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The relations between the Sombor index and Merrifield-Simmons index

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Abstract. The *Sombor index* $SO(G)$ of a graph G is defined as $SO(G) = \sum_{uv\in E(G)} (d_G(u)^2 + d_G(v)^2)^{\frac{1}{2}}$, while the *Merrifield-Simmons index* $i(G)$ of a graph G is defined as $i(G) = \sum_{k\geq 0} i(G;k)$, where $d_G(x)$ is the degree of any one given vertex x in G and $i(G;k)$ denotes the number of k-membered independent sets of G. In this paper, we investigate the relations between the Sombor index and Merrifield-Simmons index. First, we compare the Sombor index with Merrifield-Simmons index for some special graph families, including chemical graphs, bipartite graphs, graphs with restricted number of edges or cut vertices and power graphs, and so on. Second, we determine sharp bounds on the difference between Sombor index and Merrifield-Simmons index for general graphs, connected graphs and some special connected graphs, including self-centered graphs and graphs with given independence number.

1. Introduction

Throughout this paper we consider only simple graphs. For a graph $G = (V, E)$ with vertex set $V = V(G)$ and edge set $E = E(G)$, the degree of a vertex v in G, denoted by $d_G(v)$, is the number of edges incident with v. The open neighborhood of a vertex v, denoted by $N_G(v)$, is the set of vertices adjacent to v in G. The close neighborhood of a vertex v, denoted by $N_G[v]$, is equal to $N_G(v) \cup \{v\}$. Let G be a graph. A subset S of $V(G)$ is called an independent set of G if the subgraph induced by S has no edges.

A topological index is a number, which represents a chemical structure in a graph-theoretical manner through the molecular graph, if this number correlates with a molecular property. Usually, topological indices can be used to understand physicochemical properties of chemical compounds. Till now, hundreds of topological indices have been introduced, studied and recognized to be useful tools in chemical researches. Those topological indices which gained much popularity during the past decades are the Randić connectivity index, the Zagreb indices, Wiener index and Merrifield-Simmons index.

The *Merrifield-Simmons index* of G, denoted by $i(G)$, is defined to be the total number of independent subsets, that is,

$$i(G) = \sum_{k\geq 0} i(G;k),$$

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where $i(G;k)$ denotes the number of k-membered independent sets of G for $k \geq 1$ and $i(G;0) = 1$. The relationships between the Merrifield-Simmons index and other graph invariants and topological indices have been investigated by Hua et al. [16, 17] and Xu et al. [29]. For relationships between other graph invariants, the readers are referred to [2, 6, 7, 14, 15, 18].

More recently, a new degree-based topological indices named the *Sombor index*, was proposed by Gutman in [10]. The Sombor index is defined for a graph G as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2},$$

where $d_G(u)$ and $d_G(v)$ are degrees of vertices u and v, respectively. For recent results on Sombor index, the readers are referred to [4, 5, 9, 19–22, 27].

In this paper, we investigate the relations between the Sombor index and Merrifield-Simmons index. First, we compare the Sombor index with Merrifield-Simmons index for some special graph families. Second, we determine sharp bounds on the difference between Sombor index and Merrifield-Simmons index for general graphs, connected graphs and some special connected graphs.

2. Preliminary results

In this section, we give some preliminary results for Sombor index and the Merrifield-Simmons index.

We first give two lemmas concerning Merrifield-Simmons index that will be used in the proof of our results.

Lemma 2.1 ([11]). *Let G be a graph.*

(*a*) *If u is a vertex in G, then $i(G) = i(G-u) + i(G - N_G[u])$;*
(*b*) *If xy is an edge in G, then $i(G) = i(G-xy) - i(G - \{N_G[x] \cup N_G[y]\})$.*

Lemma 2.1 (*b*) implies the following result.

Lemma 2.2. *Let G be a non-complete graph. Then*

$$i(G) > i(G+e),$$

where e is an edge in $E(\overline{G})$.

