# On Mostar Index of Trees with Parameters 

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#### Abstract

The Mostar index of a graph $G$ is defined as the sum of absolute values of the differences between $n_{u}$ and $n_{v}$ over all edges $u v$ of $G$, where $n_{u}$ and $n_{v}$ are respectively, the number of vertices of $G$ lying closer to vertex $u$ than to vertex $v$ and the number of vertices of $G$ lying closer to vertex $v$ than to vertex $u$. We identify those trees with minimum and/or maximum Mostar index in the families of trees of order $n$ with fixed parameters like the maximum degree, the diameter, number of pendent vertices by using graph transformations that decrease or increase the Mostar index.


## 1. Introduction

All graphs considered in this paper are finite and simple. Let $G$ be a connected graph on $n$ vertices with vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, let $N_{G}(v)$ be the set of all neighbors of $v$ in $G$. The degree of $v \in V(G)$, denoted by $d_{G}(v)$, is the cardinality of $N_{G}(v)$. A vertex is said to be pendent if its degree is one, and an edge is said to be pendent if one end vertex is pendent. The graph formed from $G$ by deleting a vertex $v \in V(G)$ (and its incident edges) is denoted by $G-v$. A connected graph with $n$ vertices is a tree if $|E(G)|=n-1$. A caterpillar is a tree, the deletion of whose pendent vertices outside a diametral path produces a path. A vertex having degree greater than two is called branch vertex. As usual, by $S_{n}$ and $P_{n}$ we denote the star and path on $n$ vertices, respectively. For $e=u v \in E(G)$, let $N_{u}(e \mid G)$ and $N_{v}(e \mid G)$ be respectively the set of vertices of $G$ lying closer to vertex $u$ than to vertex $v$ and the set of vertices of $G$ lying closer to vertex $v$ than to vertex $u$, i.e.,

$$
\begin{aligned}
N_{u}(e \mid G) & =\left\{x \in V(G): d_{G}(u, x)<d_{G}(v, x)\right\}, \\
N_{v}(e \mid G) & =\left\{x \in V(G): d_{G}(v, x)<d_{G}(u, x)\right\} .
\end{aligned}
$$

The numbers of vertices of $N_{u}(e \mid G)$ and $N_{v}(e \mid G)$ are denoted by $n_{u}(e \mid G)$ and $n_{v}(e \mid G)$, respectively. Let $G$ be a connected graph. The Szeged index of $G$, proposed by Gutman [9], is defined as

$$
S z(G)=\sum_{e=u v \in E(G)} n_{u}(e \mid G) n_{v}(e \mid G)
$$

Now the Szeged index and its variants have been studied extensively, see, e.g., $[1-3,5,6,8,10,15,16,23$, $24,27]$. We mention that the Szeged index is a particular case of the modified Wiener index, defined as

[^0]$\sum_{e=u v \in E(G)}\left(n_{u}(e \mid G) n_{v}(e \mid G)\right)^{\lambda}$ for a nonzero real $\lambda$, see, e.g., $[11,25,26]$. If $G$ is a tree, then $S z(G)$ coincides with the Wiener index of $G$ [22]. Actually, the Wiener index of a connected graph $G$ is defined as the sum of distances between all pairs of vertices, see, e.g., [4, 19]. To measure the peripherality in a graph (i.e., how far a graph is from being distance-balanced [13, 17]), Doslić et al. [7] introduced a novel graph invariant, named as Mostar index of a graph. For a connected graph $G$, the Mostar index of $G$ is defined as
$$
\operatorname{Mo}(G)=\sum_{e=u v \in E(G)}\left|n_{u}(e \mid G)-n_{v}(e \mid G)\right| .
$$

Doslić et al. [7] studied the Mostar index of trees and unicyclic graphs, and showed how the Mostar index can be efficiently computed for various classes of chemically interesting graphs using a variant of the cut method proposed by Klavžar et al. [14]. In particular, they showed that among $n$-vertex trees, the star $S_{n}$ and path $P_{n}$ are the unique ones with maximum and minimum Mostar index, respectively. Tepeh [20] studied the Mostar index of bicyclic graphs. Hayat and Zhou [12] determined all the $n$-vertex cacti with the largest Mostar index, and obtained a sharp upper bound for the Mostar index for cacti of order $n$ with $k$ cycles, and characterize the extremal case.

