On Mostar Index of Trees with Parameters

Fazal Hayat\textsuperscript{a}, Bo Zhou\textsuperscript{a}

\textsuperscript{a}School of Mathematical Sciences, South China Normal University, Guangzhou 510631, PR China

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 \(uv\) 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 \(e = uv \in E(G)\), let \(N_u(e|G)\) and \(N_v(e|G)\) 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.,

\[ N_u(e|G) = \{ x \in V(G) : d_G(u, x) < d_G(v, x) \} , \]
\[ N_v(e|G) = \{ x \in V(G) : d_G(v, x) < d_G(u, x) \} . \]

The numbers of vertices of \(N_u(e|G)\) and \(N_v(e|G)\) are denoted by \(n_u(e|G)\) and \(n_v(e|G)\), respectively.

Let \(G\) be a connected graph. The Szeged index of \(G\), proposed by Gutman [9], is defined as

\[ Sz(G) = \sum_{e=uv \in E(G)} n_u(e|G)n_v(e|G) . \]

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
Lemma 2.3. Let $a$ and $b$ be positive integers with $a \geq b + 2$. Then $\text{Mo}(A_n(a - 1, b + 1)) < \text{Mo}(A_n(a, b))$.

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 $\text{Mo}(A_n(a, b)) > \text{Mo}(A_n(a - 1, b + 1))$, as 
$$\text{Mo}(A_n(a, b)) - \text{Mo}(A_n(a - 1, b + 1)) = |b + 1 - (n - b - 1)| - |a - (n - a)| > 0.$$

For a graph $G$ with $E_1 \subseteq E(G)$, $G - E_1$ denotes the graph with vertex set $V(G)$ and edge set $E(G) \setminus E_1$. Similarly, if $E_2 \subseteq E(\overline{G})$, then $G + E_2$ denotes the graph with vertex set $V(G)$ and edge set $E(G) \cup E_2$, where $\overline{G}$ is the complement of $G$. In particular, if $E_1 = \{e\}$ ($E_2 = \{f\}$, 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 $x'$ and $y'$ be respectively the neighbors of $x$ and $y$ in the path connecting $x$ and $y$. Let

$$G' = G - \{x_i : i = 1, \ldots, s\} + \{x' : i = 1, \ldots, s\},$$

$$G'' = G - \{y_j : i = 1, \ldots, t\} + \{y' : i = 1, \ldots, t\}.$$

Then $Mo(G < max\{Mo(G'), Mo(G'')\}$.

Proof. Let $e' = xx'$ and $e'' = yy'$. Note that, if $x$ and $y$ are adjacent, then $x' = y$ and $y' = x$. From the constructions of $G'$ and $G''$, we have $\psi_G(e) = \psi_G(e)$ for all $e \in G \setminus \{e'\}$, and $\psi_G(e) = \psi_G(e)$ for all $e \in G \setminus \{e''\}$. Let $n_i(f) = n_i(f(G))$ where $z \in \{x, x'\}$ if $f = e'$ and $z \in \{y, y'\}$ if $f = e''$. Then

$$Mo(G) - Mo(G') = \psi_G(e') - \psi_G(e') = |n_z(e') - n_z(e')| - |n_z(e') - s - (n_z(e') + s)|,$$

$$Mo(G) - Mo(G'') = \psi_G(e'') - \psi_G(e'') = |n_y(e'') - n_y(e'')| - |n_y(e'') - t - (n_y(e'') + t)|.$$

Obviously, $n_z(e') \geq n_y(e'')$ and $n_y(e'') \geq n_z(e')$. If $n_z(e') > n_y(e'')$ and $n_y(e'') > n_z(e')$, then $n_z(e') > n_y(e'') \geq n_y(e'') \geq n_z(e')$, which is a contradiction. Thus we have either $n_z(e') \leq n_y(e'')$ or $n_y(e'') \leq n_y(e'')$. In the former case, $Mo(G) - Mo(G') = n_z(e') - n_z(e') - (n_y(e'') - n_y(e') + 2s) = -2s < 0$, and in the latter case, $Mo(G) - Mo(G'') = n_y(e'') - n_y(e'') - (n_y(e'') - n_y(e'') + 2t) = -2t < 0$. Thus, $Mo(G) < Mo(G')$ or $Mo(G) < Mo(G'')$, as desired. \qed

For integer $k$, let $P_{n,d,k}$ be the tree obtained from the path $P_{d+1} = v_0v_1 \ldots v_d$ by attaching $n - d - 1$ pendent edges at $v_k$, where $1 \leq k \leq \lfloor \frac{d}{2} \rfloor$. Let $S(a_1, \ldots, a_r)$ be the tree consisting of $r$ pendent paths of lengths $a_1, \ldots, a_r$ respectively at a common vertex $u$, where $a_i \geq \cdots \geq a_r \geq 1$. If $a_i - a_j = 0, 1$ for any $i$ and $j$ with $1 \leq i < j \leq r$, then we call $S(a_1, \ldots, a_r)$ a balanced starlike tree and denoted by $BS_{n,r}$.