The following result is obvious from the definition of Sombor index.

Lemma 2.3. *Let G be a non-complete graph. Then*

$$SO(G) < SO(G+e),$$

where $e \in E(\overline{G})$.

According to Lemmas 2.2 and 2.3, we have the following result.

Lemma 2.4. *Let G be a non-complete graph. Then*

$$i(G) - SO(G) > i(G+e) - SO(G+e),$$

where $e \in E(\overline{G})$.

More recently, Gutman proved the following result on the Sombor index.

Theorem 2.5 ([10]). *Let T be a tree of order n. Then*

$$SO(T) \geq 2(n-3)\sqrt{2} + 2\sqrt{5}$$

with equality if and only if $T \cong P_n$.

Let F_n be the nth *Fibonacci number*, satisfying that $F_0 = 1$, $F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$ for $n \geq 2$. By the definition of Fibonacci number and Merrifield-Simmons index, we have $i(P_n) = F_{n+1}$.

We recall some established results on the Merrifield-Simmon index.

Theorem 2.6 ([12]). *Let G be a 2-edge-connected graph of order* $n \geq 4$. *Then*

$$i(G) \leq 2^{n-2} + 3$$

with equality if and only if $G \cong K_{2,n-2}$ *or* C_5.

Theorem 2.7 ([13]). *Let G be a connected graph of order* $n \geq 4$ *and k cut vertices. Then*

$$i(G) \geq (n-k)F_{k+1} + F_k$$

with equality if and only if $G \cong KP_{n,k}$, *where* $KP_{n,k}$ *is the graph obtained by connecting an edge between one pendent vertex of* P_k *and one vertex of the complete graph* K_{n-k}.

Theorem 2.8 ([25]). *Let T be a tree on n vertices with diameter d. Then*

$$i(T) \leq F_{d+2} + (2^{n-d-1} - 1)F_2F_d$$

with equality if and only if $T \cong W_{n,d,1}$, *where* $W_{n,d,1}$ *is the tree of diameter d obtained by attaching* $n-d-1$ *pendent vertices to* v_1 *(or* v_{d-1}*) of the path* $P_{d+1} = v_0v_1\cdots v_{d-1}v_d$.

The following result identifies the tree with the second largest Merrifield-Simmons index.

Theorem 2.9. *Let T be a tree of order* $n \geq 4$. *If* $T \ncong S_n$, *then*

$$i(G) \leq 3 \cdot 2^{n-3} + 2$$

with equality if and only if $T \cong S_{1,n-3}$.

Proof. Let d be the diameter of T. Since $T \ncong S_n$, we have $d \geq 3$. If $d = 3$, then T is the double star $S_{a,b}$ for $1 \leq a, b \leq n-3$ and $a + b = n-2$. By Lemma 2.1(a), $i(S_{a,b}) = 2^a(2^b + 1) + 2^b = 2^{n-2} + 2^a + 2^b \leq 2^{n-2} + 2^{n-3} + 2$ with equality if and only if $(a, b) = (1, n-3)$ or $(b, a) = (1, n-3)$, i.e., $T \cong S_{1,n-3}$.

From Theorem 2.8 and a result in [16] (Lemma 3.8), we know that for $d \geq 4$, we have $i(T) \leq i(W_{n,d,1}) \leq i(W_{n,4,1}) = 5 \cdot 2^{n-4} + 3$. So, $i(T) \leq 5 \cdot 2^{n-4} + 3 < 3 \cdot 2^{n-3} + 2 = i(S_{1,n-3})$.

This completes the proof. □

3. The relations between Sombor index and Merrifield-Simmons index

In this section, we investigate the relations between Sombor index and the Merrifield-Simmons index. We will proceed by dividing our discussions into two subsections.

3.1. Comparison between the Sombor index and Merrifield-Simmons index

In this subsection, we compare the Sombor index with Merrifield-Simmons index. We consider the following two examples.