In this note, we give some further properties of Mostar index of trees. We identify those trees with minimum and/or maximum Mostar index in the families of trees of order $n$ with fixed parameters like the maximum degree, the diameter, number of pendent vertices using graph transformations that decrease or increase the Mostar index.

## 2. Preliminaries

For simplicity, we set $\psi_{G}(e)=\left|n_{u}(e \mid G)-n_{v}(e \mid G)\right|$ for a connected graph $G$ with $e=u v \in E(G)$.
Let $G$ be a connected graph with a cut edge $e=u v$, and let $G / e$ be the graph obtained from $G$ by contracting the edge $e$ into a new vertex $w_{e}$ such that it is adjacent to each vertex in $N_{G}(u) \cup N_{G}(v) \backslash\{u, v\}$ and then attaching a pendent edge at $w_{e}$.

Lemma 2.1. [7] Let $G$ be a connected graph with a cut edge e. Ife is not a pendent edge, then $\operatorname{Mo}(G / e)>\operatorname{Mo}(G)$.
A path $v_{0} \ldots v_{s}$ in a graph $G$ is a pendent path of length $s\left(\right.$ at $\left.v_{0}\right)$ if $d_{G}\left(v_{0}\right) \geq 2, d_{G}\left(v_{s}\right)=1$, and if $s \geq 2$, $d_{G}\left(v_{i}\right)=2$ for $i=1, \ldots, s-1$. Evidently, a pendent path of length one is a pendent edge. Let $H$ be a nontrivial connected graph with $u \in V(H)$. For two nonnegative integers $\ell$ and $m$, let $H_{u ;, m}$ be the graph obtained from $H$ by attaching two pendent paths of length $\ell$ and $m$, respectively at $u$. In particular, $H_{u ; 0,0}=H$ and $H_{u ;,, 0}$ is obtained from $H$ by attaching a pendent path of length $\ell$. From the proof of Theorem 5 in [7], we have

Lemma 2.2. [7] Let $H$ be a nontrivial connected graph with $u \in V(H)$. If $\ell \geq m \geq 1$, then $\operatorname{Mo}\left(G_{u ;, f, m}\right)>$ $\operatorname{Mo}\left(G_{u ; \ell+1, m-1}\right)$.

Let $A_{n}(a, b)$ be the $n$-vertex tree obtained from a path by attaching $a$ and $b$ pendent vertices respectively to the two terminal vertices, where $n-a-b \geq 2$ and $a \geq b \geq 0$.

Lemma 2.3. Let $a$ and $b$ be positive integers with $a \geq b+2$. Then $\operatorname{Mo}\left(A_{n}(a-1, b+1)\right)<\operatorname{Mo}\left(A_{n}(a, b)\right)$.
Proof. If $a \leq \frac{n}{2}$, then $b+1<a \leq \frac{n}{2}$, and otherwise, $b+1<n-a<\frac{n}{2}$. Thus $\operatorname{Mo}\left(A_{n}(a, b)\right)>\operatorname{Mo}\left(A_{n}(a-1, b+1)\right)$, as $\operatorname{Mo}\left(A_{n}(a, b)\right)-\operatorname{Mo}\left(A_{n}(a-1, b+1)\right)=|b+1-(n-b-1)|-|a-(n-a)|>0$.

For a graph $G$ with $E_{1} \subseteq E(G), G-E_{1}$ denotes the graph with vertex set $V(G)$ and edge set $E(G) \backslash E_{1}$. Similarly, if $E_{2} \subseteq E(\bar{G})$, then $G+E_{2}$ denotes the graph with vertex set $V(G)$ and edge set $E(G) \cup E_{2}$, where $\bar{G}$ is the complement of $G$. In particular, if $E_{1}=\{e\}\left(E_{2}=\{f\}\right.$, respectively), then we write $G-e(G+f$, respectively) instead of $G-\{e\}(G+\{f\}$, respectively).