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 $\Delta$, $P_{n,\Delta - \Delta + 1, 1}$ 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 $Mo(T)$ is as small as possible. We only need to show that $T \equiv P_{n,\Delta - \Delta + 1, 1}$.

Choose a vertex $v \in V(T)$ with degree $\Delta$. Let $N_G(v) = \{v_1, \ldots, v_\Delta\}$. 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 $T$ 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 $T \equiv G_{\ell, m}$, 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 $Mo(T) = Mo(G_{\ell, m}) > Mo(G_{\ell, m + 1, m - 1})$, 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, $T \equiv P_{n,\Delta - \Delta + 1, 1}$. \qed

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 $d$, $P_{n,d,\lfloor \frac{d}{2} \rfloor}$ 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 $Mo(T)$ is as large as possible. We only need to show that $T \cong P_{n,d,\lfloor \frac{d}{2} \rfloor}$.

Let $P = v_0, \ldots, v_l$ be a diametric path of $T$. Suppose that $T$ is not a caterpillar. Then there exist some vertex say $w$ outside this set is adjacent to at least one member of the set). Obviously, $A$ outside this set is adjacent to at least one member of the set. Thus, $T$ is a tree of order $n$ with diameter $d$.

But by Lemma 2.1, $Mo(T) < Mo(T')$, a contradiction to the maximality of $T$. Thus, $T$ is a caterpillar.

Next, we show that all pendant 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 $Mo(T)$, which is a contradiction. Thus, all pendant 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 $1 \leq k \leq \lfloor \frac{d}{2} \rfloor$. Then $n - (2k + 2) \geq 0$. Suppose that $k < \lfloor \frac{d}{2} \rfloor$. Let $T' = P_{n,d,k+1}$. As $k - 1 < \min(d - k, n - (d - k)) \leq \frac{n}{2}$, we have $Mo(T) - Mo(T') = \psi_T(v_1v_{k+1}) - \psi_T(v_kv_{k+1}) = n - (d - k) - (d - k) - |k + 1 - (n - k - 1)| < 0$, implying that $Mo(T) < Mo(T')$, a contradiction. Therefore, $k = \lfloor \frac{d}{2} \rfloor$, i.e., $T \cong P_{n,d,\lfloor \frac{d}{2} \rfloor}$.

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 $BS_{n,r}$, we denote the starlike tree of order $n$ with $r$ pendent vertices, say $a_1, \ldots, a_r$. By Lemma 2.2, $BS_{n,r}$ is a tree of order $n$ with $r$ pendent vertices. Let $x$ be the vertex with maximum degree $r$ such that the $r$ primary paths have almost equal lengths, i.e., for any two pendant paths with length $\ell$ and $s$, $|\ell - s| = 0, 1$. Let $n - 1 = rs + t$, where $0 \leq t \leq r - 1$. Then $BS_{n,r}$ consists of $t$ pendant paths of length $s + 1$ and $r - t$ pendant paths of length $s$ at a common vertex.

Theorem 3.3. Among all trees of order $n$ with $r$ pendant vertices, $BS_{n,r}$ 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 $r$ pendant vertices such that $Mo(T)$ 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 $T - P$ containing $x$ ($y$, respectively). Assume that $n_x \geq n_y$. Obviously, $n_x \leq \frac{n}{2}$. Let $z$ be the neighbor of $y$ in $P$ and $w$ be any other neighbor of $y$. Let $n_{yw} = n_w(yw|T)$. Let $T' = T - yw + zw$. Obviously, $T'$ is a tree of order $n$ with $r$ pendant vertices. Note that $\psi_T(e) = \psi_T(e)$ for $e \in E(T) \setminus \{yz, yw\} = E(T') \setminus \{yz, zw\}$ and $\psi_T(yw) = \psi_T(zw)$. Thus

$$Mo(T) - Mo(T') = \psi_T(zw) - \psi_T(yw) = |n_y - (n - n_y)| - |(n_y - n_w) - n - (n_y - n_w)| < 0,$$

implying that $Mo(T) < Mo(T')$, a contradiction. This proves the claim.

By the claim, $T$ consists of $r$ some pendant paths at a common vertex. Let $a_1, \ldots, a_r$ be the lengths of these pendant 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 $T \cong G_{n,a_i,a_j}$, where $G$ is the graph obtained from $T$ by deleting vertices of degree two or one in two pendant paths with lengths $a_i$ and $a_j$, respectively. Obviously, $G_{n,a_i-1,a_j+1}$ is a tree of order $n$ with $r$ pendant vertices. By Lemma 2.2, $Mo(T) < Mo(G_{n,a_i-1,a_j+1})$, a contradiction. Therefore, $a_i - a_j = 0, 1$ for any $i$ and $j$ with $1 \leq i < j \leq r$. That is, $T \cong BS_{n,r}$.

