IOSR Journal of Computer Engineering (IOSR-JCE)
e-ISSN: 2278-0661, p-ISSN: 2278-8727, Volume 27, Issue 6, Ser. 2 (Nov. – Dec. 2025), PP 51-64
www.iosrjournals.org

Extremal p-Sombor Indices of Unicyclic Graphs

Ting Li[a] , Bingjun Li[b,*]
[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.*

Abstract

For a positive real number p *, the* p *-Somber index of a graph* G *, introducted by Réti et al, is defined as*

$$SOp(G) = \sum_{uv \in E(G)} (d(u)^p + d(v)^p)^{\frac{1}{p}},$$

where $d(u)$ *denotes the degree of the vertex* u *in* G *. In this paper, for* $p \geq 1$ *, we determine the first three largest* p *-Sombor indices among unicyclic graphs and characterize the corresponding extremal graphs.*

Keywords: *p-Sombor index, Unicyclic graph, Extremal values.*

Date of Submission: 25-11-2025 Date of Acceptance: 08-12-2025

I. Introduction

In a graph G , its vertex set and edge set are represented as $V(G)$ and $E(G)$ respectively. The quantity of vertices and edges in G is named as the order and the size correspondingly. We adopt n and m to stand for the order and size of G respectively. Regarding a vertex $u \in V(G)$, the degree of u , which is denoted by $d_G(u)$, refers to the amount of edges that are incident to vertex u in G . The maximum degree of G , marked as Δ , equals $\max\{d_G(u): u \in V(G)\}$. When $d_G(u) = 1, u$ is referred to as a pendant vertex, and the sole edge linked to this pendant vertex v is called a pendant edge. The notation $N_G(u)$ represents the set of neighbors of vertex u .

The Sombor index was originally proposed based on geometric principles. Although it has been extensively studied in terms of mathematical properties and chemical applications [1-5]. In the past few decades, in order to predict some important physicochemical and biological properties of compounds, hundreds of molecular structures have been introduced and studied by scholars in the fields of mathematics and chemistry. Under given constraints, finding the upper and lower bounds of topological indices for various types of graphs has become one of the hot issues that many researchers focus on. Since its introduction at the end of 2020, the Sombor index has quickly become a research hotspot in mathematical chemistry, network science, materials science and other fields. In the field of graph theory, a lot of research is devoted to exploring the Sombor index and its extremal properties in different types of graphs, see [6-16].

Gutman et al. [17] studied the problem of obtaining the maximum (or minimum) Sombor index value in trees and graphs with a specified order of n. Sun et al. [18] characterized the extremal graphs with the maximum and minimum Sombor index values based on the chromatic number γG . Wang et al. [19] determined the extrema of the p -Sombor index for trees. Zhou et al. [20], using matching number as a relevant parameter, obtained the extremal trees and unicyclic graphs with the maximum and minimum Sombor index values. Zhou et al. [21] explored the extrema of the Sombor index given the maximum degree in the same class of graphs. Das et al. [17] established bounds for the Sombor index of trees based on order, the number of pendant vertices, and so on. Liu et al. [22] determined the minimal Sombor index of tricyclic and tetracyclic graphs. Das et al. [23] provided an upper bound for the Sombor index of connected graphs with a specified independence number. Liu et al. [24] derived various bounds for the reduced Sombor index by considering different graph characteristics and parameters. They also calculated the expectation related to the reduced Sombor index in random polyphenyl chains, as well as the bounds of radius and energy of the reduced Sombor index. In addition, their work included determining the ranking of the minimal values for trees, chemical unicyclic graphs, chemical bicyclic graphs, and chemical tricyclic graphs. Moreover, they explored the application of the reduced

Sombor index in analyzing octane isomers. Inspired by the references $[20,25-27]$, we continue to study the extremal problems of the p -Sombor index of unicyclic graphs.

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 $\mathbb{U}_{n,n} = \mathbf{C}_n . \mathcal{U}_{n,k}$ denotes the graph with n vertices, girth $\kappa(3 \leq \kappa \leq n)$, and a path of length $n-k$ attached to it. $\mathcal{U}_{n,\kappa}^{n-\kappa}$ represents the graph with n vertices, girth $\kappa(3 \leq \kappa \leq n)$, and $n-\kappa$ pendant edges attached to a vertex of the cycle $\mathbf{C}_\kappa$. In a similar manner, $\mathcal{U}_{n,n-1}$ denotes the distinctive unicyclic graph with a girth $n-1$ and n vertices is concluded that $\mathbb{U}_{n,n-1} = \mathcal{U}_{n,n-1}$.