Lemma 2.4. Let $G$ be a tree with $x, y \in V(G)$. Suppose that $x_{1}, \ldots, x_{s}$ and $y_{1}, \ldots, y_{t}$ are pendent vertices adjacent to $x$ and $y$ respectively. Let $x^{\prime}$ and $y^{\prime}$ be respectively the neighbors of $x$ and $y$ in the path connecting $x$ and $y$. Let

$$
\begin{aligned}
& G^{\prime}=G-\left\{x x_{i}: i=1, \ldots, s\right\}+\left\{x^{\prime} x_{i}: i=1, \ldots, s\right\}, \\
& G^{\prime \prime}=G-\left\{y y_{i}: i=1, \ldots, t\right\}+\left\{y^{\prime} y_{i}: i=1, \ldots, t\right\} .
\end{aligned}
$$

Then $\operatorname{Mo}(G)<\max \left\{\operatorname{Mo}\left(G^{\prime}\right), \operatorname{Mo}\left(G^{\prime \prime}\right)\right\}$.
Proof. Let $e^{\prime}=x x^{\prime}$ and $e^{\prime \prime}=y y^{\prime}$. Note that, if $x$ and $y$ are adjacent, then $x^{\prime}=y$ and $y^{\prime}=x$. From the constructions of $G^{\prime}$ and $G^{\prime \prime}$, we have $\psi_{G}(e)=\psi_{G^{\prime}}(e)$ for all $e \in G \backslash\left\{e^{\prime}\right\}$, and $\psi_{G}(e)=\psi_{G^{\prime \prime}}(e)$ for all $e \in G \backslash\left\{e^{\prime \prime}\right\}$. Let $n_{z}(f)=n_{z}(f \mid G)$ where $z \in\left\{x, x^{\prime}\right\}$ if $f=e^{\prime}$ and $z \in\left\{y, y^{\prime}\right\}$ if $f=e^{\prime \prime}$. Then

$$
\begin{aligned}
\operatorname{Mo}(G)-\operatorname{Mo}\left(G^{\prime}\right) & =\psi_{G}\left(e^{\prime}\right)-\psi_{G^{\prime}}\left(e^{\prime}\right) \\
& =\left|n_{x}\left(e^{\prime}\right)-n_{x^{\prime}}\left(e^{\prime}\right)\right|-\left|n_{x}\left(e^{\prime}\right)-s-\left(n_{x^{\prime}}\left(e^{\prime}\right)+s\right)\right| \\
\operatorname{Mo}(G)-\operatorname{Mo}\left(G^{\prime \prime}\right) & =\psi_{G}\left(e^{\prime \prime}\right)-\psi_{G^{\prime \prime}}\left(e^{\prime \prime}\right) \\
& =\left|n_{y}\left(e^{\prime \prime}\right)-n_{y^{\prime}}\left(e^{\prime \prime}\right)\right|-\left|n_{y}\left(e^{\prime \prime}\right)-t-\left(n_{y^{\prime}}\left(e^{\prime \prime}\right)+t\right)\right| .
\end{aligned}
$$

Obviously, $n_{x^{\prime}}^{\prime}\left(e^{\prime}\right) \geq n_{y}\left(e^{\prime \prime}\right)$ and $n_{y^{\prime}}\left(e^{\prime \prime}\right) \geq n_{x}\left(e^{\prime}\right)$. If $n_{x}\left(e^{\prime}\right)>n_{x^{\prime}}\left(e^{\prime}\right)$ and $n_{y}\left(e^{\prime \prime}\right)>n_{y^{\prime}}\left(e^{\prime \prime}\right)$, then $n_{x}\left(e^{\prime}\right)>n_{x^{\prime}}\left(e^{\prime}\right) \geq$ $n_{y}\left(e^{\prime \prime}\right)>n_{y^{\prime}}\left(e^{\prime \prime}\right) \geq n_{x}\left(e^{\prime}\right)$, which is a contradiction. Thus we have either $n_{x}\left(e^{\prime}\right) \leq n_{x^{\prime}}^{\prime}\left(e^{\prime}\right)$ or $n_{y}\left(e^{\prime \prime}\right) \leq n_{y^{\prime}}\left(e^{\prime \prime}\right)$. In the former case, $\operatorname{Mo}(G)-\operatorname{Mo}\left(G^{\prime}\right)=n_{x^{\prime}}\left(e^{\prime}\right)-n_{x}\left(e^{\prime}\right)-\left(n_{x^{\prime}}\left(e^{\prime}\right)-n_{x}\left(e^{\prime}\right)+2 s\right)=-2 s<0$, and in the latter case, $\operatorname{Mo}(G)-\operatorname{Mo}\left(G^{\prime \prime}\right)=n_{y^{\prime}}\left(e^{\prime \prime}\right)-n_{y}\left(e^{\prime \prime}\right)-\left(n_{y^{\prime}}\left(e^{\prime \prime}\right)-n_{y}\left(e^{\prime \prime}\right)+2 t\right)=-2 t<0$. Thus, $\operatorname{Mo}(G)<\operatorname{Mo}\left(G^{\prime}\right)$ or $\operatorname{Mo}(G)<\operatorname{Mo}\left(G^{\prime \prime}\right)$, as desired.

