DOI https://doi.org/10.24297/jam.v24i.9714

Ordering Unicyclic Graphs with a Fixed Girth by p-Sombor Indices

Ting Li[a], Bingjun Li[b,1]

[a]School of Mathematics & Statistics Guizhou University of Finance and Economics, Guiyang 550025, China.

[b]School of Mathematics & Statistics Guizhou University of Finance and Economics, Guiyang 550025, China.

asltsdd@sina.com, gfkdlbj@sina.com

Abstract

The p-Sombor index of a graphs G is defined as,

$$SOp(G) = \sum_{xy \in E(G)} (d^p(x) + d^p(y))^{\frac{1}{p}},$$

where $d(x)$ represents the degree of vertex x in graph G. Our focus centers on exploring the p-Sombor index of unicyclic graphs, specifically addressing graphs with a predetermined girth. We determine the first four smallest p-Sombor index and identifying the corresponding graphs that achieve these extremes.

Key words: p-Sombor index, Unicyclic graph.

1 Introduction

In our current scholarly pursuit, we concentrate on the examination of graphs that are undirected and connected, represented as $G = (V, E)$. For each vertex x within the graph G, it possesses a degree d_x, which signifies the quantity of vertices it is directly linked to. The set of vertices that are in direct adjacency with x is denoted by $N(x)$.

Within the domain of graph theory, a plethora of academic inquiries have been dedicated to exploring the Sombor index and its maximum and minimum characteristics across a spectrum of graph types, as referenced in $[1, 2, 8, 11, 16]$. In this paper, we present a summary of our findings and suggest potential avenues for future research. A straightforward next step would involve transcending the Euclidean norm employed by Gutman in the formulation of $SO(G)$. This entails considering the p-norm variant, which we refer to as the SO_p index, with the stipulation that $p \neq 0$. Notably, SO_1 corresponds to the First Zagreb index (as detailed in [7]), and SO_2 equates to the standard Sombor index. In this study, our emphasis will be placed on scenarios where p is greater than or equal to 1.

For a positive p, the edge contributions $\varphi_p(e) = (d_x^p + d_y^p)^{\frac{1}{p}}$ to $SOp(G)$ are well known: they appear as the sums $\mathfrak{S}_p(a)$ related to p-meals in the classical monograph [**?**] on inequalities. (Here a stands for the pair (d_x, d_y) of degrees of the end-vertices of $e = xy$.)

The Gutman et al. [4] have delved into the challenge of constructing graphs with a predetermined number of vertices n, while R ´eti et al. [**?**] have concentrated their efforts on various types of connected graphs, including those with a single cycle (unicyclic), two cycles (bicyclic), three cycles (tricyclic), four cycles (tetracyclic), and five cycles (pentacyclic), all of order n. Zhang and his collaborators [17], as well as Chen and Zhu [3], have each separately pinpointed the lowest Sombor index for unicyclic graphs that possess a consistent cycle length (girth). Nithya and her associates [14] employed an alternative methodology, categorizing unicyclic graphs with a fixed girth based on their Sombor index and identifying the quartet of graphs with the smallest Sombor indices. Following a comparable strategy, we extend our investigation to the p-Sombor index, aiming to uncover the top four graphs with the smallest p-Sombor indices.

[1]Corresponding author.

In recent years, the Sombor index has gained attention and application in fields such as chemistry and bioinformatics due to its ability to effectively characterize the complexity of molecular structures and other related physicochemical properties [13]. With the widespread application of graph theory in complex network analysis, the Sombor index is also regarded as a tool for evaluating the structural characteristics of networks, which can be used to describe various types of networks, such as protein interaction networks, social networks, computer networks, etc, and may further evolve into more sophisticated variations to meet specific needs in different fields [9]. Continued research dynamics suggest that with the development of theory and more interdisciplinary collaboration, the Sombor index and its related extensions will receive in-depth research and application in more scientific and technological fields , especially in those requiring the quantification and comparison of structural differences in complex systems. Researchers may explore how to optimize computational methods and how to combine other graph theory indices to enhance the understanding and predictive capabilities of complex network characteristics. A large amount of research in graph theory is dedicated to studying the extremal properties of the Sombor index across various classes of graphs [6].

As an important parameter in graph theory, the Sombor index holds multifaceted research value in the field of chemistry, particularly in chemical graph theory, where it has been found to effectively characterize the complexity of molecular structures, such as their thermodynamic properties related to entropy and enthalpy of vaporization [15]. By calculating the Sombor index of graphs corresponding to molecular structures, scientists can predict certain properties of compounds, which aids in the design of new drugs, the selection of organic synthesis routes, and the prediction of material properties. For various types of complex networks, the Sombor index provides a concise yet powerful metric that can be used to compare global connectivity, the tightness of local structures, and other network attributes across different networks [5]. It can be utilized to identify key nodes within a network, reveal hierarchical network structures, or detect anomalous substructures [10]. Thus, the Sombor index not only enriches the foundational theories of graph theory but also offers valuable quantitative tools in practical applications, contributing to the advancement and technological innovation in multiple scientific fields.

