n$ vertices, respectively.

Let $\mathbb{S}_n$ be the star of order $n$. Denote by $\mathbb{S}_n^*$ the graph generated by associating one new edge among the leaves of the star $\mathbb{S}_n$. Let $\mathbb{S}_n^{*,k}$ be the generated graph of order $n$ constructed by associating $k$ new edges between the leaves in a star $\mathbb{S}_n$. In particular, $\mathbb{S}_n^*$ is just $\mathbb{S}_n^{*,1}$.

**Theorem 1.** *[34] Let $\Omega \in \mathbb{C}(n,k)$ be a connected graph. Then*

*(i) for $n \geq 10$ and $n < 4k$ then $Mo_e(\Omega) \leq 2n^2 - 8n + (24-4n)k$ with equality if and only if $\Omega \cong \Omega^n(\underbrace{3,3,3...,3}_{4k-n}, \underbrace{4,4,4,...,4}_{n-3k})$.*

*(ii) for $n \geq 10$ and $n \geq 4k$ then $Mo_e(\Omega) \leq n^2 - n - 12k$ with equality if and only if $\Omega \cong \Omega^n(4,4,4,...,4)$.*

*(iii) for $n = 9$, then $Mo_e(\Omega) \leq 72 - 12k$ with equality if and only if $\Omega \cong \Omega_9$.*

*(iv) for $n \leq 9$, then $Mo_e(\Omega) \leq n^2 - n - (n+3)k$ with equality if and only if $\Omega \cong \Omega^n(3,3,3,...,3)$.*

The second maximum edge Mostar index for $\mathbb{C}(n,k)$ with the following given conditions determined by Liu et al [24].

**Theorem 2.** *[34] Let $\widehat{\mathbb{C}(n,k)} \in \mathbb{C}(n,k)$ be a connected graph achieving maximum edge Mostar index for $n \geq 3k+2$, $k \geq 2$ and $n \geq 9$, $k = 1$. For any $\Omega \in \mathbb{C}(n,k)$, we have $Mo_e(\Omega) < Mo_e(\widehat{\mathbb{C}(n,k)})$.*

**Lemma 1.** *[2] Suppose that $\Omega$ is a connected graph and $K$ is an induced subgraph of $\Omega$ such that $K$ is a tree and connected with $\Omega$ by cut vertex $u$. Consider that $K$ transform* *to star graph centered at u, then Weighted vertex index $Mo_v^w(\Omega)$ increases (unless K is already such a star). Similarly, if K transform to path graph with end vertex u, then weighted vertex index $Mo_v^w(\Omega)$ decreases.*

## 3. Main results

In this section, we present our main results of this paper. More precisely, we have the following two results.

**Theorem 3.** *Among all the tree graphs in $T(n,d)$ the $T(\widehat{n,d})$, for $n \geq d+1$ and $d \geq 6$ has maximum weighted vertex Mostar index. Thus for any $\Omega \in T(n,d)$, we have*

$$Mo_v^w(\Omega) < Mo_v^w(T(\widehat{n,d}))$$

We have following result by using Theorem 3.

**Corollary 1.** *Let $\Omega \in T(n,d)$ be the tree graph with $n \geq 2$ and $d \geq 2$, then we have the following.*

$$Mo_v^w(\Omega) = \begin{cases} n^3 - 3n^2 + 2n & n \geq d+1,\ d = 2 \\ n^3 - 5n^2 + 10n - 12 & n \geq d+1,\ d = 3 \\ n^3 - (2m+1)n^2 + d^2 + 5d - 4 - 12(n-12) & n \geq d+1,\ m \geq 1, \text{ and } d \geq 6 \end{cases} \tag{1}$$

**Theorem 4.** *For any graph $\Omega \in \mathbb{C}(n,k)$ where $n \geq 2k+1$,*

$$Mo_{\mathrm{e}}^w(\Omega) \leq n^3 + (k-4)n^2 + (-3k+5)n - (2n+4), \forall n \geq 1$$

*with the equality holds if and only if $\Omega \cong \mathbb{S}_n^{*,k}$.*

## 4. Proof of main results

First of all, some basic lemmas are proved so that the main result can be proved easily. In Lemma 2, we establish a graph $\Omega_2$ by converting a cut edge $uv$ into a pendent edge $uv$ in $\Omega_1$, such that the new graph $\Omega_2$ has a greater weighted vertex Mostar invariant.