For integer $k$, let $P_{n, d, k}$ be the tree obtained from the path $P_{d+1}=v_{0} v_{1} \ldots v_{d}$ by attaching $n-d-1$ pendent edges at $v_{k}$, where $1 \leq k \leq\left\lfloor\frac{d}{2}\right\rfloor$.

Let $S\left(a_{1}, \ldots, a_{r}\right)$ be the tree consisting of $r$ pendent paths of lengths $a_{1}, \ldots, a_{r}$ respectively at a common vertex $u$, where $a_{1} \geq \cdots \geq a_{r} \geq 1$. If $a_{i}-a_{j}=0,1$ for any $i$ and $j$ with $1 \leq i<j \leq r$, then we call $S\left(a_{1}, \ldots, a_{r}\right)$ a balanced starlike tree and denoted by $B S_{n, r}$.

## 3. Results

The maximum degree of a graph is the the maximum degree of its vertices.
Theorem 3.1. Among all trees of order $n$ with maximum degree $\Delta, P_{n, n-\Delta+1,1}$ is the unique tree with minimum Mostar index, where $3 \leq \Delta \leq n-2$.

Proof. Let $T$ be a tree of order $n$ with maximum degree $\Delta$ such that $M o(T)$ is as small as possible. We only need to show that $T \cong P_{n, n-\Delta+1,1}$.

Choose a vertex $v \in V(T)$ with degree $\Delta$. Let $N_{T}(v)=\left\{v_{1}, \ldots, v_{\Delta}\right\}$. Let $T_{i}$ be the component of $T-v$ containing $v_{i}$, where $i=1, \ldots, \Delta$. Suppose that for some $i, T_{i}$ is not a path with one terminal vertex $v_{i}$. Then there is a vertex in $T_{i}$ such that its degree in $T$ is at least three. So there is a vertex $w$ in $T_{i}$ such that $d_{T}(v, w)$ is as large as possible. That is to say, there are two pendent paths, say with lengths $\ell$ and $m$ respectively at $w$ in $T$. Assume that $\ell \geq m$. So $T \cong G_{w ;, m, m}$, where $G$ is the graph obtained from $T$ by deleting the vertices of degree two and one in the two pendent paths. By Lemma 2.2, we have $M o(T)=M o\left(G_{w ; \ell, m}\right)>M o\left(G_{w ; \ell+1, m-1}\right)$, a contradiction. Therefore, for each $i=1, \ldots, \Delta, T_{i}$ is a path with one terminal vertex $v_{i}$. So $T$ consist of $\Delta$ pendent paths at $v$. By Lemma 2.2, $T \cong P_{n, n-\Delta+1,1}$.

The diameter of a graph is the largest distance between any pair of vertices.
Theorem 3.2. Among all trees of order $n$ with diameter $d, P_{\left.n, d, \lambda \frac{d}{2}\right\rfloor}$ is the unique tree with maximum Mostar index, where $3 \leq d \leq n-2$.

Proof. Let $T$ be a tree of order $n$ with diameter $d$ such that $\operatorname{Mo}(T)$ is as large as possible. We only need to show that $T \cong P_{n, d,\left\lfloor\frac{d}{2}\right\rfloor}$.

Let $P=v_{0} \ldots v_{d}$ be a diametric path of $T$. Suppose that $T$ is not a caterpillar. Then there exist some vertex say $w$ outside $P$ with $d_{T}(w) \geq 2$ such that $w v_{i} \in E(T)$ for some $1 \leq i \leq d-1$. Let $N$ be the set of neighbour of $w$ except $v_{i}$. Let $T^{\prime}=T-\{w s: s \in N\}+\left\{v_{i} s: s \in N\right\}$. It is obvious that $T$ is a tree of order $n$ with diameter $d$. But by Lemma 2.1, $\operatorname{Mo}(T)<M o\left(T^{\prime}\right)$, a contradiction to the maximality of $T$. Thus, $T$ is a caterpillar.