The p-Sombor index is a generalized version of the Sombor index, which becomes the standard Sombor index when p equals 2 [**?**]. The introduction of the p-Sombor index provides a more flexible tool for studying molecular structures, especially in exploring the impact of different parameters p on molecular properties. By adjusting the parameter p, the p-Sombor index can more finely capture changes in the strength of connections between vertices in molecular graphs, thus offering richer information about molecular structure than the traditional Sombor index. In chemistry and drug design, constructing accurate models for predicting molecular properties is crucial. The flexibility of the p-Sombor index allows researchers to select the most suitable p value according to different application scenarios, optimizing the predictive performance of the model. For instance, when searching for new drugs with specific biological activity, optimizing the model by adjusting the p value might help identify more effective drug candidates. Studying the extremal problems of the p-Sombor index, *i.e.*, determining which types of molecular structures lead to the maximum or minimum values of the p-Sombor index, is essential for understanding how molecular structure influences physical and chemical properties. This understanding not only aids chemists and materials scientists in designing molecules or materials with ideal characteristics but also enhances our knowledge of complex molecular systems existing in nature. Research on the p-Sombor index promotes interdisciplinary collaboration among mathematics, chemistry, and materials science. Through these collaborations, not only has the development of fundamental theories been advanced, but the application process of new technologies and materials has also been accelerated. In summary, the study of the p-Sombor index and its extremal problems not only deepens our understanding of the relationship between molecular structure and properties but also provides strong support for practical applications such as new drug development and material design [12].

Next we introduce certain notations and terminologies. The set $\mathbb{U}_n$, represents all unicyclic graphs that consist of at least five vertices. Subsequently, $\mathbb{U}_{n,\kappa}$ represents the subset of unicyclic graphs characterized by a fixed girth

$\kappa(3 \leq n \leq \kappa)$ and a specific number of n vertices. Interestingly, the set $\mathbb{U}_n$ can be constructed as the amalgamation of $\mathbb{U}_{n,\kappa}$ sets for varying girth values, a succinct depiction being $\mathbb{U}_n = \cup_{\kappa=3}^{n}\mathbb{U}_{n,\kappa}$. Furthermore, $\mathbf{C}_n$ denotes the cycle on n vertices, it can be inferred that $\mathbb{U}_{n,n} = \mathbf{C}_n$. In a similar manner, $\mathcal{U}_{n,n-1}^{1}$ denotes the distinctive unicyclic graph with a girth $n-1$ and n vertices is concluded that $\mathbb{U}_{n,n-1} = \mathcal{U}_{n,n-1}^{1}$. The forthcoming discussions will focus exclusively on instances where $3 \leq \kappa \leq n-2$.

2 Investigating the smallest p-Sombor indices in $\mathbb{U}_{n,\kappa}$ graphs

This section delves into the analysis of the graphs within the set $\mathbb{U}_{n,k}$, and aims to ascertain the first to fourth smallest values of the p-Sombor indices along with their corresponding extremal graphs. To facilitate this analysis, we commence by introducing several lemmas that will prove instrumental in our exploration.

Lemma 1. Let $f(x,y) = (x^p + y^p)^{\frac{1}{p}}$, where $x > 0$ and $y > 0$. The functions f and f_x are strictly increasing in x on the interval $[1,\infty)$, where f_x denotes the partical derivative function of f with respect to x. The function f_{xy} is stricly decreasing in y on the interval $[1,\infty)$, where f_{xy} denotes the second partical derivative function of f_x with respect to y.

Transformation 1. Consider G, G_1 be a non trivial connected graph. Choose two unique vertices x and y in G with $d_G(x) \geq 2$, $d_G(y) = 1$, a vertex z in G_1 with $d_{G_1}(z) \geq 1$. The two vertices x, y in G form a path V, where $V := xa_iy(i \geq 1)$, when $i = 0,\ a_0 = y$. Now, construct a graph I_1 by connecting the vertex z in graph G_1 through the vertex x in graph G; construct a graph I_2 by connecting the vertex z in graph G_1 through the vertex y in graph G.

Lemma 2. Consider the graph in Transformation 1 to be denoted by I_1 and I_2. Then

$$\begin{cases} SOp(I_1) > SOp(I_2), \text{when } i = 0 \text{ or } i = 1, \\ SOp(I_1) > SOp(I_2), \text{when } i \geq 2 \text{ and } d_z \leq d_{a_i} \text{ or } d_{a_1} \leq d_{a_i} \text{ or } d_{\alpha_i} \leq d_{a_i}. \end{cases}$$

Proof. Let $d_{I_1}(z) = \eta$, $d_{I_1}(x) = \alpha$, and $N_G(x) = N_{I_1}(x) \setminus \{z, y\} = \{x_1, x_2, ..., x_{\alpha-2}\}$ or $N_G(x) = N_{I_1}(x) \setminus \{a_1, z\} = \{x_1, x_2, ..., x_{\alpha-2}\}$. Each vertex x_i (for $1 \leq i \leq \alpha - 2$) has a degree in I_1, denoted as $d_{I_1}(x_i) = \alpha_i$. we intend to examine three scenarios, each with a different value for a_i.

Case 1. $i = 0$. (Refer to Fig. 1 for visual representation of these graphs.)