**Lemma 2.** *Suppose that two subgraphs $T_1$ and $T_2$ such that connected by an edge $uv$, where $u \in V(T_1)$ and $v \in V(T_2)$, and acquired the graph $\Omega_1$. Now, we construct the new graph $\Omega_2$ by deleting the cut edge $uv$ and associating a pendent edges at central vertex in $\Omega_1$. Then $Mo_v^w(\Omega_1) < Mo_v^w(\Omega_2)$.*

*Proof.* Suppose $T_1$ and $T_2$ be subgraphs of $\Omega_1$. By construction of $\Omega_2$, the number of closer vertices of end vertices of the fixed edge of $T_1$ and $T_2$ in $\Omega_1$ remains same in $\Omega_2$, respectively. Therefore, for an edge $xy \in E(T_m)$ for $m \in \{1,2\}$, we have $n_x(\mathrm{e}|\Omega_1)(x) = n_x(\mathrm{e}|\Omega_2)(x)$ and $n_y(\mathrm{e}|\Omega_1)(y) = n_y(\mathrm{e}|\Omega_2)(y)$.

For the cut edge $uv$ in $\Omega_1$, we have $n_u(\mathrm{e}|\Omega_1)(u) = n_v(\mathrm{e}|\Omega_1)(v) = |E(T_1)| + 1$. Similarly for graph $\Omega_2$, $n_u(\mathrm{e}|\Omega_2)(u) = |E(T_1)| + |E(T_2| + 1$ and $n_v(\mathrm{e}|\Omega_2)(v) = 1$.

By using the definition of weighted vertex Mostar index, we have

$$Mo_v^w(\Omega) = \sum_{e=uv\in E(\Omega)} (d_\Omega(u) + d_\Omega(v))|n_u(\mathrm{e}|\Omega)(v) - n_v(\mathrm{e}|\Omega)(v)|,$$

$$\begin{aligned} Mo_v^w(\Omega_1) - Mo_v^w(\Omega_2) &= (d_\Omega(u) + d_\Omega(v))|n_u(\mathrm{e}|\Omega_1)(u) - n_v(\mathrm{e}|\Omega_1)(u)| \\ &+ \sum_{m=1}^{2} \sum_{xy\in E(T_1)} (d_\Omega(x) + d_\Omega(y))|n_x(\mathrm{e}|\Omega_1)(x) - n_y(\mathrm{e}|\Omega_1)(y)| \\ &- (d_\Omega(u) + d_\Omega(v))|n_u(\mathrm{e}|\Omega_2)(u) - n_v(\mathrm{e}|\Omega_2)(v)| \\ &- \sum_{m=1}^{2} \sum_{xy\in E(T_2)} (d_\Omega(x) + d_\Omega(y))|n_x(\mathrm{e}|\Omega_2)(x) - n_y(\mathrm{e}|\Omega_2)(y)|, \\ &= |\{E(T_1) + 1\} - \{E(T_2) + 1\}| + \sum_{m=1}^{2} \sum_{xy\in E(T_1)} |n_x(\mathrm{e}|\Omega_1(x) - n_y(\mathrm{e}|\Omega_1)(y)| \\ &- |\{E(T_1) + E(T_1) + 1\} - \{1\}| - \sum_{m=1}^{2} \sum_{xy\in E(T_2)} |n_x(\mathrm{e}|\Omega_2)(x) - n_y(\mathrm{e}|\Omega_2)(y)|, \\ &= -|E(T_1)| - |E(T_2)|, \end{aligned}$$

There are two cases, if

**Case 1.** $|E(T_1)| \geq |E(T_2)|$, *then* $-2|E(T_2)| < 0$,

**Case 2.** $|E(T_2)| \geq |E(T_1)|$, *then* $-2|E(T_1)| < 0$,

In each case,

$$Mo_v^w(\Omega_1) - Mo_v^w(\Omega_2) < 0,$$

which shows maximum weighted vertex moster index. This completes the proof.

Further, we deduce new $\Omega_2$ from $\Omega_1$ moving all the pendent vertices to a central vertices such that new graph has maximum weighted vertex moster index.

**Lemma 3.** *Let $T_1$ and $T_2$ be two subgraphs constructed by adjoining $n - d - 1$ pendent vertices at central vertices with* d *(with even diameter). Consider that two subgraphs $T_1$ and $T_2$ with common $u_kv_k$ edge between them, presented by $\Omega_1$. Now construct $\Omega_2$ from $\Omega_1$ by removing all pendent vertices and $u_kv_k$ edge to central vertex. Then $Mo_v^w(\Omega_1) < Mo_v^w(\Omega_2)$.*

*Proof.* Suppose $T_1$ and $T_2$ be subgraphs of $\Omega_1$. By construction of $\Omega_2$, the number of closer vertices of end vertices of the fixed edge of $T_1$ and $T_2$ in $\Omega_1$ remains same in $\Omega_2$ respectively. Therefore, for an edge $xy \in E(T)$, $n_x(\mathrm{e}|\Omega_1)(x) = n_x(\mathrm{e}|\Omega_2)(x)$ and $n_y(\mathrm{e}|\Omega_1)(y) = n_y(\mathrm{e}|\Omega_2)(y)$ The cut edge $u_kv_k$ in $\Omega_1$ follows as,

**Case 3.** $d_{u_k} = d_{v_k} = (n-d)+1$, *and* $n_{u_k}(\mathrm{e}|\Omega_1)(u_k) = [E(T_1)+2$, $n_{v_k}(\mathrm{e}|\Omega_1)(v_k) = E(T_2)+2$.

