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More On Mostar Index*

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Abstract

For the purpose of measuring how far is a graph from being distance-balanced, Došlić *et al.* (J. Math. Chem., 56 (2018), 2995–3013) have recently introduced a new bond additive structural invariant called Mostar index as $Mo(G) = \sum_{e=uv\in E(G)} |n_u(e|G)-n_v(e|G)|$, where $n_u(e|G)$ denotes the number of vertices of G lying closer to u than to v. In this paper, we find a sharp lower bound for the Mostar index of trees in terms of their order and maximum degree and characterize the trees for which the lower bound are achieved. Moreover, we relate the Mostar index and irregularity index for graphs with diameter at most two and apply this result to find upper bounds for the Mostar index of sum, disjunction, and symmetric difference of graphs.

1 Introduction

All graphs considered in this paper are finite, simple and connected. Let G be a graph on n vertices and m edges. We denote the vertex set and edge set of G by $V(G)$ and $E(G)$, respectively. For $u \in V(G)$, we denote by $N_G(u)$ the set of all first neighbors of u in G. The cardinality of $N_G(u)$ is called the degree of u in G and denoted by $d_G(u)$. The distance $d_G(u, v)$ between the vertices $u, v \in V(G)$ is defined as the length of any shortest path in G connecting u and v. The diameter of G is the maximum distance between the pair of its vertices. Let $e = uv$ be an edge of G connecting the vertices u and v. We denote by $n_u(e|G)$ the number of vertices of G lying closer to u than to v. Note that the vertices equidistant from u and v are not counted in $n_u(e|G)$ or $n_v(e|G)$. For a vertex $z \in V(G)$, we denote by $m_z(G)$ the number of edges in G whose end-vertices have different distances from z, i.e., $m_z(G) = |\{uv \in E(G) : d_G(u, z) \neq d_G(v, z)\}|$.

A *graph invariant* (also known as *topological index*) is a numerical value associated to a graph which is structurally invariant. Some of the most important graph invariants are bond-additive which can be presented as the sum of contributions of edges in graph. The well-known *Zagreb indices* are among the oldest graph invariants firstly introduced by Gutman and Trinajstić in [15], where they examined the dependence of total π-electron energy on molecular structures, and this was elaborated on in [14]. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G are defined as

$$M_1(G) = \sum_{u\in V(G)} d_G(u)^2 \quad \text{and} \quad M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v).$$

For properties of Zagreb indices, see the recent survey [9] and the references cited therein.

A graph G is said to be *regular* if all its vertices have the same degree, otherwise it is said to be *irregular*. In order to provide a quantitative measure of graph irregularity, i.e., of the deviation of a graph from being regular, several graph topological indices have been proposed. Among the most investigated ones are the *irregularity index* [4] and the *total irregularity* [1] which are respectively defined as

$$irr(G) = \sum_{uv\in E(G)} \big|d_G(u) - d_G(v)\big| \quad \text{and} \quad irr_t(G) = \frac{1}{2} \sum_{u,v\in V(G)} \big|d_G(u) - d_G(v)\big|.$$

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We refer the reader to [2, 3, 11], for some recent results on irregularity measures.

A graph G is said to be *distance-balanced* if for every edge uv, the number of vertices lying closer to u than to v is equal to the number of vertices lying closer to v than to u. In many applications and problems of graph theory, it is of great importance to measure how far is a graph from being distance-balanced. Recently, Došlić *et al.* [13] proposed a new bond-additive structural invariant called *Mostar index* for that purpose. It was defined as

$$Mo(G) = \sum_{e=uv\in E(G)} \big|n_u(e|G) - n_v(e|G)\big|.$$

It is obvious that, a graph G is distance-balanecd if and only if $Mo(G) = 0$. So the Mostar index can be thought of as a quantitative refinement of the distance-non-balancedness of a graph. Since the Mostar index is a newly-introduced graph invariant, only a few mathematical properties of this invariant have been investigated. Došlić *et al.* [13] determined the extremal values of this invariant and characterized extremal trees and unicyclic graphs. Tepeh [17] proved a conjecture of Došlić *et al.* [13] on a characterization of bicyclic graphs with given number of vertices for which extremal values of Mostar index are attained. The purpose of this paper is to further study mathematical properties of this new graph invariant.