Fig. 1: Graphs I_1 and I_2

It follows that:

$$\begin{aligned}
SOp(I_1) - SOp(I_2) &= \sum_{i=1}^{\alpha-2}[(d_{I_1}^p(x) + d_{I_1}^p(x_i))^{\frac{1}{p}} - (d_{I_2}^p(x) + d_{I_2}^p(x_i))^{\frac{1}{p}}] \\
&+ (d_{I_1}^p(x) + d_z^p)^{\frac{1}{p}} - (d_{I_2}^p(y) + d_z^p)^{\frac{1}{p}} \\
&+ (d_{I_1}^p(x) + d_{I_1}^p(y))^{\frac{1}{p}} - (d_{I_2}^p(x) + d_{I_2}^p(y))^{\frac{1}{p}} \\
&= \sum_{i=1}^{\alpha-2}[(\alpha^p + \alpha_i^p)^{\frac{1}{p}} - ((\alpha-1)^p + \alpha_i^p)^{\frac{1}{p}}] \\
&+ (\alpha^p + \eta^p)^{\frac{1}{p}} - (2^p + \eta^p)^{\frac{1}{p}} \\
&+ (\alpha^p + 1^p)^{\frac{1}{p}} - ((\alpha-1)^p + 2^p)^{\frac{1}{p}} \\
&> (\alpha^p + 1^p)^{\frac{1}{p}} - ((\alpha-1)^p + 2^p)^{\frac{1}{p}}.
\end{aligned}$$

Note that $f(\alpha) = \alpha^p - (\alpha-1)^p$, where $\alpha \geq 3$. The function f are strictly increasing in α on the interval $[3, \infty)$, which is equivalent to

$$(\alpha^p - (\alpha-1)^p) > 2^p - 1^p. \tag{1}$$

From (1), it follows that $(\alpha^p + 1^p)^{\frac{1}{p}} - ((\alpha-1)^p + 2^p)^{\frac{1}{p}} > 0$.
Thus, $SOp(I_1) > SOp(I_2)$.

Case 2. $i = 1$. (Refer to Fig. 2 for visual representation of the graphs.)

Fig. 2: Graphs I_1 and I_2

It follows that:

$$\begin{aligned}
SOp(I_1) - SOp(I_2) = & \sum_{i=1}^{\alpha-2}[(d_{I_1}^p(x) + d_{I_1}^p(x_i))^{\frac{1}{p}} - (d_{I_2}^p(x) + d_{I_2}^p(x_i)^{\frac{1}{p}}] \\
& + (d_{I_1}^p(x) + d_z^p)^{\frac{1}{p}} - (d_{I_2}^p(y) + d_z^p)^{\frac{1}{p}} \\
& + (d_{I_1}^p(x) + d_{a_1}^p)^{\frac{1}{p}} - (d_{I_2}^p(x) + d_{a_1}^p)^{\frac{1}{p}} \\
& + (d_{I_1}^p(y) + d_{a_1}^p)^{\frac{1}{p}} - (d_{I_2}^p(y) + d_{a_1}^p)^{\frac{1}{p}} \\
= & \sum_{i=1}^{\alpha-2}[(\alpha^p + \alpha_i^p)^{\frac{1}{p}} - ((\alpha-1)^p + \alpha_i^p)^{\frac{1}{p}}] \\
& + (\alpha^p + \eta^p)^{\frac{1}{p}} - (2^p + \eta^p)^{\frac{1}{p}} + (\alpha^p + t^p)^{\frac{1}{p}} \\
& - ((\alpha-1)^p + t^p)^{\frac{1}{p}} + (1^p + t^p)^{\frac{1}{p}} - (2^p + t^p)^{\frac{1}{p}} \\
> & (\alpha^p + t^p)^{\frac{1}{p}} - ((\alpha-1)^p + t^p)^{\frac{1}{p}} \\
& - [(2^p + t^p)^{\frac{1}{p}} - (1^p + t^p)^{\frac{1}{p}}] \\
= & f(\alpha, t) - f(\alpha-1, t) - [f(2, t) - f(1, t)] \\
= & f_x(\mathbf{C}_1, t) - f_x(\mathbf{C}_2, t).
\end{aligned}$$

Note that $1 < \mathbf{C}_2 < 2 < \mathbf{C}_1 < \alpha$, by Lemma 1, we have $SOp(I_1) > SOp(I_2)$.

Case 3. $i \geq 2$. (Refer to Fig. 3 for visual representation of these graphs.)

Fig. 3: Graphs I_1 and I_2

It follows that:

$$\begin{aligned}
SOp(I_1) - SOp(I_2) &= \sum_{i=1}^{\alpha-2} [(d_{I_1}^p(x) + d_{I_1}^p(x_i))^{\frac{1}{p}} - (d_{I_2}^p(x) + d_{I_2}^p(x_i)^{\frac{1}{p}}] \\
&+ (d_{I_1}^p(x) + d_z^p)^{\frac{1}{p}} - (d_{I_2}^p(y) + d_z^p)^{\frac{1}{p}} \\
&+ (d_{I_1}^p(x) + d_{a_1}^p)^{\frac{1}{p}} - (d_{I_2}^p(x) + d_{a_1}^p)^{\frac{1}{p}} \\
&+ (d_{I_1}^p(y) + d_{a_i}^p)^{\frac{1}{p}} - (d_{I_2}^p(y) + d_{a_i}^p)^{\frac{1}{p}} \\
&= \sum_{i=1}^{\alpha-2} [(\alpha^p + \alpha_i^p)^{\frac{1}{p}} - ((\alpha-1)^p + \alpha_i^p)^{\frac{1}{p}}] \\
&+ (\alpha^p + \eta^p)^{\frac{1}{p}} - (2^p + \eta^p)^{\frac{1}{p}} \\
&+ (\alpha^p + t^p)^{\frac{1}{p}} - ((\alpha-1)^p + t^p)^{\frac{1}{p}} \\
&+ (1^p + m^p)^{\frac{1}{p}} - (2^p + m^p)^{\frac{1}{p}} \\
&> (\alpha^p + t^p)^{\frac{1}{p}} - ((\alpha-1)^p + t^p)^{\frac{1}{p}} \\
&+ (1^p + m^p)^{\frac{1}{p}} - (2^p + m^p)^{\frac{1}{p}}.
\end{aligned}$$