Furthermore, pendent edges at central vertices in $\Omega_1$ connected with $u_k$ are following as:

**Case 4.** $d_{u_k} = d_{v_k} = (n-d)+1$, *and* $n_{u_k}(\mathrm{e}|\Omega_1)(u_k) = n_{v_k}(\mathrm{e}|\Omega_1)(v_k) = [E(T)+E(T)]+3$, $d_{a_k^*} = d_{b_k^*} = 1$, *for some* $1 \le k \le n-d-1$.

Similarly, $2n-2d-1$ pendent vertices at central vertex in $\Omega_2$ by removing pendent vertices and cut edge from $\Omega_1$. Now, the pendent edges $uv_k^*$, where $1 \le k \le 2n-2d-1$ at central vertex of $\Omega_2$.

**Subcase 1.** $n_u(\mathrm{e}|\Omega_2)(u) = |E(T_1)+2|$, *and* $n_{v_k^*}(\mathrm{e}|\Omega_2)(v_k^*) = 1$.

By combining Cases 3,4 and subcase 1, and employing definition of weighted vertex Mostar index, we have

$$\begin{aligned}
Mo_v^w(\Omega_1) - Mo_v^w(\Omega_2) &= \Bigg[\sum_{m=1}^{2}\sum_{xy\in E(T_1)} (d_{\Omega_1}(x)+d_{\Omega_1}(y))|n_x(\mathrm{e}|\Omega_1)(x) - n_y(\mathrm{e}|\Omega_1)(y)| \\
&+ \sum_{k=1}^{n-d-1} (d_{\Omega_1}(a_k^*)+d_{\Omega_1}(u_k))|n_{a_k^*}(\mathrm{e}|\Omega_1)(a_k^*) - n_{u_k}(\mathrm{e}|\Omega_1)(u_k)| \\
&+ \sum_{k=1}^{n-d-1} (d_{\Omega_1}(b_k^*)+d_{\Omega_1}(v_k))|n_{b_k^*}(\mathrm{e}|\Omega_1)(b_k^*) - n_{v_k}(\mathrm{e}|\Omega_1)(v_k)|\Bigg] \\
&- \Bigg[\sum_{m=1}^{2}\sum_{xy\in E(T_1)} (d_{\Omega_2}(x)+d_{\Omega_2}a(y))|n_x(\mathrm{e}|\Omega_2)(x) - n_y(\mathrm{e}|\Omega_2(y)| \\
&- \sum_{k=1}^{2n-2d-1} (d_{\Omega_2}(u)+d_{\Omega_2}(v_k^*))|n_{v_k^*}(\mathrm{e}|\Omega_2)(v_k^*) - n_u(\mathrm{e}|\Omega_2(u)|\Bigg], \\
&\le \Bigg[\{(n-d)+2\}(E(T_1)-E(T_2)-2) + \{(n-d)+2\}(E(T_1)+E(T_2)+1)\Bigg], \\
&= \Bigg[\{(n-d)+2\}(-1)\Bigg], \\
&< 0
\end{aligned}$$

It shows, $Mo_v^w(\Omega_1) - Mo_v^w(\Omega_2) < 0$, which shows proof is complete.

**Corollary 2.** *Consider* $\Omega$ *be the graph with even diameter and* $T$ *be subgraph of* $\Omega$*, which is presented by* $\Omega_1$*. To construct* $\Omega_2$ *from* $\Omega_1$*, remove both pendent vertices connected with cut edge and attach at central vertex of* $T$*. Then* $Mo_v^w(\Omega_1) < Mo_v^w(\Omega_2)$

*Proof.* Suppose two subgraphs in $\Omega_1$ say, $T_1$ and $T_2$. By construction of $\Omega_2$, the number of closer vertices of end vertices of the fixed edge of $T_1$ and $T_2$ in $\Omega_1$ remains same in $\Omega_2$, respectively. Therefore, for an edge $xy \in E(T_r)$, where $r \in \{1,2\}$ we have $n_x(\mathrm{e}|\Omega_1)(x) = n_x(\mathrm{e}|\Omega_2)(x)$ and $n_y(\mathrm{e}|\Omega_1)(y) = n_y(\mathrm{e}|\Omega_2)(y)$. The number of closed vertices of a fixed vertex of $T$ in $\Omega_1$ is $d$ and $d-1$ in $\Omega_2$. The following case for cut edge $uv \in E(\Omega_1)$.

**Case 5.** *$d_u = d_v = 3$, and $n_u(\mathrm{e}|\Omega_1)(u) = E(T)+1$, $n_v(\mathrm{e}|\Omega_1)(v) = 3$.*

Similar results for pendent vertices adjoining at vertex $u$.