This paper is organized as follows. In Section 2, we find a sharp lower bound on the Mostar index of trees in terms of their order and maximal degree and characterize the trees which achieve this bound. In Section 3, we prove that for graphs with diameter at most two, Mostar index is equal to irregularity index and apply this result to find upper bounds for the Mostar index of some operations on graphs such as suspension, sum, disjunction, and symmetric difference.

2 Trees

In this section, we present a sharp lower bound for the Mostar index of trees in terms of their order and maximum degree. We also characterize all trees whose Mostar index achieves the lower bound.

A leaf of a tree T is a vertex of degree 1, a support vertex is a vertex adjacent to a leaf and a strong support vertex is a support vertex adjacent to at least two leaves. An end-support vertex is a support vertex whose all neighbors with exception at most one are leaves. A rooted tree is a tree having a distinguished vertex v, called the root. We denote by $\mathcal{T}_{n,\Delta}$ the set of trees of order n and maximum degree Δ. Let T be a tree of order n and let $f : E(T) \to \mathbb{Z}^+$ be a function defined by $f(uv) = |n_u(uv|T) - n_v(uv|T)|$. Hence $Mo(T) = \sum_{uv\in E(T)} f(uv)$.

Proposition 1 (**[13]**) *Let T be a tree of order n. Then*

$$Mo(P_n) = \lfloor \frac{(n-1)^2}{2} \rfloor \leq Mo(T) \leq (n-1)(n-2) = Mo(S_n),$$

with the left and the right inequality achieved if and only if $T = P_n$ and $T = S_n$, respectively.

Lemma 2 *Let T be a tree of order n with maximum degree Δ and let v be a vertex of maximum degree. If T has a vertex of degree at least three different from v, then there is a tree $T' \in \mathcal{T}_{n,\Delta}$ such that $Mo(T) > Mo(T')$.*

Proof. Let T be rooted at v. Let $u \neq v$ be a vertex of degree $d_T(u) = k \geq 3$ such that $d_T(u, v)$ is as large as possible and let $N_T(u) = \{u_1, u_2, \ldots, u_k\}$. We may assume that u_k is the parent of u. Now we distinguish three cases.

Case 1. u is an end-support vertex. Let $S = \{uu_1, uu_2\}$ and let T' be the tree obtained by attaching the path u_2u_1u to $T - \{u_1, u_2\}$. Suppose that $S' = \{uu_1, u_1u_2\}$. Clearly, $T' \in \mathcal{T}_{n,\Delta}$ and $\sum_{uv\in E(T)-S} f(uv) = \sum_{uv\in E(T')-S'} f(uv)$. By definition of the Mostar index,

$$Mo(T) = \sum_{uv\notin S} f(uv) + \sum_{uv\in S} f(uv) = \sum_{uv\in E(T)-S} f(uv) + 2|n-2|, \tag{1}$$

$$Mo(T') = \sum_{uv \notin S'} f(uv) + \sum_{uv \in S'} f(uv) = \sum_{uv \in E(T') - S'} f(uv) + |n-2| + |n-4|. \tag{2}$$

Combining Eqs. (1), (2) and the fact that $n \geq 4$, we obtain

$$Mo(T) - Mo(T') = 2(n-2) - (n-2) - (n-4) > 0.$$

Case 2. u is a support vertex. By Case 1, we may assume that u is not an end-support vertex and $d_T(u_1) = 1$. Suppose $d_T(u_2) = 2$ and T_{u_2} is the component of $T - uu_2$ containing u_2. Since, by the choice of vertex u, $d_T(u, v)$ is as large as possible, we may assume that T_{u_2} is the path $x_1x_2 \ldots x_t$, $t \geq 2$ and $u_2 = x_1$.