Next, we show that all pendent edges outside the path $P$ are adjacent to a single vertex on the path $P$. Otherwise, we may choose two vertices $v_{i}$ and $v_{j}(1 \leq i<j \leq d-1)$ on the path $P$ with degree at least three in $T$. Let $Q$ be the sub-path of $P$ from $v_{i}$ to $v_{j}$. By Lemma 2.4, we may find a tree of order $n$ with diameter $d$ whose Mostar index is larger than $M o(T)$, which is a contradiction. Thus, all pendent edges outside the path $P$ are adjacent to a single vertex on the path $P$. That is, $T \cong P_{n, d, k}$ for some $k$ with $1 \leq k \leq\left\lfloor\frac{d}{2}\right\rfloor$. Then $n-(2 k+2) \geq 0$. Suppose that $k<\left\lfloor\frac{d}{2}\right\rfloor$. Let $T^{\prime}=P_{n, d, k+1}$. As $k-1<\min \{d-k, n-(d-k)\} \leq \frac{n}{2}$, we have $\operatorname{Mo}(T)-\operatorname{Mo}\left(T^{\prime}\right)=\psi_{T}\left(v_{k} v_{k+1}\right)-\psi_{T^{\prime}}\left(v_{k} v_{k+1}\right)=|n-(d-k)-(d-k)|-|k+1-(n-k-1)|<0$, implying that $M o(T)<M o\left(T^{\prime}\right)$, a contradiction. Therefore, $k=\left\lfloor\frac{d}{2}\right\rfloor$, i.e., $\left.T \cong P_{n, d,\left\lfloor\frac{d}{2}\right\rfloor}\right\rfloor$

Next we consider the Mostar index of trees when the number of pendent vertices is fixed. We use the techniques from [25].

Recall that a starlike tree is a tree with a unique vertex of degree at least three. For $3 \leq r \leq n-2$, by $B S_{n, r}$, we denote the starlike tree of order $n$ with maximum degree $r$ such that the $r$ pendent paths have almost equal lengths, i.e., for any two pendent paths with length $\ell$ and $s,|\ell-s|=0,1$. Let $n-1=r s+t$, where $0 \leq t \leq r-1$. Then $B S_{n, r}$ consists of $t$ pendent paths of length $s+1$ and $r-t$ pendent paths of length $s$ at a common vertex.

Theorem 3.3. Among all trees of order $n$ with $r$ pendent vertices, $B S_{n, r}$ is the unique tree with maximum Mostar index, where $3 \leq r \leq n-2$.

Proof. Let $T$ be a tree of order $n$ with $r$ pendent vertices such that $M o(T)$ is as large as possible.
Claim. $T$ contains exactly one branch vertex.
Suppose on contrary that $T$ contains at least two branch vertices. Obviously, we may choose two branch vertices, say $x$ and $y$, such that $d_{T}(x, y)$ is as small as possible. Let $P$ be the path connecting $x$ and $y$. If $d_{T}(x, y)>1$, then each internal vertex of $P$ is of degree 2 . Let $n_{x}$ ( $n_{y}$, respectively) be the order of the component of $T-E(P)$ containing $x$ ( $y$, respectively). Assume that $n_{x} \geq n_{y}$. Obviously, $n_{y} \leq \frac{n}{2}$. Let $z$ be the neighbor of $y$ in $P$ and $w$ be any other neighbor of $y$. Let $n_{w}=n_{w}(y w \mid T)$. Let $T^{\prime}=T-y w+z w$. Obviously, $T^{\prime}$ is a tree of order $n$ with $r$ pendent vertices. Note that $\psi_{T}(e)=\psi_{T^{\prime}}(e)$ for $e \in E(T) \backslash\{z y, y w\}=E\left(T^{\prime}\right) \backslash\{z y, z w\}$ and $\psi_{T}(y w)=\psi_{T^{\prime}}(z w)$. Thus

$$
\operatorname{Mo}(T)-\operatorname{Mo}\left(T^{\prime}\right)=\psi_{T}(z w)-\psi_{T^{\prime}}(z w)=\left|n_{y}-\left(n-n_{y}\right)\right|-\left|\left(n_{y}-n_{w}\right)-n-\left(n_{y}-n_{w}\right)\right|<0
$$

implying that $M o(T)<M o\left(T^{\prime}\right)$, a contradiction. This proves the claim.
By the claim, $T$ consists of $r$ some pendent paths at a common vertex. Let $a_{1}, \ldots, a_{r}$ be the lengths of these pendent paths, where $a_{1} \geq \cdots \geq a_{r} \geq 1$.