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 $m - 1$ pendant paths of length two and $n - 2(m - 1)$ pendant edges at a common vertex. Obviously, $A_{n,m} = BS_{n,m-m}$ for $1 \leq m \leq \frac{n}{2}$.
Corollary 3.4. Among trees of order \( n \) with matching number \( s \) (domination number \( t \), respectively), \( A_{n,s} \) (\( A_{n,t} \), respectively) is the unique tree with maximum Mostar index, where \( 1 \leq s \leq \frac{n}{2} \) (\( 1 \leq t \leq \frac{n}{2} \), 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 \( Mo(B_{n,s}) < Mo(B_{n+1,s}) \). 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 \( BS_{n,r} \) and \( v \) a neighbor of \( u \) in a pendent path of length at least two. By Lemma 2.1 or 2.2, we have \( Mo(B_{n,r}) < Mo(B_{n+1,r}) \). Note that \( BS_{n,r} \) consists of \( r + 1 \) pendent paths at a common vertex \( u \). Now, by Lemma 2.2, \( Mo(B_{n+1,r}) \) is as small as possible. \( Mo(B_{n+1,r}) \) follows that \( Mo(B_{n+2,r}) < Mo(B_{n,r+1}) \) 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, \( T \equiv BS_{n,s} \) with \( n = n - s \), i.e., \( T \equiv BS_{n,n-s} = A_{n,s} \).

If \( T \) maximizes the Mostar index among trees of order \( n \) with domination number \( t \), then, by Theorem 3.3 and the above claim, \( T \equiv BS_{n,t} \) with \( n = n - t \) i.e., \( T \equiv BS_{n,n-t} = A_{n,t} \). \( \square \)

Theorem 3.5. Among trees of order \( n \) with \( r \) pendent vertices, \( A_{n}([\frac{n}{2}], [\frac{n}{2}]) \) 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 \( Mo(T) \) 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 \( T' = T - \{z_i : i = 1, \ldots, p\} + \{y_i : i = 1, \ldots, p\} \). Evidently, \( T' \) is a tree of order \( n \) with \( r \) pendent vertices. Let \( n' \) 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 \( n_y + s - i < \min(n_y + n_x' + s - i, n - n_y + n_x' + s - i) \leq \frac{n}{2} \), implying that \( \psi_T(z_i - z_j) = \max(|n_y + s - i|, n_x + n_x' + s - i) \geq n_x + n_x' + s - i \). Therefore, \( Mo(T) - Mo(T') = \sum_{j=1}^{s} (\psi_T(z_i - z_j) - \psi_T(z_j - z_i)) > 0 \), i.e., \( Mo(T) > Mo(T') \), 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, \( T \equiv A_n(r - 1, 1) \). By Lemma 2.3, we have \( r = 3 \) and \( T \equiv A_n([\frac{3}{2}], [\frac{3}{2}]) \).

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 \( y_0 \ldots y_t \) be this path, where \( y_0 = y \). Let \( T'' = T - \{y_i : i \in N\} + \{y_i : i \in N\} \), where \( N \) is the set of pendent neighbors of \( y \). Obviously, \( T'' \) is a tree of order \( n \) with \( r \) pendent vertices. As \( t < n_y - 1 - \frac{3}{2} \), we have

\[ Mo(T'') = \psi_T(y_0y_1) - \psi_T(y_0y_t) = |t - (n - t)| - |n_y - 1 - (n - n_y + 1)| > 0, \]

i.e., \( Mo(T) > Mo(T'') \), 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 \( T' = T - xu + yu \). Note that \( T' \) is a tree of order \( n \) with \( r \) pendent vertices, and that

\[ Mo(T'') = \psi_T(z_s - z_1) = |n_y - (n - n_y)| - |n_x - 1 - (n - n_x + 1)|.\]
If \( n_x > \frac{n}{2} \), i.e., \( n_x \geq \frac{n}{2} + 1 \) then, as \( n_y < n - n_x + 1 \leq \frac{n}{2} \), we have \( Mo(T) - Mo(T^*) > 0 \), i.e., \( Mo(T) > Mo(T^*) \), a contradiction. Thus, \( n_x = \frac{n}{2} + 1 \) and then \( n_y = \frac{n}{2} - r \). If \( s \geq 2 \), then \( n_y < n_x - 1 < \frac{n}{2} \), implying that \( Mo(T) > Mo(T^*) \), also a contradiction. Therefore, we have \( s = 1 \), and then \( n_y = n_x - 1 \), implying that \( Mo(T) = Mo(T^*) \). Now consider the tree \( T^* \). Suppose that \( a \geq 3 \). Then the order of the component of \( T^* - xy \) 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 \( Mo(T^*) > Mo(T^{**}) \). Then \( Mo(T) > Mo(T^{**}) \), a contradiction. Therefore, we are left with the case \( a = 2 \), and then \( T^* \equiv A_0(1, b + 1) \) with \( b + 2 = r \geq 4 \).

By Lemma 2.3, \( Mo(T) = Mo(T^*) > Mo(A_0(\lceil \frac{n}{2}\rceil, \lceil \frac{n}{2}\rceil)) \), a contradiction. Therefore, all pendent paths at \( x \) of length one (which follows by similar argument as above if \( n_x \leq \frac{n}{2} \)). Then \( T \equiv A_0(a, b) \), where \( a + b = r \) and \( a \geq b \geq 2 \). By Lemma 2.3, we have \( T \equiv A_0(\lceil \frac{n}{2}\rceil, \lceil \frac{n}{2}\rceil) \).

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References