Let T' be the tree obtained from $T - uu_2$ by adding the path $u_1x_1x_2 \ldots x_t$ to this graph. Let $S = \{uu_1, uu_2\}$ and $S' = \{uu_1, u_1u_2\}$. Clearly, $T' \in \mathcal{T}_{n,\Delta}$ and $\sum_{uv \in E(T)-S} f(uv) = \sum_{uv \in E(T')-S'} f(uv)$. By definition of the Mostar index,

$$Mo(T) = \sum_{uv \notin S} f(uv) + |n-2| + |n-2t|, \tag{3}$$

$$Mo(T') = \sum_{uv \notin S'} f(uv) + |n-2t| + |n-2t-2|. \tag{4}$$

If $n \geq 2t+2$, by Eqs. (3) and (4), we have

$$Mo(T) - Mo(T') = (n-2) + (n-2t) - (n-2t) - (n-2t-2) > 0.$$

If $n < 2t+2$, by Eqs. (3), (4) and the fact that $n > t+2$, we have

$$Mo(T) - Mo(T') = (n-2) + |n-2t| - |n-2t| + (n-2t-2) = 2n-2t-4 > 0.$$

Case 3. u is not a support vertex. Suppose T_{u_1} and T_{u_2} are the components of $T - \{uu_1, uu_2\}$ containing u_1 and u_2, respectively. By the choice of vertex u, we may assume that $T_{u_1} = x_1x_2 \ldots x_t$, $t \geq 2$, $u_1 = x_1$ and $T_{u_2} = y_1y_2 \ldots y_s$, $t \geq 2$, $u_2 = y_1$. Then $d_T(x_i) = d_T(y_j) = 2$, $1 \leq i \leq s-1$, $1 \leq j \leq t-1$, and $d_T(x_s) = d_T(y_t) = 1$.

Let T' be the tree obtained from $T - T_{u_2}$ by adding the path $x_ty_sy_{s-1} \ldots y_2u_2$ to this graph. Let

$$S = \{uu_1, x_1x_2, \ldots, x_{t-1}x_t\} \cup \{uu_2, y_1y_2, \ldots, y_{s-1}y_s\},$$

$$S' = \{uu_1, x_1x_2, \ldots, x_{t-1}x_t\} \cup \{x_ty_s, y_sy_{s-1}, \ldots, y_2u_2\}.$$

Clearly, $T' \in \mathcal{T}_{n,\Delta}$ and $\sum_{uv \in E(T)-S} f(uv) = \sum_{uv \in E(T')-S'} f(uv)$. By definition of the Mostar index,

$$Mo(T') = \sum_{uv \notin S} f(uv) + |n-2t| + \sum_{i=1}^{t-1} |n-2t-2i| + |n-2s| + \sum_{j=1}^{s-1} |n-2s-2j|, \tag{5}$$

$$Mo(T') = \sum_{uv \notin S'} f(uv) + |n-2(t+s)| + \sum_{i=1}^{s+t-1} |n-2(t+s)-2i|. \tag{6}$$

If $n \geq 2(t+s)$, by Eqs. (5) and (6), we have

$$Mo(T) - Mo(T') = t(n-2t) - t(n-2t-2s) = 2ts > 0.$$

If $n < 2(t+s)$, by Eqs. (5), (6) and the fact that $n > t+s+1$, we have

$$Mo(T) - Mo(T') = t(n-2t) + t(t-1) + t(n-2t-2s) + t(t-1) = 2t(n-t-s-1) > 0.$$

This completes the proof. ■

A spider is a tree with at most one vertex of degree more than two, called the center of the spider (if no vertex is of degree more than two, then any vertex can be the center). A leg of a spider is a path from the center to a vertex of degree 1.