II. Preface

In this section, we will introduce some propositions that are frequently used in subsequent chapters.

Lemma 2.1. Let the function $f(x,y) = (x^p + y^p)^{\frac{1}{p}}$, where $p \geq 1, x \geq 1, y \geq 1$. The function $f(x,y)$ is strictly increasing with respect to x, y . The function f_x is the first partial derivative of $f(x,y)$ with respect to x , then the function f_x is strictly increasing with respect to x and strictly decreasing with respect to y .

Proof: $f_x = \frac{1}{p}(x^p + y^p)^{\frac{1-p}{p}} p x^{p-1} = x^{p-1}(x^p + y^p)^{\frac{1-p}{p}} > 0$.

$$f_{xx} = (p-1)x^{p-2}(x^p + y^p)^{\frac{1-p}{p}} + x^{p-1}\frac{1-p}{p} p x^{p-1}(x^p + y^p)^{\frac{1-2p}{p}}$$

$$= (p-1)x^{p-2}(x^p + y^p)^{\frac{1-p}{p}} + (1-p)x^{2p-2}(x^p + y^p)^{\frac{1-2p}{p}}.$$

Since $(p-1)x^{p-2}(x^p + y^p)^{\frac{1-p}{p}} > (p-1)x^{2p-2}(x^p + y^p)^{\frac{1-2p}{p}}$

$$(x^p + y^p)^{\frac{1-p}{p}} > x^p(x^p + y^p)^{\frac{1-2p}{p}}$$

$$1 > x^p(x^p + y^p)^{-1}.$$

Given $x^p + y^p > x^p$, therefore $f_{xx} > 0$.

$$f_{xy} = x^{p-1}\frac{1-p}{p}(x^p + y^p)^{\frac{1-2p}{p}} p y^{p-1} = (1-p)x^{p-1}y^{p-1}(x^p + y^p)^{\frac{1-2p}{p}} < 0.$$

Thus, the proof is complete.

Lemma2.2. Let the function $\phi(x,y,z) = ((x+y-2)^p + z^p)^{\frac{1}{p}} - (x^p + z^p)^{\frac{1}{p}}$, where $x \geq 1, y \geq 1, z \geq 1, p \geq 1$, the function $\phi(x,y,z)$ is strictly decreasing with respect to z .

Proof:

$$\phi_z = \frac{1}{p}((x+y-2)^p + z^p)^{\frac{1-p}{p}} p z^{p-1} - \frac{1}{p}(x^p + z^p)^{\frac{1-p}{p}} p z^{p-1}$$

$$= z^{p-1}\left[(x+y-2)^p + z^p)^{\frac{1-p}{p}} - (x^p + z^p)^{\frac{1-p}{p}}\right] < 0.$$

Thus, the proof is complete.

Lemma2.3. Let the function $g(x,y) = (2^p + x^p)^{\frac{1}{p}} - (y^p + x^p)^{\frac{1}{p}}$, where $x \geq 1, y \geq 2, p \geq 1$. Then the function $g(x,y)$ is increasing with respect to x .

Proof:

$$g_x = \frac{1}{p}(2^p + x^p)^{\frac{1-p}{p}} p x^{p-1} - \frac{1}{p}(y^p + x^p)^{\frac{1-p}{p}} p x^{p-1}$$

$$= x^{p-1}\left((2^p + x^p)^{\frac{1-p}{p}} - (y^p + x^p)^{\frac{1-p}{p}}\right) \geq 0.$$

Thus, the proof is complete.

Lemma2.4. Let the function $h(x,y) = (x + y - 1)^p - x^p$, where $x \geq 1, y \geq 1, p \geq 1$, the function $h(x,y)$ is increasing with respect to x .

Proof:

$$h_x = p(x + y - 1)^{p-1} - p x^{p-1} = p((x + y - 1)^{p-1} - x^{p-1}) > 0.$$

Thus, the proof is complete.