**Case 6.** *$n_v(\mathrm{e}|\Omega_1)(v) = E(T)+3$, and $n_{u_1^*}(\mathrm{e}|\Omega_1)(u_1^*) = n_{u_2^*}(\mathrm{e}|\Omega_1)(u_2^*) = 1$.*

There are following cases in $\Omega_2$, for pendent edges $uv \in E(\Omega_2)$.

**Case 7.** *$d_u = 3$, $d_v = d_{u_2^*} = d_{u_1^*} = 1$.*

**Case 8.** *$n_u(\mathrm{e}|\Omega_2)(u) = E(T)+3$, and $n_v(\mathrm{e}|\Omega_2)(v) = n_{u_1^*}(\mathrm{e}|\Omega_2)(u_1^*) = n_{u_2^*}(\mathrm{e}|\Omega_2)(u_2^*) = 1$.*

By combining Cases 5, 6, 7 and 8, and employing definition of weighted vertex Mostar index, we have,

$$
\begin{aligned}
Mo_v^w(\Omega_1) - Mo_v^w(\Omega_2) = \Bigg[ &\sum_{m=1}^{2} \sum_{xy \in E(T_1)} (d_{\Omega_1}(x) + d_{\Omega_1}(y))|n_x(\mathrm{e}|\Omega_1)(x) - n_y(\mathrm{e}|\Omega_1)(y)| \\
&+ (d_{\Omega_1}(u) + d_{\Omega_1}(v))|n_v(\mathrm{e}|\Omega_1)(v) - n_u(\mathrm{e}|\Omega_1)(u)| \\
&+ (d_{\Omega_1}(u_1^*) + d_{\Omega_1}(v))|n_{u_1^*}(\mathrm{e}|\Omega_1)(u_1^*) - n_v(\mathrm{e}|\Omega_1)(v)| \\
&+ (d_{\Omega_1}(u_2^*) + d_{\Omega_1}(v))|n_{u_2^*}(\mathrm{e}|\Omega_1)(u_2^*) - n_v(\mathrm{e}|\Omega_1)(v)| \\
&- (d_{\Omega_2}(v) + d_{\Omega_2}(u))|n_v(\mathrm{e}|\Omega_2)(v) - n_u(\mathrm{e}|\Omega_2)(u)| \\
&- (d_{\Omega_2}(u_1^*) + d_{\Omega_2}(u))|n_{u_1^*}(\mathrm{e}|\Omega_2)(u_1^*) - n_u(\mathrm{e}|\Omega_2)(u)| \\
&- (d_{\Omega_2}(u_2^*) + d_{\Omega_2}(u))|n_{u_2^*}(\mathrm{e}|\Omega_2)(u_2^*) - n_u(\mathrm{e}|\Omega_2)(u)| \\
&- \sum_{r=1}^{2} \sum_{xy \in E(T_2)} (d_{\Omega_2}(x) + d_{\Omega_2}(y))|n_x(\mathrm{e}|\Omega_2)(x) - n_y(\mathrm{e}|\Omega_2)(y)| \Bigg], \\
&= \Bigg[(3+3)(|3-|E(T)|-1|) + (3+1)(|1-|E(T)|-3|) + (3+1)(|1-|E(T)|-3|) \\
&- (3+1)(|1-|E(T)|-3|) - (3+1)(|1-|E(T)|-3|) - (3+1)(|1-|E(T)|-3|)\Bigg], \\
&\leq -6|E(T)| + 4|E(T)| + 20, \\
&< 0
\end{aligned}
$$

It shows, $Mo_v^w(\Omega_1) - Mo_v^w(\Omega_2) < 0$, which shows the maximum weighted vertex Mostar index.

**Lemma 4.** *Consider $\Omega$ be the graph with even diameter and $T$ be subgraph of $\Omega$, which is presented by $\Omega_1$. To construct $\Omega_2$ from $\Omega_1$, remove all $n-d-1$ pendent vertices and identifying at central vertex of $T$. Then $Mo_v^w(\Omega_1) < Mo_v^w(\Omega_2)$.*

*Proof.* By use of corollary 2, we can easily extend the graph up-to $n-d-1$ pendent vertices linked with cut edge and proof is obvious.

Next, we turn to the proof of Theorem 3.