Lemma 3 *Let T be a spider of order n with $k \geq 3$ legs. If T has two legs of length at least 2, then there is a spider T' of order n with k legs such that $Mo(T) > Mo(T')$.*

Proof. Let v be the center of T and $N_T(v) = \{v_1, v_2, \ldots, v_k\}$. Root T at v. Assume, without loss of generality, that $d_T(v_1) = d_T(v_2) = 2$ and let $vx_1x_2\ldots x_t$, $v_1 = x_1$ and $vy_1y_2\ldots y_s$, $v_2 = y_1$ be two legs of T. Let T' be the tree obtained from T by deleting the edges $x_1x_2, \ldots, x_{t-1}x_t$ and adding the edges $y_sx_1, x_1x_2, \ldots, x_{t-1}x_t$. Suppose

$$S = \{vv_1, x_1x_2, \ldots, x_{t-1}x_t\} \cup \{vv_2, y_1y_2, \ldots, y_{s-1}y_s\},$$

$$S' = \{vv_1, y_tx_2, \ldots, x_{t-1}x_t\} \cup \{vv_2, y_1y_2, \ldots, y_{s-1}y_s\}.$$

Clearly, $\sum_{uv\in E(T)-S} f(uv) = \sum_{uv\in E(T')-S'} f(uv)$. By definition of the Mostar index, we have

$$Mo(T') = \sum_{uv\notin S} f(uv) + |n-2t| + \sum_{i=1}^{t-1} |n-2t-2i| + |n-2s| + \sum_{j=1}^{s-1} |n-2s-2j|, \tag{7}$$

$$Mo(T') = \sum_{uv\notin S'} f(uv) + |n-2(t+s)| + \sum_{i=1}^{s+t-1} |n-2(t+s)-2i|. \tag{8}$$

By Eqs. (7), (8) and the fact that $n > s+t+1$, we obtain $Mo(T) > Mo(T')$. ■

We are now ready to prove the main theorem of this section.

Theorem 4 *For any tree $T \in \mathcal{T}_{n,\Delta}$ of order $n \geq 2$,*

$$Mo(T) \geqslant \begin{cases} (\Delta-1)(2n-\Delta-2) & \text{if } \Delta > \frac{n}{2}, \\ \frac{n}{2}(\frac{n-2}{2}) + (\frac{n}{2}-\Delta)(\frac{n+2}{2}-\Delta) + (\Delta-1)(n-2) & \text{if } \Delta \leq \frac{n}{2} \text{ and } 2 \mid n, \\ (\frac{n-1}{2})^2 + (\frac{n+1}{2}-\Delta)^2 + (\Delta-1)(n-2) & \text{if } \Delta \leq \frac{n}{2} \text{ and } 2 \nmid n. \end{cases}$$

The equality holds if and only if T is a spider with at most one leg of length at least two.

Proof. Let T_1 be a tree of order $n \geq 2$ with maximum degree Δ such that

$$Mo(T_1) = \min\{Mo(T) : T \text{ is a tree of order } n \text{ with maximum degree } \Delta\}.$$

Let v be a vertex with maximum degree Δ. Root T_1 at v. If $\Delta = 2$, then T_1 is a path of order n and by Proposition 1,

$$Mo(P_n) = \lfloor \frac{(n-1)^2}{2} \rfloor = \begin{cases} \frac{n}{2}(\frac{n-2}{2}) + (\frac{n}{2}-2)(\frac{n+2}{2}-2) + (n-2) & \text{if } 2 \mid n, \\ (\frac{n-1}{2})^2 + (\frac{n+1}{2}-2)^2 + (n-2) & \text{if } 2 \nmid n. \end{cases}$$