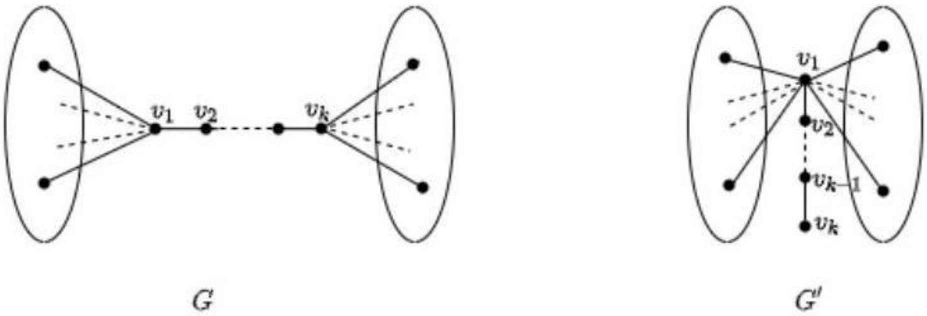

Figure 1: Graphs G, G'

Lemma2.5. Let a graph G containing an induced path $p = v_1 v_2 \dots v_\kappa, d_G(v_1) \geq 2 \geq d_G(v_\kappa) \geq 2$. $G' = G - \{v_\kappa \omega : \omega \in N_{(v_\kappa)} \setminus \{v_{\kappa-1}\} + \{v_1 \omega : \omega \in N_{(v_\kappa)} \setminus \{v_{\kappa-1}\}$. The process of transforming G into G' is called a path upgrade transformation. We have $S(G) < S(G')$.

Proof: For convenience, let $d_G(v_1) = x, d_G(v_\kappa) = y$.

Case 1. $\kappa > 2$.

$$\begin{aligned} S(G) - S(G') &= (2^p + x^p)^{\frac{1}{p}} + (2^p + y^p)^{\frac{1}{p}} + \sum_{\omega \in N_G(v_1) \setminus \{v_2\}} \left(x^p + d_G^p(\omega)\right)^{\frac{1}{p}} + \sum_{\omega \in N_G(v_\kappa) \setminus \{v_\kappa - 1\}} \left(y^p + d_G^p(\omega)\right)^{\frac{1}{p}} \\ &\quad - (1^p + 2^p)^{\frac{1}{p}} - (2^p + (x+y-1)^p)^{\frac{1}{p}} - \sum_{\omega \in N_G(v_1) \cup N_G(v_\kappa) \setminus \{v_2, v_{\kappa-1}\}} \left((x+y-1)^p + d_G^p(\omega)\right)^{\frac{1}{p}} \\ &< (2^p + x^p)^{\frac{1}{p}} + (2^p + y^p)^{\frac{1}{p}} - (1^p + 2^p)^{\frac{1}{p}} - (2^p + (x+y-1)^p)^{\frac{1}{p}} \\ &= f(y,2) - f(1,2) - [f(x+y-1,2) - f(x,2)] \quad = f_x(\mathbf{C}_1, 2) - f_x(\mathbf{C}_2, 2). \end{aligned}$$

Since $1 < \mathbf{C}_1 < y \le x < \mathbf{C}_2 < x + y - 1, f_x(\mathbf{C}_1, 2) - f_x(\mathbf{C}_2, 2) < 0. S(G) < S(G')$.

Case 2. $\boldsymbol{\kappa = 2}$.

$$\begin{aligned} S(G) - S(G') &= (x^p + y^p)^{\frac{1}{p}} + \sum_{\omega \in N_G(v_1) \setminus \{v_2\}} \left(x^p + d_G^p(\omega)\right)^{\frac{1}{p}} + \sum_{\omega \in N_G(v_2) \setminus \{v_1\}} \left(y^p + d_G^p(\omega)\right)^{\frac{1}{p}} \\ &\quad - (1^p + (x+y-1)^p)^{\frac{1}{p}} - \sum_{\omega \in N_G(v_1) \cup N_G(v_2) \setminus \{v_1, v_2\}} \left((x+y-1)^p + d_G^p(\omega)\right)^{\frac{1}{p}} \\ &< (x^p + y^p)^{\frac{1}{p}} - (1^p + (x+y-1)^p)^{\frac{1}{p}}. \end{aligned}$$

By lemma 2.4, we have $(x+y-1)^p + 1^p - x^p - y^p > 0. S(G) - S(G') < 0, S(G) < S(G')$.