Example 3.1. *For complete graph K_n, we have $SO(K_n) = \frac{\sqrt{2}n(n-1)^2}{2} > n + 1 = i(K_n)$ for $n \geq 3$.*

Example 3.2. *For star graph S_n, we have $SO(S_n) = (n-1)\sqrt{n^2 - 2n + 2} < n(n-1) < 2^{n-1} + 1 = i(S_n)$ for $n \geq 6$, while $SO(S_4) = 3\sqrt{10} > 9 = i(S_4)$.*

Two examples given above indicate that the Sombor index and Merrifield-Simmons index are incomparable for general connected graphs, even for trees. So, we aim to find that the relationship between the Merrifield-Simmons index and Sombor index for some special graph families.

We first give an upper bound for the Sombox index of graphs.

Proposition 3.3 ([23, 24]). *Let G be graph of order n and size m with maximum degree $\triangle$. Then*

$$SO(G) \leq \sqrt{2}\triangle m.$$

Next, we provide some present comparative results for the Sombor index and Merrifield-Simmons index.

Theorem 3.4. *Let G be a graph of order n and size m. If $m \leq \frac{n}{2}$, then*

$$i(G) > SO(G).$$

Proof. Let $\triangle$ be the maximum degree of G. Then $\triangle \leq \frac{n}{2}$. By assumption and Proposition 3.3, we have

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

Note that $i(G;2) = \frac{1}{2}\sum_{v \in V(G)}(n - 1 - d_G(v)) = \frac{1}{2}n(n-1) - m$. Thus,

$$\begin{aligned} i(G) &\geq i(G;0) + i(G;1) + i(G;2) \\ &= 1 + n + \frac{1}{2}n(n-1) - m \\ &\geq 1 + n + \frac{1}{2}n(n-1) - \frac{n}{2} \\ &= 1 + \frac{n^2}{2}. \end{aligned}$$

So, $i(G) > SO(G)$, as desired. □

A graph is said to be a *chemical graph* if the maximum degree of this graph is no more than 4.

Theorem 3.5. *Let G be a connected chemical graph with at least 26 vertices. Then*

$$i(G) > SO(G).$$

Proof. Let n and m be the order and size of G, respectively. According to the definition of chemical graph, we have $m \leq 2n$. Also, for each edge uv, we have $\sqrt{d_G(u)^2 + d_G(v)^2} \leq 4\sqrt{2}$. Thus, $SO(G) \leq 8\sqrt{2}n$. Similar to the proof of Theorem 3.4, we have

$$i(G) \geq 1 + n + \frac{1}{2}n(n-1) - m \geq 1 + n + \frac{1}{2}n(n-1) - 2n > \frac{1}{2}n(n-3).$$

Since $n \geq 26$, we have $i(G) > SO(G)$, as desired. □

For a graph G with $X \subseteq V(G)$ and $Y \subseteq V(G)$ such that $X \cap Y = \emptyset$, we let $e(X, Y)$ be the number of edges whose two end-vertices are in X and Y, respectively. Also, we let $\alpha(G[X])$ and $\alpha(G[Y])$ be the independence number of the subgraphs of G induced by X and Y, respectively.

Theorem 3.6. *Let G be a graph of order $n \geq 24$ with independence number α. If G satisfies*
(1) $e(X, V(G) \setminus X) \leq \alpha(G[X]) + \alpha(G[V(G) \setminus X]) - 1$ *for any vertex subset* $X \subseteq V(G)$, *and*
(2) $\alpha \geq \frac{n}{2}$,
then

$$i(G) > SO(G).$$

Proof. Let m be the size of of G. On the one hand, for any given vertex $v \in V(G)$, we let $X = \{v\}$. By (1), we have

$$d_G(v) = e(X, V(G) \setminus X) \leq 1 + \alpha(G[V(G) \setminus X]) - 1 = \alpha(G[V(G) \setminus X]).$$

Note that $\alpha(G[V(G) \setminus X]) \leq \alpha(G) = \alpha$. So, $d_G(v) \leq \alpha$ for each $v \in V(G)$.

