Solutions to Some Open Problems About Four Sombor–Index–Like Graph Invariants

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Abstract

This paper gives solutions to most of the open problems posed in the very recent paper [Z. Tang, Q. Li, H. Deng, Trees with extremal values of the Sombor-index-like graph invariants, *MATCH Commun. Math. Comput. Chem.* **90** (2023) 203–222].

1 Introduction and statements of problems

Throughout this paper, only finite graphs are considered. For notation and terminology from (chemical) graph theory, we refer the reader to relevant standard books; for example, [1, 2, 10, 11].

A graph invariant I_g is a function defined on the set of all graphs with the following property: $I_g(G_1) = I_g(G_2)$ whenever G_1 and G_2 are

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isomorphic. Recently, Gutman [6] proposed six graph invariants in view of geometric considerations and referred them to as Sombor-index-like graph invariants. (Detail about the classical Sombor indices can be found in [4,5,8].) This paper is concerned with four such Sombor-index-like graph invariants, which are defined for a graph G as

$$SO_{3}(G) = \sqrt{2}\pi \sum_{vw \in E(G)} \frac{d_{v}^{2} + d_{w}^{2}}{d_{v} + d_{w}},$$
$$SO_{4}(G) = \frac{\pi}{2} \sum_{uv \in E(G)} \left(\frac{d_{v}^{2} + d_{w}^{2}}{d_{v} + d_{w}}\right)^{2},$$
$$SO_{5}(G) = 2\pi \sum_{uv \in E(G)} \frac{|d_{v}^{2} - d_{w}^{2}|}{\sqrt{2} + 2\sqrt{d_{v}^{2} + d_{w}^{2}}},$$
$$SO_{6}(G) = \pi \sum_{uv \in E(G)} \left(\frac{d_{v}^{2} - d_{w}^{2}}{\sqrt{2} + 2\sqrt{d_{v}^{2} + d_{w}^{2}}}\right)^{2}$$

where E(G) denotes the set of edges of G and d_u represents the degree of a vertex u in G.

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By a chemical tree, we mean a tree of maximum degree at most 4. Let \mathcal{T}_n , \mathcal{CT}_n and \mathcal{CG}_n be the classes of all trees, chemical trees and connected graphs, respectively, of order n. Quite recently, Tang et al. [9] investigated some extremal properties of Sombor-index-like graph invariants and posed following open problems.

Problem 1. Find the extremal values of the graph invariants SO_5 and SO_6 in the classes \mathcal{T}_n and \mathcal{CT}_n .

Problem 2. Find the maximum value of the graph invariants SO_4 in the class \mathcal{T}_n .

Problem 3. Find the extremal values of the graph invariants SO_5 and SO_6 in the class CG_n .

Problem 4. Find the maximum values of the graph invariants SO_3 and SO_4 in the class CG_n .

In this paper, Problems 2 and 4 are solved completely. Also, partial solutions to Problems 1 and 3 are provided; more precisely, Problem 1 is solved for the class \mathcal{T}_n (this solution also resolve the minimal part of Problem 1 regarding \mathcal{CT}_n) and a solution to the minimal part of Problem 3 is indicated.

2 Results

A vertex x in a graph is said to be a pendent vertex if $d_x = 1$. An edge incident to a pendent vertex is known as a pendent edge. For an edge vw of a graph, define

$$SO_5(vw) = \frac{2\pi \left| d_v^2 - d_w^2 \right|}{\sqrt{2} + 2\sqrt{d_v^2 + d_w^2}}.$$

The following result gives the solution to the minimal part of Problem 1.

Proposition 1. If T is a tree of order at least 3, then

$$SO_5(T) \ge \frac{12\pi}{\sqrt{2} + 2\sqrt{5}}$$
 and $SO_6(T) \ge \frac{18\pi}{\left(\sqrt{2} + 2\sqrt{5}\right)^2}$,

where the equality in any of these two inequalities holds if and only if T is a path graph. Particularly, the path graph P_n uniquely attains the minimum values of SO_5 and SO_6 in the classes \mathcal{T}_n and \mathcal{CT}_n for each $n \in \{4, 5, 6, \ldots\}$.