*Proof.* Assume $\Omega \in T(n,d)$ be a graph with $d \geq 1$ and $n \geq 2$. If $T(n,d) \ncong \Omega$ and $\Omega$ has cut edge then repeatedly by using Lemma 2, we acquire sequence of new tree graphs $\Omega_1, \Omega_2, \Omega_3, ..., \Omega_\alpha$, where $\Omega_\alpha$ be a tree graph without edge with largest degree sequence such that $Mo_v^w(\Omega_1) < Mo_v^w(\Omega_2) < Mo_v^w(\Omega_3) < ... < Mo_v^w(\Omega_\alpha)$. Now, If $Mo_v^w(\Omega_\alpha) \ncong T(\widehat{n,d})$ and $Mo_v^w(\Omega_\alpha)$ has subgraph with $n-d-1$, pendent vertices with even diameter then repeatedly using Lemma 3, we can acquire sequence of tree graph such that $\Omega_{\alpha_1}$,$\Omega_{\alpha_2}$,$\Omega_{\alpha_3}$,.., $\Omega_{\alpha_\beta}$, satisfying $Mo_v^w(\Omega_{\alpha_1}) < Mo_v^w(\Omega_{\alpha_2}) < Mo_v^w(\Omega_{\alpha_3}) < ... < Mo_v^w(\Omega_{\alpha_\beta})$, where $\Omega_{\alpha_\beta}$ be a tree graph such that degree of central vertex with even diameter greater than 3.

If $\Omega_{\alpha_\beta} \ncong T(\widehat{n,d})$, then repeatedly using Lemma 4, and corollary 2, we have $\Omega_{\alpha_{\beta_1}}, \Omega_{\alpha_{\beta_2}}, \Omega_{\alpha_{\beta_3}}, ..., \Omega_{\alpha_{\beta_\gamma}}$, satisfying $Mo_v^w(\Omega_{\alpha_{\beta_1}}) < Mo_v^w(\Omega_{\alpha_{\beta_2}}) < Mo_v^w(\Omega_{\alpha_{\beta_3}}) < ... < Mo_v^w(\Omega_{\alpha_{\beta_\gamma}})$, where $Mo_v^w(\Omega_{\alpha_{\beta_\gamma}}) \cong T(\widehat{n,d})$.
This completes the proof.

**Transformation 1.** *Suppose that $k_1$ and $k_2$ are two graphs with $h_l \in V_\Omega(k_l)$ for $l = \{1,2\}$. Suppose that $\mathbb{P}_n$, $\mathbb{T}_n$, $\mathbb{S}_n$ are path, tree and star of the same order $n$ such that $\mathbb{T}_n \ncong \mathbb{P}_n$ and $\mathbb{T}_n \ncong \mathbb{S}_n$. Let $\Omega$ be a generated graph by associating the node $h_1$ with one end of $\mathbb{P}_n$ and associating the node $h_2$ with the other end of $\mathbb{P}_n$.*

*Next, Let $\Omega'$ be a transformed graph by associating the vertex $h_1$ and $h_2$ as a new vertex $h$, and then fix the vertex $h$ with the center of $\mathbb{S}_n$.*

**Lemma 5.** *We say that $\Omega$ and $\Omega'$ are graphs.Then $Mo_e^w(\Omega) < Mo_e^w(\Omega')$.*

*Proof.* Since $\mathbb{T}_n \ncong \mathbb{P}_n$ and $\mathbb{T}_n \ncong \mathbb{S}_n$, $n \geq 4$

For any edge $e = gh_1 \in E(k_1)$, $m_g(e|\Omega) - m_{h_1}(e|\Omega) = m_g(e|\Omega') - m_{h_1}(e|\Omega')$ and $d_\Omega(g) + d_\Omega(h_1) \leq d_{\Omega'}(g) + d_{\Omega'}(h_1)$. Therefore,

$$\sum_{e=gh_1 \in E(k_1)} d_\Omega(g) + d_\Omega(h_1)|m_g(e|\Omega) - m_{h_1}(e|\Omega)|,$$
$$< \sum_{e=gh_1 \in E(k_1)} d_{\Omega'}(g) + d_{\Omega'}(h_1)|m_g(e|\Omega') - m_{h_1}(e|\Omega')|,$$

Similarly, for any edge $e = g'h_2 \in E(k_1)$, $m_{g'}(e|\Omega) - m_{h_2}(e|\Omega) = m_{g'}(e|\Omega') - m_{h_2}(e|\Omega')$ and $d_\Omega(g') + d_\Omega(h_2) \leq d_{\Omega'}(g') + d_{\Omega'}(h_2)$. Therefore,

$$\sum_{e=g'h_2 \in E(k_1)} d_\Omega(g') + de_\Omega(h_2)|m_{g'}(e|\Omega) - m_{h_2}(e|\Omega)|,$$

$$< \sum_{e=g' h_2 \in E(k_1)} d_{\Omega'}(g') + d_{\Omega'}(h_2)|m_{g'}(e|\Omega') - m_{h_2}(e|\Omega')|,$$

For any edge $e = hk \in E(\mathbb{P}_n)$, $m_h(e|\Omega) - m_k(e|\Omega) = |\Omega|$. Similarly, $e = hk \in E(\mathbb{S}_n)$, $m_h(e|\Omega') - m_k(e|\Omega') = |\Omega'|$. Therefore,

$$\sum_{e=hk \in E(\mathbb{P}_n)} d_{\Omega}(h) + d_{\Omega}(k)|m_h(e|\Omega) - m_k(e|\Omega)|,$$
$$< \sum_{e=hk \in E(\mathbb{S}_n)} d_{\Omega'}(h) + d_{\Omega'}(k)|m_h(e|\Omega') - m_k(e|\Omega')|,$$

Which is obvious to show that $Mo_e^w(\Omega) < Mo_e^w(\Omega') < 0$. The proof is complete.