On the other hand, for any given vertex $v \in S$, we have $d_G(v) \leq n - \alpha$, where S is one maximum independent set in G. Thus, by our assumption that $\alpha \geq \frac{n}{2}$, $d_G(v) \leq \min\{\alpha, n - \alpha\} = n - \alpha$ for each $v \in S$. So

$$m \leq \frac{1}{2}[(n-\alpha)\alpha + \alpha(n-\alpha)] = (n-\alpha)\alpha \leq \frac{n^2}{4},$$

and then $SO(G) \leq \frac{n^2}{4} \cdot \sqrt{2}\alpha = \frac{\sqrt{2}n^2\alpha}{4}$.

If $G \cong \overline{K}_n$, then $i(G) = 2^n > 0 = SO(G)$, as desired. So, we assume that $G \ncong \overline{K}_n$. Then $i(G) > \binom{\alpha}{0} + \binom{\alpha}{1} + +\binom{\alpha}{2} + \cdots + \binom{\alpha}{\alpha} = 2^\alpha$. Since $n \geq 24$, we have $\alpha \geq \frac{n}{2} \geq 12$. Thus,

$$i(G) > 2^\alpha \geq \sqrt{2}\alpha^3 \geq \frac{\sqrt{2}n^2\alpha}{4} \geq SO(G).$$

This completes the proof. □

Theorem 3.7. *Let G be a bipartite graph with at least 24 vertices. Then*

$$i(G) > SO(G).$$

Proof. Let n, m and $\triangle$ be the order, size and maximum degree of G, respectively. Suppose that S and T are the bipartite partition sets of $V(G)$, respectively. Let $|S| = s$ and $|T| = t$. Assume without loss of generality that $t \geq s$. If $s = 1$, then $G \cong S_n$. Since $n \geq 24$, by Example 3.2, we have $i(G) > SO(G)$. Now, we assume that $s \geq 2$. Then $n = s + t \geq 4$. Since $\triangle \leq n - 2$ and $m \leq st$, by Proposition 3.3,

$$\begin{aligned} SO(G) &\leq \sqrt{2}\triangle m \\ &\leq \sqrt{2}\triangle st \\ &\leq \sqrt{2}\triangle \cdot \Big(\frac{s+t}{2}\Big)^2 \\ &= \frac{\sqrt{2}\triangle n^2}{4} \\ &\leq \frac{\sqrt{2}(n-2)n^2}{4}. \end{aligned} \tag{1}$$

According to Lemma 2.2, adding edges into a graph will decrease the Merrifield-Simmons index. By Lemma 2.1, we have

$$\begin{aligned} i(G) &\geq i(K_{s,t}) \\ &= 2^s + 2^t - 1 \\ &\geq 2 \cdot 2^{\frac{s+t}{2}} - 1 \\ &= 2^{\frac{n}{2}+1} - 1. \end{aligned} \tag{2}$$