Suppose that $a_{i}-a_{j} \geq 2$ for some pair of $i$ and $j$ with $1 \leq i<j \leq r$. Let $u$ be the vertex with maximum degree $r$. Then $T \cong G_{u ; a_{i}, a_{j}}$, where $G$ is the graph obtained from $T$ by deleting vertices of degree two or one in two pendent paths with lengths $a_{i}$ and $a_{j}$, respectively. Obviously, $G_{u ; a_{i}-1, a_{j}+1}$ is a tree of order $n$ with $r$ pendent vertices. By Lemma 2.2, $\operatorname{Mo}(T)<\operatorname{Mo}\left(G_{u ; a_{i}-1, a_{j}+1}\right)$, a contradiction. Therefore, $a_{i}-a_{j}=0,1$ for any $i$ and $j$ with $1 \leq i<j \leq r$. That is, $T \cong B S_{n, r}$.

The matching number of a graph is the number of edges in a maximum matching (i.e., set of disjoint edges with maximum number of edges). The domination number of a graph is the number of vertices in a minimum dominating set (a set of vertices with minimum number of vertices such that every vertex outside this set is adjacent to at least one member of the set).

For $1 \leq m \leq \frac{n}{2}$, let $A_{n, m}$ be the tree consists of $m-1$ pendent paths of length two and $n-2(m-1)$ pendent edges at a common vertex. Obviously, $A_{n, m}=B S_{n, n-m}$ for $1 \leq m \leq \frac{n}{2}$.

Corollary 3.4. Among trees of order $n$ with matching number $s$ (domination number $t$, respectively), $A_{n, s}\left(A_{n, t}\right.$, respectively) is the unique tree with maximum Mostar index, where $1 \leq s \leq \frac{n}{2}\left(1 \leq t \leq \frac{n}{2}\right.$, respectively).

Proof. It is trivial if $n=2$ as $A_{2,1}=P_{2}$. Suppose that $n \geq 3$. Let $T$ be a tree of order $n$ with matching number $s$ and domination number $t$. By König's theorem, $s$ is equal to the minimum cardinality of a covering of $T$. As a covering of $T$ is also a dominating set of $T$. So $t \leq s$. Then $n-s \leq n-t$. Denote by $r$ the number of pendent vertices of $T$. Note that $r \leq n-s \leq n-t$.

We claim that $\operatorname{Mo}\left(B_{n, r}\right)<\operatorname{Mo}\left(B_{n, r+1}\right)$. This is clearly true if $r=2$ as $B_{n, 2}=P_{n}$. Suppose that $r \geq 3$. For $3 \leq r \leq n-2$, let $u$ be the vertex of degree $r$ in $B S_{n, r}$ and $v$ a neighbor of $u$ in a pendent path of length at least two. By Lemma 2.1 or 2.2, we have $M o\left(B_{n, r}\right)<M o\left(B_{n, r} / u v\right)$. Note that $B_{n, r} / u v$ consists of $r+1$ pendent paths at a common vertex $u$. Now, by Lemma 2.2, $M o\left(B_{n, r} / u v\right)<M o\left(B S_{n, r+1}\right)$ if $B_{n, r} / u v \neq B S_{n, r+1}$. It follows that $\operatorname{Mo}\left(B_{n, r}\right)<\operatorname{Mo}\left(B_{n, r+1}\right)$ for $2 \leq r \leq n-2$.

If $T$ maximizes the Mostar index among trees of order $n$ with matching number $s$, then, by Theorem 3.3 and the above claim, $T \cong B S_{n, r}$ with $r=n-s$, i.e., $T \cong B S_{n, n-s}=A_{n, s}$.

If $T$ maximizes the Mostar index among trees of order $n$ with domination number $t$, then, by Theorem 3.3 and the above claim, $T \cong B S_{n, r}$ with $r=n-t$, i.e., $T \cong B S_{n, n-t}=A_{n, t}$.