**Transformation 2.** *Let $K$ be a graph with $u' \in V(K)$, and $\mathbb{C}_p$ be a cycle of order $p$. The graph $K(u')\mathbb{C}_p$ is constructed by associating the vertex $u'$ with a vertex of $\mathbb{C}_p$. Let $\Omega$ be a graph generated from $K(u')\mathbb{C}_p$ by connecting pendent edges to the vertices of $\mathbb{C}_p$ other than $u'$.*

*Next, Let $\Omega'$ be a generated graph from $\Omega$ by moving all pendent edges, which are attached at vertices of $\mathbb{C}_p$ other than $u'$, on $u'$. Given that, $|\Omega| = |\Omega'|$.*

**Lemma 6.** *Suppose that two graphs denoted by $\Omega$ and $\Omega'$. Then $Mo_e^w(\Omega) < Mo_e^w(\Omega')$.*

*Proof.* Suppose $|\Omega| = |\Omega'| = n$. In $\Omega$ and $\Omega'$, suppose the vertices of $\mathbb{C}_p$ are $u'_o(u')u'_1u'_2, .., u'_{p-1}$ subsequently. In $\Omega$, suppose that $y_j$ pendant edges rooted on $u'_j$ for $1 \le j \le p-1$ and $\sum_{j=1}^{p-1} y_j = y$.

Since, $d_{\Omega}(u') = d_{\Omega}(u') - y$. For any edge $e = wu' \in E(K)$, $d_{\Omega}(w) + d_{\Omega}(u') < d_{\Omega'}(w) + d_{\Omega'}(u')$, and $n_w(e|\Omega) - n_{u'}(e|\Omega) = n_w(e|\Omega') - n_{u'}(e|\Omega')$. Therefore,

$$= \sum_{wu' \in E(K)} (d_{\Omega}(w) + d_{\Omega}(u'))|n_w(e|\Omega) - n_{u'}(e|\Omega)|,$$
$$- \sum_{wu' \in E(K)} d_{\Omega'}(w) + de_{\Omega'}(u')n_w(e|\Omega') - n_{u'}(e|\Omega'),$$
$$< 0$$

In $\Omega$, for pendant edge, $e = u_j u'_j$ rooted on $u'_j$ $(1 \le j \le p-1)$, $d_{\Omega}(u_j) + d_{\Omega}(u'_j) = y_j + 2 + 1 = y_j + 3$ and $n_{u_j}(e|\Omega) - n_{u'_j}(e|\Omega) = n - d$.

$$\sum_{j-1}^{p-1} \sum_{u_j u'_j \in E(\Omega)} d_{\Omega}(u_j) + d_{\Omega}(u'_j)|n_{u_j}(e|\Omega) - n_{u'_j}(e|\Omega)| = (n-d) \sum_{j=1}^{p=1} y_j(y_j+3),$$

In $\Omega^{'}$, for pendant edge $e = uu^{'}$ rooted on $u^{'}$ which is not in $E(K)$ and $d_{\Omega^{'}}(u) = 1$, $d_{\Omega^{'}}(u) + d_{\Omega^{'}}(u^{'}) = d_{\Omega}(u^{'}) + y + 1$ and $n_u(\mathrm{e}|\Omega^{'}) - n_{u^{'}}(\mathrm{e}|\Omega^{'}) = n - d$.

$$\sum_{uu^{'} \in E(\Omega^{'})} d_{\Omega^{'}}(u) + d_{\Omega^{'}}(u^{'})|n_u(\mathrm{e}|\Omega^{'}) - n_{u^{'}}(\mathrm{e}|\Omega^{'})| = y(n-d)(d_{\Omega} + y + 1),$$

There is two possibilities, either $p$ is even or $p$ is odd. First we suppose $p$ is even. For any edge $e = u_j^{'}u_{j+1}^{'}$ $(0 \leq j \leq p-1)$ of $\mathbb{C}_p$ in $\Omega$, $d_{\Omega}(u_j^{'}) + d_{\Omega}(u_{j+1}^{'}) = y_j + y_{j+1} + 4$ when $1 \leq j \leq p-2$, $d_{\Omega}(u_0^{'}) + d_{\Omega}(u_1^{'}) = d_{\Omega}(u^{'}) + y_1 + 2$ when $j = 0$, $d_{\Omega}(u_{p-1}^{'}) + d_{\Omega}(u_0^{'}) = d_{\Omega}(u^{'}) + y_{p-1} + 2$ when $j = p-1$. Since $p$ is even $n_{u_j^{'}}(e|\Omega) - n_{u_{j+1}^{'}}(e|\Omega) = n - d$.