By (1) and (2),

$$i(G) - SO(G) \geq 2^{\frac{n}{2}+1} - 1 - \frac{\sqrt{2}(n-2)n^2}{4}.$$

Now, we consider the function $f(x) = 2^{\frac{x}{2}+1} - 1 - \frac{\sqrt{2}(x-2)x^2}{4}$. Then $f'(x) = \ln 2 \cdot 2^{\frac{x}{2}} - \frac{\sqrt{2}}{4}(3x^2 - 4x) = \ln 4 \cdot 2^{\frac{x}{2}-1} - \frac{\sqrt{2}}{4}(3x^2 - 4x) > 2^{\frac{x}{2}-1} - (3x^2 - 4x)$. Further, we consider the function $g(y) = 2^y - 12y^2 - 16y - 4$. Then $g'(y) = 2^y \ln 2 - 24y - 16$ and $g''(y) = 2^y(\ln 2)^2 - 24 > 2^{y-2} - 24$. It is easy to see that for $y \geq 7$, $g''(y) > 2^{y-2} - 24 > 0$. So, when $y \geq 7$, $g'(y)$ is a strictly increasing function, and then $g'(y) > g'(9) = 2^9 \ln 2 - 24 \times 9 - 16 > 2^8 - 232 = 24 > 0$. Now, when $y \geq 9$, $g(y)$ is a strictly increasing function, and then $g(y) > g(11) = 2^{11} - 12 \times 11^2 - 16 \times 11 - 8 > 0$. Therefore, when $x \geq 24$, we have $f'(x) > 2^{\frac{x}{2}-1} - (3x^2 - 4x) = g(\frac{x}{2} - 1) \geq g(11) > 0$. So, $f(x)$ is a strictly increasing function when $x \geq 24$. Since $n \geq 24$,

$$i(G) - SO(G) \quad \geq \quad f(n) \geq f(24) > 0.$$

This completes the proof. □

Theorem 3.8. *Let G be a graph with maximum degree* $\triangle$. *If there exists a vertex u in G such that* $i(G-u) \geq SO(G-u)$ *and* $i(G - N_G[u]) \geq (\sqrt{2}+1)\triangle^2$, *then*

$$i(G) > SO(G).$$

Proof. Let

$$\Psi_1 = \sum_{v \in N_G(u)} \sum_{w \in N_G(v) \setminus N_G(u)} \left(\sqrt{d_G(w)^2 + d_G(v)^2} - \sqrt{d_G(w)^2 + (d_G(v)-1)^2} \right)$$

and

$$\Psi_2 = \frac{1}{2} \sum_{v \in N_G(u)} \sum_{w \in N_G(v) \cap N_G(u)} \left(\sqrt{d_G(w)^2 + d_G(v)^2} - \sqrt{(d_G(w)-1)^2 + (d_G(v)-1)^2} \right).$$

Since

$$\sqrt{d_G(w)^2 + d_G(v)^2} - \sqrt{d_G(w)^2 + (d_G(v)-1)^2}$$

$$\begin{aligned} &= \frac{2d_G(v) - 1}{\sqrt{d_G(w)^2 + d_G(v)^2} + \sqrt{d_G(w)^2 + (d_G(v)-1)^2}} \\ &< \frac{2d_G(v) - 1}{d_G(v) + (d_G(v) - 1)} = 1, \end{aligned}$$

we have

$$\Psi_1 < \sum_{v \in N_G(u)} \sum_{w \in N_G(v) \setminus N_G(u)} 1.$$

Since

$$\sqrt{d_G(w)^2 + d_G(v)^2} - \sqrt{(d_G(w)-1)^2 + (d_G(v)-1)^2}$$

$$\begin{aligned} &= \frac{2(d_G(v) + d_G(w) - 1)}{\sqrt{d_G(w)^2 + d_G(v)^2} + \sqrt{(d_G(w)-1)^2 + (d_G(v)-1)^2}} \\ &< \frac{2(d_G(v) + d_G(w) - 1)}{d_G(v) + (d_G(w) - 1)} = 2, \end{aligned}$$

we have

$$\Psi_2 < \frac{1}{2} \sum_{v \in N_G(u)} \sum_{w \in N_G(v) \cap N_G(u)} 2 = \sum_{v \in N_G(u)} \sum_{w \in N_G(v) \cap N_G(u)} 1.$$

So

$$\Psi_1 + \Psi_2 < \sum_{v \in N_G(u)} \sum_{w \in N_G(v) \setminus N_G(u)} 1 + \sum_{v \in N_G(u)} \sum_{w \in N_G(v) \cap N_G(u)} 1 = \sum_{v \in N_G(u)} d_G(v) \leq \triangle^2.$$