Proof. Since the proofs of both desired inequalities are similar to each other, we prove one of them; namely, the one involving SO_5 . Consider a pendent vertex $u \in V(T)$ adjacent to a vertex v. Then

$$SO_5(uv) = \frac{2\pi(d_v^2 - 1)}{\sqrt{2} + 2\sqrt{d_v^2 + 1}} \ge \frac{6\pi}{\sqrt{2} + 2\sqrt{5}}$$

where the equation $SO_5(uv) = 6\pi/(\sqrt{2} + 2\sqrt{5})$ holds if and only if $d_v = 2$. Denote by $P_E(T)$ the set consisting of all pendent edges in T. By utilizing the definition of SO_5 , we have

$$SO_{5}(T) = \sum_{uv \in P_{E}(T)} SO_{5}(uv) + \sum_{xy \in E(T) \setminus P_{E}(T)} SO_{5}(xy)$$

$$\geq \sum_{uv \in P_{E}(T)} \frac{6\pi}{\sqrt{2} + 2\sqrt{5}} + \sum_{xy \in E(T) \setminus P_{E}(T)} (0) \qquad (1)$$

$$= \frac{6\pi}{\sqrt{2} + 2\sqrt{5}} |P_{E}(T)|$$

$$\geq \frac{12\pi}{\sqrt{2} + 2\sqrt{5}}. \qquad (2)$$

Certainly, the equality in (1) holds if and only if $\max\{d_v, d_u\} = 2$ for each edge $uv \in P_E(T)$ and $d_y = d_x$ for each edge $xy \in E(T) \setminus P_E(T)$. Note also that the equality in (2) holds if and only if the set $P_E(T)$ has only two elements.

Remark. The proof of Proposition 1 suggests slightly general lower bounds on SO_5 and SO_6 as given below. For a connected graph G with at least two edges and with n_1 pendent vertices, the following inequalities hold

$$SO_5(G) \ge \frac{6\pi}{\sqrt{2} + 2\sqrt{5}} n_1$$
 and $SO_6(G) \ge \frac{9\pi}{\left(\sqrt{2} + 2\sqrt{5}\right)^2} n_1$,

where the equality in any of these two inequalities holds if and only if G is either a path graph or a regular graph.

Next, we move towards a solution to the maximal part of Problem 1 for the case of trees. For this, we need the following lemma.

Lemma 1. The functions f and g defined by

$$f(x,y) = \frac{2\pi |x^2 - y^2|}{\sqrt{2} + 2\sqrt{x^2 + y^2}} \quad and \quad g(x,y) = \pi \left(\frac{x^2 - y^2}{\sqrt{2} + 2\sqrt{x^2 + y^2}}\right)^2$$

are strictly decreasing in x whenever $1 \le x \le y$.

The next lemma not only provides the solution to the maximal part of Problem 1 (take m = n - 1) concerning the class \mathcal{T}_n but also indicates the trivial solution to the minimal part of Problem 3.

Lemma 2. For $n \ge 3$, if G is a connected graph of order n and size m, then

$$0 \le SO_5(G) \le \frac{2\pi m \left((n-1)^2 - 1 \right)}{\sqrt{2} + 2\sqrt{(n-1)^2 + 1}} \tag{3}$$

and

$$0 \le SO_6(G) \le \pi m \left(\frac{(n-1)^2 - 1}{\sqrt{2} + 2\sqrt{(n-1)^2 + 1}}\right)^2 \tag{4}$$

where the left equality in either of the inequalities (3) and (4) holds if and only if G is regular, while the right equality in either of the inequalities (3) and (4) holds if and only if G is the star graph S_n .

Proof. Since the proofs of both desired inequalities are similar to each other, we prove one of them; namely, the inequality (3). It is obvious that $SO_5(G) \ge 0$ with equality if and only if G is regular. Now, consider an arbitrary edge $uv \in E(G)$ with the condition $d_u \le d_v$. By utilizing the function f defined in Lemma 1, we have

$$f(d_u, d_v) \le f(1, d_v) \le f(1, n-1)$$

where the equation $f(d_u, d_v) = f(1, n - 1)$ holds if and only if $(d_u, d_v) = (1, n - 1)$. Thus,

$$SO_5(G) = \sum_{uv \in E(G)} f(d_u, d_v) \le \sum_{uv \in E(G)} f(1, n-1) = m f(1, n-1),$$

where the equation $SO_5(G) = m f(1, n-1)$ holds if and only if G is the star graph S_n .