Theorem 3.5. Among trees of order $n$ with $r$ pendent vertices, $A_{n}\left(\left\lceil\frac{r}{2}\right\rceil,\left\lfloor\frac{r}{2}\right\rfloor\right)$ is the unique tree with minimum Mostar index, where $3 \leq r \leq n-2$.

Proof. Let $T$ be a tree of order $n$ with $r$ pendent vertices such that $M o(T)$ is as small as possible.
Claim. $T$ has at most two branch vertices.
Suppose on contrary that $T$ contains at least three branch vertices. Obviously, we may choose two branch vertices, say $x$ and $y$, such that $d_{T}(x, y)$ is as large as possible. Let $P$ be the path connecting $x$ and $y$. Let $n_{x}$ ( $n_{y}$, respectively) be the order of the component of $T-E(P)$ containing $x$ ( $y$, respectively). Obviously, some internal vertex of $P$ is a branch vertex of $T$. So we may choose branch vertices $w$ and $z$ in $P$ such that both $d_{T}(x, w)$ and $d_{T}(z, y)$ are as small as possible. Assume that $n_{x}+d_{T}(x, w) \geq n_{y}+d_{T}(z, y)$. Then $n_{y}+d_{T}(z, y) \leq \frac{n}{2}$. Let $s=d_{T}(z, y)$ and let $z_{0} \ldots z_{s}$ be the path from $z$ to $y$, where $z_{0}=z$ and $z_{s}=y$. Let $u_{1}, \ldots u_{p}$ be the neighbors of $z$ outside $P$ in $T$, where $p=d_{T}(z)-2$. Let $T^{\prime}=T-\left\{z u_{i}: i=1, \ldots, p\right\}+\left\{y u_{i}: i=1, \ldots, p\right\}$. Evidently, $T^{\prime}$ is a tree of order $n$ with $r$ pendent vertices. Let $n_{z}^{\prime}$ be the total number of vertices of the components of $T-z$ containing one of $u_{1}, \ldots, u_{p}$. For $i=0, \ldots, s$, we have $n_{y}+s-i<\min \left\{n_{y}+n_{z}^{\prime}+s-i, n-\left(n_{y}+n_{z}^{\prime}+s-i\right)\right\} \leq \frac{n}{2}$, implying that $\psi_{T}\left(z_{i-1} z_{i}\right)=\left|\left(n_{y}+s-i\right)-\left(n-\left(n_{y}+s-i\right)\right)\right|>\left|n_{y}+n_{z}^{\prime}+s-i-\left(n-\left(n_{y}+n_{z}^{\prime}+s-i\right)\right)\right|=\psi_{T^{\prime}}\left(z_{i-1} z_{i}\right)$. Therefore, $\operatorname{Mo}(T)-\operatorname{Mo}\left(T^{\prime}\right)=\sum_{i=1}^{s}\left(\psi_{T}\left(z_{i-1} z_{i}\right)-\psi_{T^{\prime}}\left(z_{i-1} z_{i}\right)\right)>0$, i.e., $M o(T)>\operatorname{Mo}\left(T^{\prime}\right)$, a contradiction. This proves the claim.

By the claim, $T$ has at most two branch vertices. If $T$ has exactly one branch vertex, then $T$ consists of $r$ pendent paths at a common vertex. By Lemma 2.2, $T \cong A_{n}(r-1,1)$. By Lemma 2.3, we have $r=3$ and $T \cong A_{n}\left(\left\lceil\frac{r}{2}\right\rceil,\left\lfloor\frac{r}{2}\right\rfloor\right)$.

Suppose that $T$ has exactly two branch vertices, say $x$ and $y$. Let $a=d_{T}(x)-1$ and $b=d_{T}(y)-1$. Obviously, $a, b \geq 2$, and there are $a$ pendent paths at $x$ and $b$ pendent paths at $y$. By Lemma 2.2, among the $a$ ( $b$, respectively) pendent paths at $x$ ( $y$, respectively), all except one are of length one. As early, let $P$ be the path connecting $x$ and $y$, and let $n_{x}$ ( $n_{y}$, respectively) be the order of the component of $T-E(P)$ containing $x$ ( $y$, respectively). Assume that $n_{x} \geq n_{y}$. Then $n_{y} \leq \frac{n}{2}$.