We construct a function $f(t) = (\alpha^p + t^p)^{\frac{1}{p}} - ((\alpha-1)^p + t^p)^{\frac{1}{p}}$, where $t \geq 0$. The function f is strictly decreasing in t on the interval $[0, \infty)$, we assume $t \leq m$.

$$\begin{aligned}
SOp(I_1) - SOp(I_2) &> (\alpha^p + m^p)^{\frac{1}{p}} - ((\alpha-1)^p + m^p)^{\frac{1}{p}} \\
&- [(2^p + m^p)^{\frac{1}{p}} - (1^p + m^p)^{\frac{1}{p}}] \\
&= f(\alpha, m) - f(\alpha-1, m) - [f(2, m) - f(1, m)] \\
&= f_x(\mathbf{C}_1, m) - f_x(mathbfC_2, m).
\end{aligned}$$

Because $1 < \mathbf{C}_2 < 2 < \mathbf{C}_1 < \alpha$, by lemma 1, we have $SOp(I_1) > SOp(I_2)$. In the same way, we also have

$$\begin{aligned}
SOp(I_1) - SOp(I_2) &> (\alpha^p + \alpha_i^p)^{\frac{1}{p}} - ((\alpha-1)^p + \alpha_i^p)^{\frac{1}{p}} \\
&- [(2^p + m^p)^{\frac{1}{p}} - (1^p + m^p)^{\frac{1}{p}}]
\end{aligned}$$

or

$$\begin{aligned}
SOp(I_1) - SOp(I_2) &> (\alpha^p + \eta^p)^{\frac{1}{p}} - (2^p + \eta^p)^{\frac{1}{p}} \\
&- [(2^p + m^p)^{\frac{1}{p}} - (1^p + m^p)^{\frac{1}{p}}].
\end{aligned}$$

So when $\alpha_i \leq m$ or $\eta \leq m$, we have $SOp(I_1) > SOp(I_2)$. In conclusion, $t \leq m$ or $\alpha_i \leq m$ or $\eta \leq m$, $SOp(I_1) > SOp(I_2)$. Hence this concludes the proof.

The graph known as $\mathcal{U}_{n,\kappa}$ is referred to as a unicyclic graph comprising n vertices and girth of κ, with $3 \leq \kappa \leq n-1$. As can be seen in Fig. 4, this graph is constructed by joining a vertex x to a cycle $\mathbf{C}_\kappa$ via a path that has a length of $n - \kappa$.

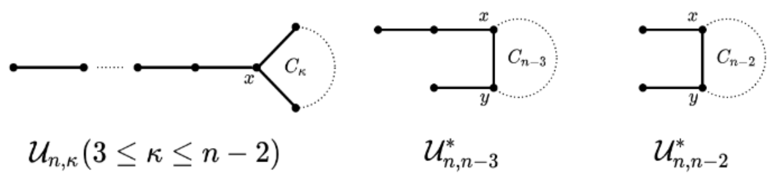

Fig. 4: The set of graphs $\mathcal{U}_{n,\kappa}(3 \le \kappa \le n-2)$, $\mathcal{U}^*_{n,n-3}$ and $\mathcal{U}^*_{n,n-2}$

Theorem 1. Consider $G \in \mathbb{U}_{n,\kappa}$ when $3 \le \kappa \le n-2$. For such graphs the following inequalities hold:

$$SOp(G) \ge (n-4)(2*2^p)^{\frac{1}{p}} + 3(3^p + 2^p)^{\frac{1}{p}} + (2^p + 1^p)^{\frac{1}{p}}.$$

Equality is maintained, if and only if $G \cong \mathcal{U}_{n,\kappa}$.

Proof. Consider $\mathbf{C} := y_1 y_2 y_3 ... y_\kappa y_1$, be the cycle graph in G. It follows that there is at least one vertex in $\{y_1, y_2, ..., y_\kappa\}$ of degree at least 3.

Assume to the contrary that at least two vertices in $\{y_1, y_2, ..., y_\kappa\}$ have degree at least three. In accordance with Lemma 2, we have $SOp(G) > SOp(\mathcal{U}_{n,\kappa})$, which is a contradiction. Thus, we may assume that the set $\{y_1, y_2, ..., y_\kappa\}$ contains exactly one vertex of degree at least 3, say y_i. If $d(y_i) \ge 4$ base on Lemma 2 $SOp(G) > SOp(\mathcal{U}_{n,\kappa})$, which is also a contradiction. Hence $d(y_i) = 3$ and by Lemma 2, equality is true if and only if $G \cong \mathcal{U}_{n,\kappa}$ and that $SO(G) \ge SO(\mathcal{U}_{n,\kappa})$.
Consequently,

$$SOp(\mathcal{U}_{n,\kappa}) = (n-4)(2*2^p)^{\frac{1}{p}} + 3(3^p + 2^p)^{\frac{1}{p}} + (2^p + 1^p)^{\frac{1}{p}}.$$

The proof for Theorem 1 is now concluded.