Now let $\Delta \geq 3$. By the choice of T_1, we deduce from Lemma 2 that T_1 is a spider with center v. It follows from Lemma 3 and the choice of T_1 that T_1 has at most one leg of length at least two. First let all legs of T_1 have length one. Then T_1 is a star of order n and the result follows by Proposition 1. Now let T_1 have only one leg of length at least two. Then

$$Mo(T_1) = \begin{cases} (\Delta-1)(2n-\Delta-2) & \text{if } \Delta > \frac{n}{2}, \\ \frac{n}{2}(\frac{n-2}{2}) + (\frac{n}{2}-\Delta)(\frac{n+2}{2}-\Delta) + (\Delta-1)(n-2) & \text{if } \Delta \leq \frac{n}{2} \text{ and } 2 \mid n, \\ (\frac{n-1}{2})^2 + (\frac{n+1}{2}-\Delta)^2 + (\Delta-1)(n-2) & \text{if } \Delta \leq \frac{n}{2} \text{ and } 2 \nmid n. \end{cases}$$

This completes the proof. ■

3 Graphs with Diameter at Most Two

In this section, we study the Mostar index of graphs with diameter at most two and apply our results to compute the Mostar index of some graph operations.

Theorem 5 *Let G be a graph with diameter at most two. Then*

$$Mo(G) = irr(G).$$

Proof. Let $e = uv \in E(G)$. It is easy to see that, the vertex u and all the vertices of G other than v which are adjacent to u but not to v are lying closer to u than to v. Hence

$$n_u(e|G) = 1 + (d_G(u) - 1) - |N_u(G) \cap N_v(G)| = d_G(u) - |N_u(G) \cap N_v(G)|.$$

Similarly,

$$n_v(e|G) = d_G(v) - |N_u(G) \cap N_v(G)|.$$

Now by definition of the Mostar index, we have

$$\begin{aligned} Mo(G) &= \sum_{e=uv\in E(G)} \big|n_u(e|G) - n_v(e|G)\big| \\ &= \sum_{e=uv\in E(G)} \big|\big(d_G(u) - |N_u(G)\cap N_v(G)|\big) - \big(d_G(v) - |N_u(G)\cap N_v(G)|\big)\big| \\ &= \sum_{uv\in E(G)} \big|d_G(u) - d_G(v)\big| = irr(G). \end{aligned}$$

This completes the proof. ■

Now we apply Theorem 5 to compute the Mostar index of some graph operations. Readers interested in more information on topological indices of graph operations can be refereed to [2, 5, 6, 7, 8, 10, 12, 16].

The *sum* (also called *join*) of graphs G_1 and G_2, denoted by $G_1 + G_2$, is a graph obtained from G_1 and G_2 by joining each vertex of G_1 to all vertices of G_2. The definition can easily be generalized to $k \geq 3$ graphs.

At first, we consider the *suspension* of a given graph G which is defined as the sum of the trivial graph K_1 and G.

Theorem 6 *Let G be a graph of order n and size m. Then*

$$Mo(K_1 + G) = irr(G) + n(n-1) - 2m. \tag{9}$$

Proof. Since $K_1 + G$ is of diameter at most two, by Theorem 5, we have

$$\begin{aligned} Mo(K_1 + G) =& irr(K_1 + G) = \sum_{uv\in E(K_1+G)} \big|d_{K_1+G}(u) - d_{K_1+G}(v)\big| \\ =& \sum_{uv\in E(G)} \big|(d_G(u)+1) - (d_G(v)+1)\big| + \sum_{u\in V(G)} \big|n - (d_G(u)+1)\big| \\ =& \sum_{uv\in E(G)} \big|d_G(u) - d_G(v)\big| + \sum_{u\in V(G)} \big(n - 1 - d_G(u)\big) \\ =& irr(G) + n(n-1) - 2m, \end{aligned}$$

and Eq. (9) holds. ■

Fan graph F_n, *wheel graph* W_n, and *Windmill graph* $D_n^{(m)}$ are suspension of P_{n-1}, C_{n-1}, and mK_{n-1}, respectively, where mK_{n-1} denotes the union of m copies of the complete graph on $n-1$ vertices. Using Theorem 6, we easily arrive at:

Corollary 7 *For $n \geq 4$,*

1. $Mo(F_n) = n^2 - 5n + 8$;
2. $Mo(W_n) = (n-1)(n-4)$;
3. $Mo(D_n^{(m)}) = m(m-1)(n-1)^2$.

