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Modified Sombor index of trees with a given diameter

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ABSTRACT: The modified Sombor index of a graph G is defined as the sum of weights $1/\sqrt{d_u^2+d_v^2}$ over all edges uv of G, where d_u and d_v are the degrees of the vertices u and v in G, respectively. In this paper, we give some relations between the modified Sombor index and diameter of graphs.

Key Words: Modified Sombor index, Diameter of graphs.

1. Introduction

Let G be a simple graph with vertex set $V = V(G)$ and edge set $E(G)$. The integers $n = n(G) = |V(G)|$ and $m = m(G) = |E(G)|$ are the *order* and the *size* of the graph G, respectively. The *open neighborhood* of vertex v is $N_G(v) = N(v) = \{u \in V(G)|uv \in E(G)\}$ and the *degree* of v is $d_G(v) = d_v = |N(v)|$. An edge v_1v_2 is called *local maximum* if its weight $\frac{1}{\sqrt{d_{v_1}^2+d_{v_2}^2}}$ is maximum in its neighborhood, in other words

$$\frac{1}{\sqrt{d_{v_1}^2+d_{v_2}^2}} \geq \frac{1}{\sqrt{d_{v_i}^2+d_u^2}}$$

for any edge v_iu for $i = 1, 2$.

A pendant vertex is a vertex of degree one. The distance between two vertices is the number of edges in the shortest path connecting them and the diameter $D(G)$ of G is the distance between any two furthest vertices in G. A diametral path is the shortest path in G connecting two vertices whose distance is $D(G)$.

Topological indices have been used and have been shown to give a high degree of predictability of pharmaceutical properties.

Recently, a new topological index, named as Sombor index [3], was introduced by Gutman, which is defined as

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2+d_v^2}.$$

Kulli and Gutman also proposed the modified Sombor index [5], which is defined as

$${}^mSO(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u^2+d_v^2}}.$$

In [7] authors obtained the first fourteen minimum chemical trees for Sombor indices. In [9] the authors studied chemical applicability of Sombor indices. In [2] obtained the extremal Sombor indices for chemical graphs, chemical trees and hexagonal systems. Chen et al. [1] studied extremal Sombor indices for tree and Huang and Liu [4] obtained some bounds for the modified Sombor index of graphs with given parameters. For more details, see [6,8]. In this work, we give several relations between the modified Sombor index and the diameter of graphs.

Main Results

In this section, we obtain the relationship between the modified Sombor index and the diameter. We start with proving the following lemma that will be needed to obtain our main result.

Lemma 1.1 *Let v_1v_2 be a local maximum edge in graph G. Then*

$${}^mSO(G) -{}^m SO(G - v_1v_2) > 0.$$

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Proof: By the definition of modified Sombor index, we have

$$\begin{aligned}
{}^{m}SO(G) -{}^{m} SO(G - v_1v_2) &= \frac{1}{\sqrt{d_{v_1}^2 + d_{v_2}^2}} + \sum_{u\in N_G(v_1)\setminus\{v_2\}} \left(\frac{1}{\sqrt{d_{v_1}^2 + d_u^2}} - \frac{1}{\sqrt{d_u^2 + (d_{v_1} - 1)^2}} \right) \\
&+ \sum_{v\in N_G(v_2)\setminus\{v_1\}} \left(\frac{1}{\sqrt{d_{v_2}^2 + d_v^2}} - \frac{1}{\sqrt{d_v^2 + (d_{v_2} - 1)^2}} \right) \\
&\geq \frac{1}{\sqrt{d_{v_1}^2 + d_{v_2}^2}} + (d_{v_1} - 1) \left(\frac{1}{\sqrt{d_{v_1}^2 + d_{v_2}^2}} - \frac{1}{\sqrt{d_{v_2}^2 + (d_{v_1} - 1)^2}} \right) \\
&+ (d_{v_2} - 1) \left(\frac{1}{\sqrt{d_{v_2}^2 + d_{v_1}^2}} - \frac{1}{\sqrt{d_{v_1}^2 + (d_{v_2} - 1)^2}} \right) \\
&= \frac{d_{v_1} + d_{v_2} - 1}{\sqrt{d_{v_1}^2 + d_{v_2}^2}} - \frac{d_{v_1} - 1}{\sqrt{d_{v_2}^2 + (d_{v_1} - 1)^2}} - \frac{d_{v_2} - 1}{\sqrt{d_{v_1}^2 + (d_{v_2} - 1)^2}} > 0.
\end{aligned}$$

It is not difficult to see that $\frac{d_{v_1}+d_{v_2}-1}{\sqrt{d_{v_1}^2+d_{v_2}^2}} > \frac{d_{v_1}-1}{\sqrt{d_{v_2}^2+(d_{v_1}-1)^2}} + \frac{d_{v_2}-1}{\sqrt{d_{v_1}^2+(d_{v_2}-1)^2}}$. □

If v_1v_2 is a leaf of G , i.e., at least one of $\{v_1v_2\}$ has degree one, we can see that it is a local maximum edge. Hence, by Lemma 1.1, we get the next result.