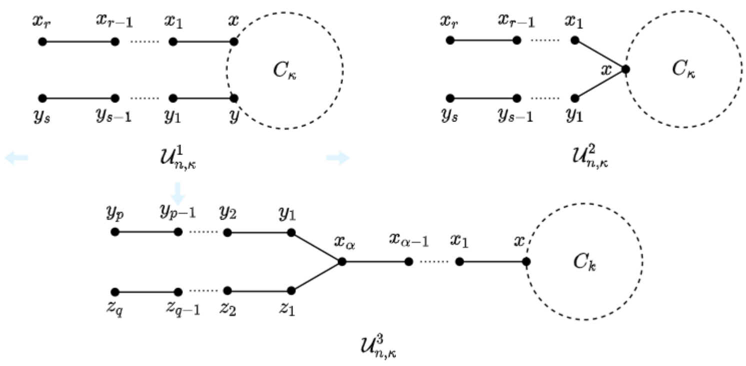

Fig. 5: The set of graphs $\mathcal{U}^1_{n,\kappa}$, $\mathcal{U}^2_{n,\kappa}(3 \le \kappa \le n-2)$ and $\mathcal{U}^3_{n,\kappa}(3 \le \kappa \le n-3)$

Supposing that for every integer κ where $3 \le \kappa \le n-2$, we can define three distinct sets of unicyclic graphs with n vertices. As can be seen in Fig. 5, within a cycle $\mathbf{C}_\kappa$, two paths of lengths r and s are attached to two separate vertices x and y to form the graphs $\mathcal{U}^1_{n,\kappa}$, where $r \ge s \ge 1$ and $r + s = n - \kappa$.

In the cycle $\mathbf{C}_\kappa$, two paths of lengths r and s are connected to a single vertex x to create the graphs $\mathcal{U}^2_{n,\kappa}$, where $r \geq s \geq 1$ and $r+s=n-\kappa$.

Additionally, a path of length a connects a vertex x from $\mathbf{C}_\kappa$ to another vertex y, which is not a pendant vertex. There are two more paths, y_p and z_q, where $p,q \geq 1$ and their combined length is $p+q=b$, which are connected to y. This configuration results in the graphs $\mathcal{U}^3_{n,\kappa}$, where $b \geq 2$, $a \geq 1$, and $a+b=n-\kappa$.

Lemma 3. Consider $G \in \mathcal{U}^1_{n,\kappa} \cup \mathcal{U}^2_{n,\kappa}$, when $3 \leq \kappa \leq n-4$. For such graphs, the following inequalities hold:

$$SOp(G) \geq (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (2*3^p)^{\frac{1}{p}} + 2(2^p+1^p)^{\frac{1}{p}}.$$

Equality is maintained, if and only if $G \in \mathcal{U}^1_{n,\kappa}$, for the edge xy belongs to the graph G with $r \geq s > 1$.

Proof. Suppose $G \in \mathcal{U}^1_{n,\kappa}$.
In the case where the edge xy belongs to the graph G. this implies that

$$SOp(G) = \begin{cases} (n-6)(2*2^p)^{\frac{1}{p}} + 3(3^p+2^p)^{\frac{1}{p}} + (2*3^p)^{\frac{1}{p}} + (3^p+1^p)^{\frac{1}{p}} \\ +(2^p+1^p)^{\frac{1}{p}}, \text{when } r > s = 1, \qquad (2) \\ (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (2*3^p)^{\frac{1}{p}} + 2(2^p+1^p)^{\frac{1}{p}}, \\ \text{when } r \geq s > 1. \qquad (3) \end{cases}$$

when $xy \notin E(G)$, then

$$SOp(G) = \begin{cases} (n-7)(2*2^p)^{\frac{1}{p}} + 5(3^p+2^p)^{\frac{1}{p}} + (3^p+1^p)^{\frac{1}{p}} + (2^p+1^p)^{\frac{1}{p}}, \\ \text{when } r > s = 1, \qquad (4) \\ (n-8)(2*2^p)^{\frac{1}{p}} + 6(3^p+2^p)^{\frac{1}{p}} + 2(2^p+1^p)^{\frac{1}{p}}, \\ \text{when } r \geq s > 1. \qquad (5) \end{cases}$$

Given that $G \in \mathcal{U}^2_{n,\kappa}$. It follows that

$$SOp(G) = \begin{cases} (n-5)(2*2^p)^{\frac{1}{p}} + 3(4^p+2^p)^{\frac{1}{p}} + (4^p+1^p)^{\frac{1}{p}} + (2^p+1^p)^{\frac{1}{p}}, \\ \text{when } r > s = 1, \qquad (6) \\ (n-6)(2*2^p)^{\frac{1}{p}} + 4(4^p+2^p)^{\frac{1}{p}} + 2(2^p+1^p)^{\frac{1}{p}}, \\ \text{when } r \geq s > 1. \qquad (7) \end{cases}$$

By

$$\begin{aligned}(2)-(3) &= (n-6)(2*2^p)^{\frac{1}{p}} + 3(3^p+2^p)^{\frac{1}{p}} + (2*3^p)^{\frac{1}{p}} \\ &+ (3^p+1^p)^{\frac{1}{p}} + (2^p+1^p)^{\frac{1}{p}} - [(n-7)(2*2^p)^{\frac{1}{p}} \\ &+ 4(3^p+2^p)^{\frac{1}{p}} + (2*3^p)^{\frac{1}{p}} + 2(2^p+1^p)^{\frac{1}{p}}] \\ &= (2*2^p)^{\frac{1}{p}} - (1^p+2^p)^{\frac{1}{p}} - [(2^p+3^p)^{\frac{1}{p}} - (1^p+3^p)^{\frac{1}{p}}].\end{aligned}$$

Because the function $f(t) = (\alpha^p + t^p)^{\frac{1}{p}} - ((\alpha-1)^p + t^p)^{\frac{1}{p}}$, where $t \geq 0$. The function f is strictly decreasing in t on the interval $[0, \infty)$. We find $(2) > (3)$. By the similar way, We can find the smallest p-Sombor index is

$SOp(G) = (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (2*3^p)^{\frac{1}{p}} + 2(2^p+1^p)^{\frac{1}{p}}$. Thus, we can conclude the proof.