Note that $SO(G) = SO(G-u) + \sum_{v\in N_G(u)} \sqrt{d_G(u)^2 + d_G(v)^2} + \Psi_1 + \Psi_2$. Thus,

$$\begin{aligned} SO(G) &< SO(G-u) + \sum_{v\in N_G(u)} \sqrt{d_G(u)^2 + d_G(v)^2} + \triangle^2 \\ &\le SO(G-u) + (\sqrt{2}+1)\triangle^2 \\ &\le i(G-u) + i(G-N_G[u]) \\ &= i(G), \end{aligned}$$

completing the proof. □

Next, we use the number of cut vertices in a graph to give a sufficient condition for a graph having larger Merrifield-Simmons index than Sombor index.

Theorem 3.9. *Let G be a connected graph of order $n \ge 20$ and k cut vertices. If $k \ge \frac{n}{2}$, then*

$$i(G) > SO(G).$$

Proof. By Theorem 2.7, we have $i(G) \ge (n-k)F_{k+1} + F_k$. Since G has k cut vertices, then $\triangle \le n-k$. So, $\sqrt{d_G(u)^2 + d_G(v)^2} \le \sqrt{2}(n-k)$ for each edge $uv \in E(G)$. Also, we have $2m \le n\triangle \le n(n-k)$, that is, $m \le \frac{n(n-k)}{2}$. Thus, $SO(G) \le \frac{\sqrt{2}}{2}n(n-k)^2$. Then

$$i(G) - SO(G) \ge (n-k)F_{k+1} + F_k - \frac{\sqrt{2}}{2}n(n-k)^2 > (n-k)F_{k+1} - \frac{\sqrt{2}}{2}n(n-k)^2.$$

Since $k \ge \frac{n}{2}$, we have

$$i(G) - SO(G) > (n-k)F_{k+1} - \sqrt{2}k(n-k)^2. \tag{3}$$

We have the following claim.

Claim 3.10. *For $k \ge 10$, $F_{k+1} \ge \sqrt{2}k^2$.*

Proof. We proceed by induction on k. When $k = 10$, $F_{k+1} = F_{11} = 144 > \sqrt{2}k^2$. When $k = 11$, $F_{k+1} = F_{12} = 233 > \sqrt{2}k^2$. Now, we assume that $k \ge 12$ and assume that Claim 3.10 holds for smaller values of k. So, by induction hypothesis, we have

$$\begin{aligned} F_{k+1} &= F_k + F_{k-1} \\ &\ge \sqrt{2}(k-1)^2 + \sqrt{2}(k-2)^2 \\ &> \sqrt{2}k^2. \end{aligned}$$

This proves the claim. □

Since $n \ge 20$, we have $k \ge 10$. Thus, by Claim 3.10 and (3), we have

$$i(G) - SO(G) > (n-k)F_{k+1} - \sqrt{2}k(n-k)^2 \ge \sqrt{2}k(n-k)(2k-n) \ge 0,$$

as expected. □

At the end of this subsection, we compare the Sombor index with Merrifield-Simmons index for a special graph family.

For a positive integer k, the *kth power* of a graph G (see [1]), denoted by G^k, is a graph whose vertex set is the same as that of G such that two vertices are adjacent in G^k if and only if their distance is at most k in G. When $k = 1$, we set $G^k = G$.

Theorem 3.11. *For any positive integer k, let G be a graph and G^k be the kth power of G. If $i(G) < SO(G)$, then*

$$i(G^k) < SO(G^k).$$

Proof. By Lemmas 2.2, 2.3 and the definition of the kth power graph, we clearly have $i(G^k) < i(G)$ and $SO(G^k) > SO(G)$. So, the result follows as expected. □

3.2. The difference between the Sombor index and Merrifield-Simmons index

In this subsection, we study the the difference between the Sombor index and Merrifield-Simmons index. More specifically, we determine sharp bounds on the difference between the Sombor index and Merrifield-Simmons index for general graphs, connected graphs and some special connected graphs.