Suppose that there is a pendent path at $y$ whose length is at least two. Let $y_{0} \ldots y_{\ell}$ be this path, where $y_{0}=y$. Let $T^{\prime \prime}=T-\{y v: v \in N\}+\left\{y_{1} v: v \in N\right\}$, where $N$ is the set of pendent neighbors of $y$. Obviously, $T^{\prime \prime}$ is a tree of order $n$ with $r$ pendent vertices. As $\ell<n_{y}-1<\frac{n}{2}$, we have

$$
\operatorname{Mo}(T)-\operatorname{Mo}\left(T^{\prime}\right)=\psi_{T}\left(y_{0} y_{1}\right)-\psi_{T^{\prime \prime}}\left(y_{0} y_{1}\right)=|\ell-(n-\ell)|-\left|n_{y}-1-\left(n-n_{y}+1\right)\right|>0,
$$

i.e., $M o(T)>M o\left(T^{\prime \prime}\right)$, a contradiction. Thus, all pendent paths at $y$ are of length one.

Suppose that $n_{x}>\frac{n}{2}$ and there is a pendent path at $x$ whose length is at least two. Let $P=z_{0} \ldots z_{s}$, where $z_{0}=x$ and $z_{s}=y$. Let $u$ be a pendent neighbor of $x$. Let $T^{*}=T-x u+y u$. Note that $T^{*}$ is a tree of order $n$ with $r$ pendent vertices, and that

$$
\operatorname{Mo}(T)-\operatorname{Mo}\left(T^{*}\right)=\psi_{T}\left(z_{s-1} z_{s}\right)-\psi_{T^{*}}\left(z_{0} z_{1}\right)=\left|n_{y}-\left(n-n_{y}\right)\right|-\left|n_{x}-1-\left(n-n_{x}+1\right)\right| .
$$

If $n_{x}>\frac{n+1}{2}$, i.e., $n_{x} \geq \frac{n}{2}+1$ then, as $n_{y}<n-n_{x}+1 \leq \frac{n}{2}$, we have $\operatorname{Mo}(T)-\operatorname{Mo}\left(T^{*}\right)>0$, i.e., $\operatorname{Mo}(T)>\operatorname{Mo}\left(T^{\prime}\right)$, a contradiction. Thus, $n_{x}=\frac{n+1}{2}$ and then $n_{y}=\frac{n+1}{2}-r$. If $s \geq 2$, then $n_{y}<n_{x}-1<\frac{n}{2}$, implying that $\operatorname{Mo}(T)>\operatorname{Mo}\left(T^{*}\right)$, also a contradiction. Therefore, we have $s=1$, and then $n_{y}=n_{x}-1$, implying that $M o(T)=M o\left(T^{*}\right)$. Now consider the tree $T^{*}$. Suppose that $a \geq 3$. Then the order of the component of $T^{*}-x y$ containing $x$ is smaller than $\frac{n}{2}$. By similar argument as above by deleting all pendent edges at $x$ in $T^{*}$ and adding the same number of pendent edges at the neighbor of $x$ in the pendent path with length at least two to get a tree $T^{* *}$ of order $n$ with $r$ pendent vertices such that $\operatorname{Mo}\left(T^{*}\right)>\operatorname{Mo}\left(T^{* *}\right)$. Then $\operatorname{Mo}(T)>M o\left(T^{* *}\right)$, a contradiction. Therefore, we are left with the case $a=2$, and then $T^{*} \cong A_{n}(1, b+1)$ with $b+2=r \geq 4$. By Lemma 2.3, $\operatorname{Mo}(T)=\operatorname{Mo}\left(T^{*}\right)>\operatorname{Mo}\left(A_{n}\left(\left\lceil\frac{r}{2}\right\rceil,\left\lfloor\frac{r}{2}\right\rfloor\right)\right)$, a contradiction. Therefore, all pendent paths at $x$ are of length one (which follows by similar argument as above if $n_{x} \leq \frac{n}{2}$ ). Then $T \cong A_{n}(a, b)$, where $a+b=r$ and $a \geq b \geq 2$. By Lemma 2.3, we have $T \cong A_{n}\left(\left\lceil\frac{r}{2}\right\rceil,\left\lfloor\frac{r}{2}\right\rfloor\right)$.

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