Lemma 4. Consider $G \in \mathcal{U}^3_{n,\kappa}$, when $3 \leq \kappa \leq n-4$. For such graphs, the following inequalities hold:

$$SOp(G) \geq (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (2*3^p)^{\frac{1}{p}} + 2(2^p+1^p)^{\frac{1}{p}}.$$

Where equalitiy is achieved only under the condition that the edge xy belongs to the graph G *i.e.*, $a = 1$ and vertex $y \sim y_p$ and $y \sim z_q$, where $p > 1$ and $q > 1$.

Proof. Initially assume that $a = 1$. In this scenario, it can be deduced $b \geq 3$ and vertex $y \sim y_p$ and $y \sim z_q$ either $p = 1,\ q > 1$ or $q = 1,\ p > 1$. Hence,

$$SOp(G) = \begin{cases} (n-6)(2*2^p)^{\frac{1}{p}} + 3(3^p+2^p)^{\frac{1}{p}} + (2*3^p)^{\frac{1}{p}} + (3^p+1^p)^{\frac{1}{p}} \\ +(1^p+2^p)^{\frac{1}{p}}, \text{when } p = 1 \text{ or } q = 1, \\ (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(1^p+2^p)^{\frac{1}{p}}, \\ \text{when } p > 1 \text{ and } q > 1. \end{cases}$$

Assume that $a > 1$. Then

$$SOp(G) = \begin{cases} (n-6)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + 2(3^p+1^p)^{\frac{1}{p}}, \\ \text{when } p = 1 \text{ and } q = 1, \\ (n-7)(2*2^p)^{\frac{1}{p}} + 5(3^p+2^p)^{\frac{1}{p}} + (3^p+1^p)^{\frac{1}{p}} + (2^p+1^p)^{\frac{1}{p}}, \\ \text{when } p = 1 \text{ or } q = 1, \\ (n-8)(2*2^p)^{\frac{1}{p}} + 6(3^p+2^p)^{\frac{1}{p}} + 2(2^p+1^p)^{\frac{1}{p}}, \\ \text{when } p > 1 \text{ and } q > 1. \end{cases}$$

Though comparison, we find the smallest p-Sombor index is $SOp = (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(1^p+2^p)^{\frac{1}{p}}$. The lemma is true as a result.

Unicyclic graphs with a girth ranging from 3 to $n-4$, and having n vertices, are labeled as $\mathcal{U}^*_{n,\kappa}$. The construction of these graphs follows two unique methods: first, by attaching two paths, each no shorter than two units in length, to two adjacent vertices, labeled as x and y, on the cycle $\mathbf{C}_\kappa$; second, by creating an edge that links a vertex x in $\mathbf{C}_\kappa$ to another vertex y, which is part of a path with a length of $n-\kappa-1$.

Fig. 6 visually illustrates that y is positioned such that it does not border any of the pendant vertices. It is evident that the set $\mathcal{U}^*_{n,\kappa}$ is a subset of the union of $\mathcal{U}^1_{n,\kappa}$ and $\mathcal{U}^3_{n,\kappa}$. And $SOp(\mathcal{U}^*_{n,\kappa}) \geq (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p + 3^p)^{\frac{1}{p}} + 2*(1^p+2^p)^{\frac{1}{p}}$.

Further elaboration is as follows: when $\kappa = n-3$, the graph $\mathcal{U}^*_{n,n-3}$ is formed by appending a path of length 2 and an additional edge (a pendant edge) that connects two adjacent vertices, labeled as x and y, within the cycle $\mathbf{C}_{n-3}$. Similarly, when $\kappa = n-2$, it is feasible to construct the graph $\mathcal{U}^*_{n,n-2}$ by connecting two additional edges (pendant edges) to two adjacent vertices, labeled as x and y, on the cycle $\mathbf{C}_{n-2}$. This process is depicted in Fig. 4Fig. We can determine the second-smallest p-Sombor indices for the graphs within the set $\mathbb{U}_{n,\kappa}$ by applying reasoning similar to that used in the proof of Theorem 1.

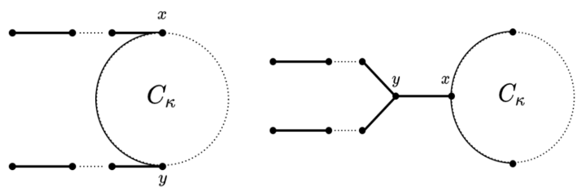

Fig. 6: Two categories of graphs in the set $\mathcal{U}^*_{n,\kappa}(3 \leq \kappa \leq n-4)$

Theorem 2. Consider $G \in \mathbb{U}_{n,\kappa}$ and $G \ncong \mathcal{U}_{n,\kappa}$. The following inequalities apply for such graphs:
(1) If $3 \leq \kappa \leq n-4$, then

$$SOp(G) \geq (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(1^p+2^p)^{\frac{1}{p}}.$$

Equality is maintained, if and only if $G \in \mathcal{U}^*_{n,\kappa}$.
(2) If $\kappa = n-3$, then

$$SOp(G) \geq (n-6)(2*2^p)^{\frac{1}{p}} + 3(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + (3^p+1^p)^{\frac{1}{p}} + (1^p+2^p)^{\frac{1}{p}}.$$

Equality is maintained, if and only if $G \cong \mathcal{U}^*_{n,n-3}$.
(3) If $\kappa = n-2$, then

$$SOp(G) \geq (n-5)(2*2^p)^{\frac{1}{p}} + 2(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(3^p+1^p)^{\frac{1}{p}}.$$

Equality is maintained, if and only if $G \cong \mathcal{U}^*_{n,n-2}$.