We first give sharp bounds on the difference between the Sombor index and Merrifield-Simmons index of general graphs.

Theorem 3.12. *Let G be a graph of order n. Then*

$$n + 1 - \frac{\sqrt{2}n(n-1)^2}{2} \leq i(G) - SO(G) \leq 2^n \tag{4}$$

with the left-hand side equality if and only if $G \cong K_n$, and the right-hand side equality if and only if $G \cong \overline{K_n}$.

Proof. By Lemma 2.4, adding edges into a graph will strictly decrease the value of $i(G)-SO(G)$ and removing edges from a graph will strictly increase the value of $i(G) - SO(G)$. So, we obtain the desired result. □

Second, we give sharp bounds on the difference between Sombor index and Merrifield-Simmons index of connected graphs.

Theorem 3.13. *Let G be a connected graph of order n.*

(1) *For $n \geq 2$,*

$$i(G) - SO(G) \geq n + 1 - \frac{\sqrt{2}n(n-1)^2}{2}$$

with equality if and only if $G \cong K_n$;

(2) *For $n \geq 9$,*

$$i(G) - SO(G) \leq 2^{n-1} + 1 - (n-1)\sqrt{n^2 - 2n + 2}$$

with equality if and only if $G \cong S_n$.

Proof. The lower bound is the same as that obtained in Theorem 3.12. Now, we consider the upper bound.

Let G be a graph attaining the maximum value of $i(G) - SO(G)$. We claim that G is a tree. Suppose to the contrary that G has at least one cycle and let e be any one edge in a cycle of G. By Lemma 2.4, $i(G) - SO(G) < i(G-e) - SO(G-e)$, a contradiction to our choice of G. So, G is a tree. Next, we shall prove that if $G \ncong S_n$, then

$$i(G) - SO(G) < 2^{n-1} + 1 - (n-1)\sqrt{n^2 - 2n + 2}.$$

Since $G \ncong S_n$, we have $i(G) \leq i(S_{1,n-3}) = 3 \cdot 2^{n-3} + 2$ by Theorem 2.9. Also, $SO(G) \geq 2(n-3)\sqrt{2} + 2\sqrt{5}$ by Theorem 2.5. So, for $G \ncong S_n$,

$$i(G) - SO(G) \leq 3 \cdot 2^{n-3} + 2 - 2(n-3)\sqrt{2} - 2\sqrt{5}.$$

Now, it suffices to prove that

$$2^{n-1} + 1 - (n-1)\sqrt{n^2 - 2n + 2} > 3 \cdot 2^{n-3} + 2 - 2(n-3)\sqrt{2} - 2\sqrt{5},$$

that is,

$$2^{n-3} - (n-1)\sqrt{n^2 - 2n + 2} - 1 + 2(n-3)\sqrt{2} + 2\sqrt{5} > 0.$$

Further, as $n \geq 2$, we need only to prove that

$$2^{n-3} - (n-1)n - 1 + 2(n-3)\sqrt{2} + 2\sqrt{5} > 0.$$

Let $f(x) = 2^{x-3} - (x-1)x - 1 + 2(x-3)\sqrt{2} + 2\sqrt{5}$. Then $f'(x) = 2^{x-3}\ln 2 - 2x + 1 + 2\sqrt{2}$, $f''(x) = (2\ln 2)^2 \cdot 2^{x-3} - 2$. When $x \geq 4$, $f''(x) = (2\ln 2)^2 \cdot 2^{x-3} - 2 > 2^{x-3} - 2 \geq 0$. So, $f'(x)$ is a strictly increasing function on the interval $[4, +\infty)$. When $x \geq 8$, $f'(x) = 2^{x-3}\ln 2 - 2x + 1 + 2\sqrt{2} > 2^{x-4} - 2x + 1 + 2\sqrt{2} > 0$. Then $f(x)$ is a strictly increasing function on the interval $[8, +\infty)$. Thus, $f(x) \geq f(9) = -9 + 12\sqrt{2} + 2\sqrt{5} > 0$. Since $n \geq 9$, we have

$$2^{n-3} - (n-1)n - 1 + 2(n-3)\sqrt{2} + 2\sqrt{5} = f(n) \geq f(9) > 0.$$

This completes the proof. □

Finally, we give sharp bounds on the difference between the Sombor index and Merrifield-Simmons index of some special connected graphs.