From Lemma 2, the next result follows.

Proposition 2. The star graph S_n uniquely attains the maximum values of SO_5 and SO_6 in the class \mathcal{T}_n for each $n \in \{4, 5, 6, \ldots\}$.

Now, we pay attention to solving Problem 2. For this, we need the following lemma.

Lemma 3. If G is a connected graph of order at least 3 with the minimum degree 1 and the maximum degree Δ , then

$$SO_4(G) \le \frac{\pi(\Delta^2 + 1)}{2\left(\Delta + 1\right)^2} F(G)$$

with equality if and only if $\{d_v, d_w\} = \{1, \Delta\}$ for every edge $vw \in E(G)$, where $F(G) = \sum_{x \in V(G)} d_x^3$, known as the forgotten topological index [3].

Proof. Note that the function f defined by

$$f(x,y) = \frac{\pi(x^2 + y^2)}{2(x+y)^2},$$

is strictly decreasing in x whenever $1 \leq x \leq y$. Thereby, for any edge $vw \in E(G)$ with $d_v \leq d_w$, it holds that

$$f(d_v, d_w) \le f(1, d_w) \le f(1, \Delta) \tag{5}$$

where the equation $f(d_v, d_w) = f(1, \Delta)$ holds if and only if $d_v = 1$ and $d_w = \Delta$. From (5) it follows that

$$\frac{\pi}{2} \left(\frac{d_v^2 + d_w^2}{d_v + d_w} \right)^2 \le (d_v^2 + d_w^2) f(1, \Delta).$$
(6)

Now, applying the summation over the edge set E(G) on (6) yields the desired result.

From a general result of [7], it follows that the inequality $F(T) < F(S_n)$ holds for any tree T of order n different from the star graph S_n . Also, for $\Delta \leq n-1$, it holds that

$$\frac{\pi(\Delta^2 + 1)}{2\left(\Delta + 1\right)^2} \le \frac{\pi((n-1)^2 + 1)}{2n^2}$$

with equality if and only if $\Delta = n - 1$. These observations together with Lemma 3 give the next result, which provides the solution to Problem 2.

Proposition 3. For $n \ge 3$, if T is a tree of order n different from the star graph S_n , then

$$SO_4(T) < \frac{\pi (n-1)((n-1)^2 + 1)^2}{2n^2}.$$

Particularly, the star graph S_n uniquely attains the maximum value of SO_4 in the class \mathcal{T}_n for each $n \in \{4, 5, 6, \ldots\}$.

Finally, in order to providing the solution to Problem 4, we give the following lemma.

Lemma 4. If G is a connected graph with the maximum degree Δ and size m, then

$$SO_3(G) \le \sqrt{2}\pi\Delta m$$
 and $SO_4(G) \le \frac{\pi\Delta^2 m}{2}$,

where the equality in either of the two inequalities holds if and only if G is a Δ -regular graph.

Proof. For any edge $vw \in E(G)$, it holds that $d_v^2 + d_w^2 \leq \Delta d_v + \Delta d_w$ and $(d_v^2 + d_w^2)^2 \leq (\Delta d_v + \Delta d_w)^2$, where the equality in either of the two inequalities holds if and only if $d_v = d_w = \Delta$.

The next result gives the solution to Problem 4.

Proposition 4. If G is a connected graph of order n, then

$$SO_3(G) \le \frac{\pi n(n-1)^2}{\sqrt{2}}$$
 and $SO_4(G) \le \frac{\pi n(n-1)^3}{4}$

where the equality in either of the two inequalities holds if and only if G is the complete graph K_n .

Proof. Let Δ and m be the maximum degree and size of G. Then, by utilizing Lemma 4, we get

$$SO_3(G) \le \sqrt{2\pi\Delta m} \le \frac{\pi n(n-1)^2}{\sqrt{2}}$$
 and $SO_4(G) \le \frac{\pi \Delta^2 m}{2} \le \frac{\pi n(n-1)^3}{4}$.

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