Proof. Consider a unique cycle $\mathbf{C}$ in G, represented as $\mathbf{C} := y_1y_2y_3...y_\kappa$
y_1, then a cycle with at least a degree of three must formed by at least one vertex from the set $\{y_1, y_2, y_3, ..., y_\kappa\}$.

If the cycle $\mathbf{C}$ in the graph G has a length that satisfies $3 \leq \kappa \leq n-4$, and if at least three vertices within the set $\{y_1, y_2, y_3, ..., y_\kappa\}$ have a degree of at least three, then by applying Lemmas 2 and 3, it can be concluded that there exists a graph G_1 in $\mathcal{U}^1_{n,\kappa}$ such that $SOp(G) > SOp(G_1) \geq (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(1^p+2^p)^{\frac{1}{p}}$. If exactly two vertices in the set $\{y_1, y_2, y_3, ..., y_\kappa\}$ have a degree of at least three, then according to Lemmas 2 and 3, there exists a graph G_2 in $\mathcal{U}^1_{n,\kappa}$ such that $SOp(G) \geq SOp(G_2) \geq (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(1^p+2^p)^{\frac{1}{p}}$. In the scenario where equality is achieved, this occurs if and only if G is an element of the intersection of $\mathcal{U}^1_{n,\kappa}$ and $\mathcal{U}^*_{n,\kappa}$.

According to Lemmas 2 and 3, if there is a vertex y_i in the set of vertices $\{y_1, y_2, y_3, ..., y_\kappa\}$ that have a degree of at least three and $d(y_i) \geq 5$, then it implies the existence of a graph $G_3 \in \mathcal{U}^2_{n,\kappa}$ such that $SOp(G) > SOp(G_3) > (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(1^p+2^p)^{\frac{1}{p}}$. In a similar way, if $d(y_i) = 4$, then there must be a graph $G_4 \in \mathcal{U}^2_{n,\kappa}$ such that $SOp(G) > SOp(G_4) > (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(1^p+2^p)^{\frac{1}{p}}$.

Therefore, we can deduce that $d(y_i) = 3$. Given that G is not isomorphic to $\mathcal{U}_{n,\kappa}$, it is necessary for the cycle $\mathbf{C}$ to exist that at least one vertex outside the cycle has a degree of at least three; otherwise, the cycle would not be possible. If there are at least two vertices outside of the cycle $\mathbf{C}$, each with a degree of at least three, then by applying Lemmas 2 and 4, we can infer that there exists a graph G_5 in $\mathcal{U}^3_{n,\kappa}$ such that $SOp(G) > SOp(G_5) \geq (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(1^p+2^p)^{\frac{1}{p}}$.

Consequently, we can assume that there is at least one vertex with a degree of at least three outside the cycle $\mathbf{C}$, indicating that G belongs to the set $\mathcal{U}^3_{n,\kappa}$. Then by utilizing Lemma 4, we can deduce that $SOp(G) \geq (n-7)(2*2^p)^{\frac{1}{p}} + 4(3^p+2^p)^{\frac{1}{p}} + (3^p+3^p)^{\frac{1}{p}} + 2(1^p+2^p)^{\frac{1}{p}}$.

Equality is maintained if and only if $G \in \mathcal{U}^*_{n,\kappa}$. Because $\mathcal{U}^*_{n,\kappa} \subseteq \mathcal{U}^1_{n,\kappa} \cup \mathcal{U}^3_{n,\kappa}$, the assertion 1 in the theorem must hold true. When considering scenarios where $\kappa = n-2$ or $\kappa = n-3$, similar reasoning shows that assertions 2 and 3 are also valid. Consequently, the theorem can be proven.

Given that

$$SOp(\mathcal{U}_{n,n-1}) = (n-3)(2\cdot 2^p)^{\frac{1}{p}} + 2(3^p+2^p)^{\frac{1}{p}} + (3^p+1^p)^{\frac{1}{p}}.$$

For the cycle $\mathbf{C}_n$, $SOp(\mathbf{C}_n) = n(2\cdot 2^p)^{\frac{1}{p}}$. The following conclusions can be readily drawn by applying Theorem 1 and Theorem 2.

Corollary 1. Let the graphs specified above be $\mathcal{U}_{n,\kappa}$ and $\mathcal{U}^*_{n,\kappa}$.
(1) If $n = 5$, then
$SOp(\mathcal{U}^*_{5,3}) > SOp(\mathcal{U}_{5,4}) > SOp(\mathcal{U}_{5,3}) > SOp(\mathbf{C}_5)$.
(2) If $n = 6$, then
$SOp(\mathcal{U}^*_{6,4}) > SOp(\mathcal{U}^*_{6,3}) > SOp(\mathcal{U}_{6,5}) > SOp(\mathcal{U}_{6,4}) > SOp(\mathbf{C}_6)$.
(3) If $n \geq 7$, then
$SOp(\mathcal{U}^*_{n,n-2}) > SOp(\mathcal{U}^*_{n,n-3}) > SOp(\mathcal{U}^*_{n,n-4}) = ... = SOp(\mathcal{U}^*_{n,3})$
$> SOp(\mathcal{U}_{n,n-1}) > SOp(\mathcal{U}_{n,3}) = ... = SOp(\mathcal{U}_{n,n-2}) > SOp(\mathbf{C}_n)$.