$$\begin{aligned}
&= \sum_{j=0}^{p-1} d_{\Omega}(u_j^{'}) + d_{\Omega}(u_{j+1}^{'})|n_{u_j^{'}}(\mathrm{e}|\Omega) - n_{u_{j+1}^{'}}(\mathrm{e}|\Omega)|,\\
&= 2(n-d)(d_{\Omega}(u^{'}) + y + 2(p-1)),
\end{aligned}$$

Similarly in $\Omega^{'}$, after simplification we have,

$$\begin{aligned}
&= \sum_{j=0}^{p-1} d_{\Omega^{'}}(u_j^{'}) + d_{\Omega^{'}}(u_{j+1}^{'})|n_{u_j^{'}}(\mathrm{e}|\Omega^{'}) - n_{u_{j+1}^{'}}(\mathrm{e}|\Omega^{'})|,\\
&= 2(n-d)(d_{\Omega^{'}}(u^{'}) + 2(p-1))\\
&= 2(n-d)(d_{\Omega^{'}}(u^{'}) + y + 2(p-1)),
\end{aligned}$$

By using the above calculations, we have straightforward result

$$\begin{aligned}
Mo_{\mathrm{e}}^{w}(\Omega) - Mo_{\mathrm{e}}^{w}(\Omega^{'}) &= \sum_{j=0}^{p-1} d_{\Omega}(u_j^{'}) + d_{\Omega}(u_{j+1}^{'})|n_{u_j^{'}}(\mathrm{e}|\Omega) - n_{u_{j+1}^{'}}(\mathrm{e}|\Omega)|,\\
&- \sum_{j=0}^{p-1} d_{\Omega^{'}}(u_j^{'}) + d_{\Omega^{'}}(u_{j+1}^{'})|n_{u_j^{'}}(\mathrm{e}|\Omega^{'}) - n_{u_{j+1}^{'}}(\mathrm{e}|\Omega^{'})|,\\
&< 0,
\end{aligned}$$

The result $Mo_{\mathrm{e}}^{w}(\Omega) < Mo_{\mathrm{e}}^{w}(\Omega^{'})$ is obvious similar for $p$ is odd. The proof is complete.

**Transformation 3.** *Let $K$ be a graph with $u \in V(K)$ such that $d_K(u) \geq 2$, and $\mathbb{C}_p$ be a cycle of order p such that $p \geq 4$. Let $\Omega$ be a generated graph from $K(u)\mathbb{C}_p$ by combining a vertices of $\mathbb{C}_p$ with $u$.*

*Next, Let $\Omega^{'}$ be the graph obtained from $\Omega$ by exchanging $\mathbb{C}_p$ for $\mathbb{C}_3$ and $p-3$ pendent edges. Note that, $|\Omega| = |\Omega^{'}|$.*

**Lemma 7.** *Let $\Omega$ and $\Omega^{'}$ be two connected graphs explained in Transformation 3. Then $Mo_{\mathrm{e}}^{w}(\Omega) < Mo_{\mathrm{e}}^{w}(\Omega^{'})$.*

*Proof.* Suppose $|\Omega| = |\Omega^{'}| = n$ without loss of generality. Note that $d_{\Omega}(u) = d_{\Omega^{'}}(u) - (p-3)$. For any edge $\mathrm{e} = uu^{'} \in E(K)$, $d_{\Omega}(u) + d_{\Omega}(u^{'}) < d_{\Omega^{'}}(u) + d_{\Omega^{'}}(u^{'})$, and $m_u(\mathrm{e}|\Omega) - m_{u^{'}}(\mathrm{e}|\Omega) = m_u(\mathrm{e}|\Omega^{'}) - m_{u^{'}}(\mathrm{e}|\Omega^{'})$. Therefore,

$$\begin{aligned}
&= \sum_{\mathrm{e}=uu^{'}\in E(K)} d_{\Omega}(u) + d_{\Omega}(u^{'})|m_u(\mathrm{e}|\Omega) - m_{u^{'}}(\mathrm{e}|\Omega)|, \\
&- \sum_{\mathrm{e}=uu^{'}\in E(K)} d_{\Omega^{'}}(u) + d_{\Omega^{'}}(u^{'})|m_u(\mathrm{e}|\Omega^{'}) - m_{u^{'}}(\mathrm{e}|\Omega^{'})|, \\
&< 0
\end{aligned}$$

When $p$ is odd, for the edges in $\mathbb{C}_p$ of $\Omega$

$$\begin{aligned}
&= \sum_{j=0}^{p-1} d_{\Omega}(u_j) + d_{\Omega}(u_{j+1})|m_{u_j}(\mathrm{e}|\Omega) - m_{u_{j+1}}(\mathrm{e}|\Omega), \\
&= 4(p-1) + (n-1)[2(d_{\Omega}(u)+2) + 4(p-3)],
\end{aligned}$$