Corollary 1.1 *Let v_1v_2 be a leaf in the graph G. Then*

$${}^{m}SO(G) -{}^{m} SO(G - v_1v_2) > 0.$$

Now we gave the relation of modified Sombor index and diameter of trees as follows.

Theorem 1.1 *Let T be a tree with order $n \geq 4$ diameter $D(T)$. Then*

$$\begin{aligned}
{}^{m}SO(T) - D(T) &\geq \frac{n(\sqrt{2} - 4)}{4} - \frac{3\sqrt{2}}{4} + \frac{2\sqrt{5}}{5} + 1, \\
\frac{{}^{m}SO(T)}{D(T)} &\geq \frac{\sqrt{5}n - 3\sqrt{5} + 4\sqrt{2}}{2\sqrt{10}\,(n - 1)},
\end{aligned}$$

where equalities hold iff $T \cong P_n$.

Proof: Let $T = P_n$, then, we have ${}^{m}SO(T) = \frac{\sqrt{2}(n-3)}{4} + \frac{2\sqrt{5}}{5}$ and $D(T) = n - 1$. Therefore, our result holds. Now we let that $T \neq P_n$, then, $D(T) \leq n - 2$ and there are at least three pendent vertices in T. So, we can let that $P = u_0, u_1, \ldots, u_D$ be the longest path in T. Then at least one pendant vertex, say v_1, is not contained in P. Now we start an operation on T, i.e., we continually delete pendant vertices which are not contained in P until the resulting tree is P. Assume $v_1, v_2, \ldots, v_k$ are the vertices in the order they were deleted, we have

$${}^{m}SO(T) >{}^{m} SO(T - v_1) > \cdots >{}^{m} SO(T - \bigcup_{i=1}^{k} v_k) ={}^{m} SO(P) = \frac{\sqrt{2}D}{4} + \frac{2\sqrt{5}}{\sqrt{5}} - \frac{\sqrt{2}}{2}$$

by Corollary 1.1 and

$$D(T) = D(T - v_1) = \cdots = D(T - \bigcup_{i=1}^{k} v_k) = D.$$

Thus, we have

$$
\begin{aligned}
{}^{m}SO(T)-D(T) &>^{m} SO(P)-D(P)\\
&\geq \frac{(D+1)(\sqrt{2}-4)}{4}+\frac{2\sqrt{5}}{5}-\frac{(\sqrt{2}-4)}{4}-\frac{\sqrt{2}}{2}\\
&\geq \frac{(n-1)(\sqrt{2}-4)}{4}+\frac{2\sqrt{5}}{5}-\frac{(\sqrt{2}-4)}{4}-\frac{\sqrt{2}}{2}\\
&= \frac{(n-1)(\sqrt{2}-4)}{4}+\frac{2\sqrt{5}}{5}-\frac{3\sqrt{2}}{4}+1\\
&> \frac{n(\sqrt{2}-4)}{4}-\frac{3\sqrt{2}}{4}+\frac{2\sqrt{5}}{5}+1.
\end{aligned}
$$

Similarly to the above we can write that

$$
\begin{aligned}
\frac{{}^{m}SO(T)}{D(T)} &> \frac{{}^{m}SO(P)}{D(P)}\\
&= \frac{\frac{(D+1)\sqrt{2}}{4}+\frac{2\sqrt{5}}{5}-\frac{\sqrt{2}}{4}-\frac{\sqrt{2}}{2}}{D}\\
&= \frac{\frac{(D+1)\sqrt{2}}{4}+\frac{2\sqrt{5}}{5}-\frac{3\sqrt{2}}{4}}{D}\\
&\geq \frac{\frac{n\sqrt{2}}{4}+\frac{2\sqrt{5}}{5}-\frac{3\sqrt{2}}{4}}{n-1}\\
&= \frac{\sqrt{5}n-3\sqrt{5}+4\sqrt{2}}{2\sqrt{10}\,(n-1)}.
\end{aligned}
$$

□

This result seems true for any connected graph with order and we propose as a conjecture as follows:

Conjecture 1.1 *Let G be a connected graph with order $n \geq 4$ and diameter D. Then*

$$
{}^{m}SO(G)-D(G) \geq \frac{n(\sqrt{2}-4)}{4}-\frac{3\sqrt{2}}{4}+\frac{2\sqrt{5}}{5}+1.
$$

The following result was obtained from [4].

Lemma 1.2 *Let G be a simple graph with n vertices. Then*

$$
{}^{m}SO(G) \leq \frac{\sqrt{2}}{4}n
$$

with equality iff G is a regular graph.

Note that the complete graph K_n is a regular graph with diameter one, hence, by this fact and Lemma 1.2, we immediately get to the following result.

Lemma 1.3 *Let G be a simple graph with n vertices. Then*

$$
{}^{m}SO(G)-D(G) \leq \frac{\sqrt{2}}{4}n-1
$$

with equality iff $G \cong K_n$.

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