3 Conclusion

By using Theorem 1 and 2, along with Corollary 1, we can further deduce the following conclusions: The unique graphs in the $\mathcal{U}_{n,\kappa}$ set where $3 \leq \kappa \leq n-2$, that have the second-smallest p-Sombor indices, and the unique graphs in the $\mathcal{U}_{n,n-1}$ set that have the third-smallest p-Sombor indices, are all included in the $\mathbb{U}_n$ set. Moreover, the graphs in $\mathcal{U}^*_{5,3}$ have the fourth-smallest p-Sombor indices among all graphs in $\mathbb{U}_5$, and the graphs in $\mathcal{U}^*_{6,3}$ have the fourth-smallest p-Sombor indices among all graphs in $\mathbb{U}_6$. Lastly, for $n \geq 7$, the $\mathcal{U}^*_{n,\kappa}$ graph set with $3 \leq \kappa \leq n-4$ possess the fourth-smallest p-Sombor indices among all graphs in $\mathbb{U}_n$.

This work was supported by Natural Science Foundation of Guizhou Province (no. ZK2021019) and Guizhou University of Finance and Economics (no. 2024ZXSY225).

References

[1] Aarman Aashtab, Saieed Akbari, Saba Madadinia, Matineh Noei, and Fatemeh Salehi. On the graphs with minimum sombor index. *MATCH Commun. Math. Comput. Chem*, 88(3):553–559, 2022. `https://doi.org/10.46793/match.88-3.553A`.

[2] Hanlin Chen, Wenhao Li, and Jing Wang. Extremal values on the sombor index of trees. *MATCH Commun. Math. Comput. Chem*, 87(1):23–49, 2022. https://doi.org/10.46793/match.87-1.023C.

[3] Meng Chen and Yan Zhu. Extremal unicyclic graphs of sombor index. *Applied Mathematics and Computation*, 463:128374, 2024. https://doi.org/10.1016/j.amc.2023.128374.

[4] Kinkar Chandra Das and Ivan Gutman. On sombor index of trees. *Applied Mathematics and Computation*, 412:126575, 2022. https://doi.org/10.1016/j.amc.2021.126575.

[5] Kinkar Chandra Das, Ahmet Sinan Çevik, Ismail Naci Cangul, and Yilun Shang. On sombor index. *Symmetry*, 13(1):140, 2021. https://doi.org/10.3390/sym13010140.

[6] Hanyuan Deng, Zikai Tang, and Renfang Wu. Molecular trees with extremal values of sombor indices. *International Journal of Quantum Chemistry*, 121(11):e26622, 2021. https://doi.org/10.1002/qua.26622.

[7] Boris Furtula and Ivan Gutman. A forgotten topological index. *Journal of Mathematical Chemistry*, 53:1184–1190, 2015. https://doi.org/10.1007/s10910-015-0480-z.

[8] Ivan Gutman. Geometric approach to degree-based topological indices: Sombor indices. *MATCH Commun. Math. Comput. Chem*, 86(1):11–16, 2021. https://doi.org/10.46793/match.88-3.553A.

[9] Hechao Liu, Hanlin Chen, Qiqi Xiao, Xiaona Fang, and Zikai Tang. More on sombor indices of chemical graphs and their applications to the boiling point of benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, 121(17):e26689, 2021. https://doi.org/10.1002/qua.26689.

[10] Hechao Liu, Ivan Gutman, Lihua You, and Yufei Huang. Sombor index: review of extremal results and bounds. *Journal of Mathematical Chemistry*, 60:771–798, 2022. https://doi.org/10.1007/s10910-022-01342-9.

[11] Hechao Liu, Lihua You, and Yufei Huang. Extremal sombor indices of tetracyclic (chemical) graphs. *MATCH Commun. Math. Comput. Chem*, 88(3):573–581, 2022. https://doi.org/10.46793/match.88-3.573L.

[12] Hechao Liu, Lihua You, and Yufei Huang. Ordering chemical graphs by sombor indices and its applications. *MATCH Communications in Mathematical and in Computer Chemistry*, 87(1):5–22, 2022. https://doi.org/10.46793/match.87-1.005L.

[13] J. A. Méndez-Bermúdez, R. Aguilar-Sánchez, Edil D. Molina, and José M. Rodríguez. Mean sombor index. *Discrete Mathematics Letters*, 9:18–25, 2022. https://doi.org/10.47443/dml.2021.s204.

[14] Palaniyappan Nithya, Suresh Elumalai, Selvaraj Balachandran, and Mesfin Masre. Ordering unicyclic graphs with a fixed girth by sombor indices. *MATCH Commun. Math. Comput. Chem*, 92(1):205–224, 2024. https://doi.org/10.46793/match.92-1.205N.

[15] Izudin Redžepović. Chemical applicability of sombor indices. *Journal of the Serbian Chemical Society*, 86(5):445–457, 2021. https://doi.org/10.2298/JSC201215006R.

[16] B Senthilkumar, YB Venkatakrishnan, S Balachandran, Akbar Ali, Tariq A Alraqad, and Amjad E Hamza. On the maximum sombor index of unicyclic graphs with a fixed girth. *Journal of Mathematics*, (1):8202681, 2022. https://doi.org/10.1155/2022/8202681.

[17] Wanping Zhang, Jixiang Meng, and Na Wang. Extremal graphs for sombor index with given parameters. *Axioms*, 12(2):203, 2023. https://doi.org/10.3390/axioms12020203.