When $p$ is even, for the edges in $\mathbb{C}_p$ of $\Omega$

$$\begin{aligned}
&= \sum_{j=0}^{p-1} d_{\Omega}(u_j) + d_{\Omega}(u_{j+1})|m_{u_j}(\mathrm{e}|\Omega) - m_{u_{j+1}}(\mathrm{e}|\Omega)|, \\
&= n[2(d_{\Omega}(u)+2) + 4(p-2)],
\end{aligned}$$

For any pendant edge $uu^{'}$ rooted on $u$ in $\Omega^{'}$, $d_{\Omega^{'}}(u) + d_{\Omega^{'}}(u^{'}) = d_{\Omega^{'}}(u) + p - 2$, and $m_u(\mathrm{e}|\Omega^{'}) - m_{u^{'}}(\mathrm{e}|\Omega^{'}) = n - d$ and $d_{\Omega^{'}} = 1$. Therefore,

$$\begin{aligned}
&= \sum_{\mathrm{e}=uu^{'}\in E(\Omega^{'})\setminus E(K)} d_{\Omega^{'}}(u) + d_{\Omega^{'}}(u^{'})|n_u(\mathrm{e}|\Omega^{'}) - n_{u^{'}}(\mathrm{e}|\Omega^{'})|, \\
&= (p-3)n[(d_{\Omega}(u)) + (p-2)],
\end{aligned}$$

For the edges in $\mathbb{C}_3$ of $\Omega^{'}$

$$\begin{aligned}
&= \sum_{j=0}^{2} d_{\Omega^{'}}(u_j) + de_{\Omega^{'}}(u_{j+1})|m_{u_j}(\mathrm{e}|\Omega^{'}) - m_{u_{j+1}}(\mathrm{e}|\Omega^{'})|, \\
&= 8 + [2(d_{\Omega^{'}}(u)+2)(n-1)], \\
&= 8 + 2(d_{\Omega^{'}}(u)+p-1)(n-1),
\end{aligned}$$

By using the above calculations, we have straightforward result $Mo_e^w(\Omega) - Mo_e^w(\Omega^{'}) < 0$, which completes proof.

**Transformation 4.** *Assume that $K$ is a graph and $\mathbb{C}_p$ is a cycle of order $p$. The graph formed by associating the vertex $u$ with a vertex of $\mathbb{C}_p$ is denoted by $K(u)\mathbb{C}_p$. Let $\Omega$ be the graph formed from $K(u)\mathbb{C}_p$ by attaching some triangles and (or) some pendent edges to the vertices of $\mathbb{C}_p$ except $u$.*

*Now, Let $\Omega^{'}$ be the graph formed from $\Omega$ by shifting all triangles and pendent edges rooted on vertices of $\mathbb{C}_p$ except for $u$ to $u$. Given that $|\Omega| = |\Omega^{'}|$.*

**Lemma 8.** *Suppose that $\Omega$ and $\Omega^{'}$ are two graphs. Then $Mo_e^w(\Omega) < Mo_e^w(\Omega^{'})$.*

We leave to the reader the proof of Lemma 8, since it is similar to the proof of Lemma 6.

**Transformation 5.** *Let $C_k$ be a cycle with $r \geq 4$ and $u^{'}, u_1^{'}, ..., u_{k-1}^{'}$ are the vertices of $C_k$ subsequently. Let $K_o$ be a cactus graph such that $d(K_o) \geq 2$ and all cycles in $K_o$ are triangles. Suppose $w, x$ are two vertices of $V(K_o)$ such that $w, x$ are in some triangles of $K_o$ and $d(K_o)(w) = d(K_o)(x) = 2$. Let $\Omega$ be the resulting graph by associating $u^{'}$ and $x$ via a path (the length of the path $\geq 0$), and fix $u_j^{'}$ where $i \neq 0$ with one vertex of a graph $K$.*

*Next, Let $\Omega^{'}$ be a generated graph from $\Omega$ by exclude the edge $u_j^{'}y$ for any $y \in V_K$ and addition of edge $wy$.*

**Lemma 9.** *Suppose $\Omega$ and $\Omega^{'}$ are two graphs. Then $Mo_e^w(\Omega) > Mo_e^w(\Omega^{'})$.*

The proof of Lemma 9, leave to readers, since it is evidently analogous to the proof of Lemma 7.

Next, we turn to the proof of Theorem 4.

*Proof.* By using Lemmas 1, 5, 6, 7, 8, and 9 for any graph $\Omega \in \mathbb{C}(n, k)$, $Mo_{\mathrm{e}}^w(\Omega) < Mo_{\mathrm{e}}^w(\mathbb{S}_n^{*,k})$ and the equality holds if and only if $\Omega \cong \mathbb{S}_n^{*,k}$. It is easy to compute that $Mo_{\mathrm{e}}^w(\Omega) = n^3 + (k-4)n^2 + (-3k+5)n - (2n+4)$. The proof completes.

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