Now, we consider the sum of two non-trivial graphs.

Theorem 8 *Let G_1 and G_2 be non-trivial graphs of order n_1 and n_2, respectively. If $n_1 \geq n_2$, then*

$$Mo(G_1 + G_2) \leq irr(G_1) + irr(G_2) + n_2(n_1 - 1)(n_1 - 2). \tag{10}$$

Moreover, the bound is sharp.

Proof. The sum $G_1 + G_2$ is of diameter at most two. Eq. (10) now follows from Theorem 5 and the upper bound given in [2, Theorem 2] for $irr(G_1 + G_2)$. ■

The *complete r-partite graph* $K_{n_1,n_2,\ldots,n_r}$ is a sum of the empty graphs $\bar{K}_{n_1}, \ldots, \bar{K}_{n_r}$ and by Theorem 5, we arrive at:

Corollary 9

$$Mo(K_{n_1,n_2,\ldots,n_r}) = irr(K_{n_1,n_2,\ldots,n_r}) = \sum_{i=1}^{r-1} \sum_{j=i+1}^{r} n_i n_j |n_j - n_i|.$$

The *disjunction* of graphs G_1 and G_2, denoted by $G_1 \vee G_2$, is a graph with vertex set $V(G_1) \times V(G_2)$ in which the vertex (u_1, u_2) is adjacent to the vertex (v_1, v_2) if and only if $u_1v_1 \in E(G_1)$ or $u_2v_2 \in E(G_2)$.

Theorem 10 *Let G_1 and G_2 be graphs of order n_1 and n_2 and size m_1 and m_2, respectively. Then*

$$\begin{aligned} Mo(G_1 \vee G_2) \leq & \big({n_2}^3 - M_1(G_2)\big)irr(G_1) + \big({n_1}^3 - M_1(G_1)\big)irr(G_2) \\ & + \big(2n_2m_2 + M_1(G_2)\big)irr_t(G_1) + \big(2n_1m_1 + M_1(G_1)\big)irr_t(G_2). \end{aligned} \tag{11}$$

Proof. Note that $G_1 \vee G_2$ is of diameter at most two. Eq. (11) now follows from Theorem 5 and the upper bound given in [2, Theorem 9] for $irr(G_1 \vee G_2)$. ■

The *symmetric difference* of graphs G_1 and G_2, denoted by $G_1 \oplus G_2$, is a graph with vertex set $V(G_1) \times V(G_2)$ in which the vertex (u_1, u_2) is adjacent to the vertex (v_1, v_2) if and only if $u_1v_1 \in E(G_1)$ or $u_2v_2 \in E(G_2)$, but not both.

Theorem 11 *Let G_1 and G_2 be graphs of order n_1 and n_2 and size m_1 and m_2, respectively. Then*

$$\begin{aligned} Mo(G_1 \oplus G_2) \leq & \big({n_2}^3 - 4M_1(G_2)\big)irr(G_1) + \big({n_1}^3 - 4M_1(G_1)\big)irr(G_2) \\ & + 2\big(n_2m_2 + M_1(G_2)\big)irr_t(G_1) + 2\big(n_1m_1 + M_1(G_1)\big)irr_t(G_2). \end{aligned} \tag{12}$$

Proof. Note that $G_1 \oplus G_2$ is of diameter two. Eq. (12) now follows from Theorem 5 and the upper bound given in [2, Theorem 10] for $irr(G_1 \oplus G_2)$. ■

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