Recall that a self-centered graph has two vertices is just the path P_2, and the self-centered graph having three vertices is just the cycle C_3. So, we assume that a self-centered graph has at least four vertices in the following result.

Theorem 3.14. *Let G be a self-centered graph of order $n \geq 4$. Then*

$$n + 1 - \frac{\sqrt{2}n(n-1)^2}{2} \leq i(G) - SO(G) \leq 2^{n-2} + 3 - 2\sqrt{2}n \tag{5}$$

with the left-hand side equality if and only if $G \cong K_n$, and the right-hand side equality if and only if $G \cong C_5$.

Proof. The lower bound is obvious from Theorem 3.13, as the complete graph K_n is self-centered. Now, we consider the upper bound.

Since G is a self-centered graph, G has no cut vertex, for otherwise, G is not a self-centered graph, a contradiction. Since G has no cut vertex, G is a 2-connected. Thus, G is also 2-edge-connected. By Theorem 2.6, $i(G) \leq 2^{n-2} + 3$ with equality if and only if $G \cong K_{2,n-2}$ or C_5. Let m be the size of G. As G is 2-connected, the minimum degree of G is at least two, and then $SO(G) \geq 2\sqrt{2}m \geq 2\sqrt{2}n = SO(C_n)$ with equality if and only if $m = n$ and all vertices of G have degree two, that is, $G \cong C_n$. So,

$$i(G) - SO(G) \leq 2^{n-2} + 3 - 2\sqrt{2}n$$

with equality if and only if $G \cong C_5$. □

Theorem 3.15. *Let G be a graph of order n with independence number α. Then*

$$i(G) - SO(G) \geq n + 2^{\alpha} - \alpha - \alpha(n-\alpha)\sqrt{2n^2 - 2n(\alpha+1) + \alpha^2 + 1} + \frac{\sqrt{2}}{2}(n-1)(n-\alpha)(n-\alpha-1)$$

with equality if and only if $G \cong K_{n-\alpha} \vee \alpha K_1$.

Proof. Take G to be a graph with the smallest value of $i(G) - SO(G)$. Let S be a maximum independent set in G. Then $|S| = \alpha$. By our choice of G, the subgraph $G[V(G) \setminus S]$ is a complete subgraph, for otherwise, by Lemma 2.4, adding edges into $G[V(G) \setminus S]$ will decrease the value of $i(G) - SO(G)$, a contradiction. Similarly, for any u in S and any v in $V(G) \setminus S$, there exists an edge connecting u and v. Thus, $G \cong K_{n-\alpha} \vee \alpha K_1$, and

$$i(G) - SO(G) = n + 2^{\alpha} - \alpha - \alpha(n-\alpha)\sqrt{2n^2 - 2n(\alpha+1) + \alpha^2 + 1} + \frac{\sqrt{2}}{2}(n-1)(n-\alpha)(n-\alpha-1).$$

This completes the proof. □

4. Concluding remarks

In this paper, we have investigated the relations between the Sombor index and Merrifield-Simmons index. First, we compared the Sombor index and Merrifield-Simmons index for some special graphs. Second, we determined sharp bounds on the difference between Sombor index and Merrifield-Simmons index for general graphs, connected graphs and some special connected graphs.

Recall that most of our results in Section 2 deal with sufficient conditions for a graph G satisfying the inequality $i(G) > SO(G)$. We end the paper by proposing the following problem.

Problem 4.1. *Find all graphs G such that* $SO(G) > i(G)$.

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