Thus, the proof is complete.

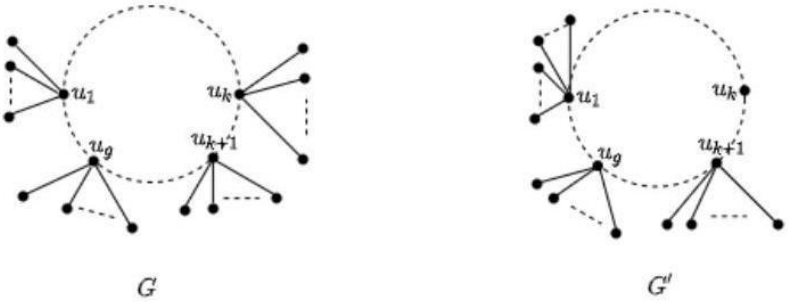

Figure 2: Graphs G, G'

Lemma2.6. Let G be a graph consisting of a cycle of length g and some pendant edges, where $\{u_1, \ldots, u_{\kappa-1}, u_\kappa, u_{\kappa+1}, \ldots, u_g\}$ is the set of vertices on the cycle of length g , and $d_T(u_1) = \Delta. G' = G - \{u_\kappa \omega \colon \omega \in N_G(u_\kappa) \setminus \{u_{\kappa-1}, u_{\kappa+1}\} + \{u_1 \omega \colon \omega \in N_G(u_\kappa) \setminus \{u_{\kappa-1}, u_{\kappa+1}\}$. We have $S(G) < S(G')$.

Proof: For convenience, let $d_T(u_1) = x \ge 3, d_T(u_\kappa) = y \ge 2, x \ge y$.

Case 1. When $\kappa = 2$, then $u_{\kappa-1} = u_1, u_{\kappa+1} = u_3$.

$$
\begin{aligned}
S(G')-S(G) = & \sum_{\omega\in N_G(u_1)\backslash\{u_2,u_g\}}\left[\left(d_{G'}^p(u_1)+d_{G'}^p(\omega)\right)^{\frac{1}{p}}-\left(d_G^p(u_1)+d_G^p(\omega)\right)^{\frac{1}{p}}\right] \\
& +\sum_{\omega\in N_G(u_2)\backslash\{u_1,u_{\kappa+1}\}}\left[\left(d_{G'}^p(u_1)+d_{G'}^p(\omega)\right)^{\frac{1}{p}}-\left(d_G^p(u_2)+d_G^p(\omega)\right)^{\frac{1}{p}}\right]+\left(d_{G'}^p(u_1)+d_{G'}^p(u_2)\right)^{\frac{1}{p}} \\
& -\left(d_G^p(u_1)+d_G^p(u_2)\right)^{\frac{1}{p}}+\left(d_{G'}^p(u_2)+d_{G'}^p(u_3)\right)^{\frac{1}{p}}-\left(d_G^p(u_2)+d_G^p(u_3)\right)^{\frac{1}{p}} \\
& +\left(d_{G'}^p(u_1)+d_{G'}^p(u_g)\right)^{\frac{1}{p}}-\left(d_G^p(u_1)+d_G^p(u_g)\right)^{\frac{1}{p}} \\
& =(x-2)\left[((x+y-2)^p+1^p)^{\frac{1}{p}}-(x^p+1^p)^{\frac{1}{p}}\right] \\
& +(y-2)\left[((x+y-2)^p+1^p)^{\frac{1}{p}}-(y^p+1^p)^{\frac{1}{p}}\right]+((x+y-2)^p+2^p)^{\frac{1}{p}}-(x^p+y^p)^{\frac{1}{p}} \\
& +\left((x+y-2)^p+d_{G'}^p(u_g)\right)^{\frac{1}{p}}-\left(x^p+d_G(u_g)^p\right)^{\frac{1}{p}}+\left(2^p+d_{G'}^p(u_3)\right)^{\frac{1}{p}}-\left(y^p+d_G^p(u_3)\right)^{\frac{1}{p}} \\
& >((x+y-2)^p+1^p)^{\frac{1}{p}}-(x^p+1^p)^{\frac{1}{p}}+\left(2^p+d_{G'}^p(u_3)\right)^{\frac{1}{p}}-\left(y^p+d_G^p(u_3)\right)^{\frac{1}{p}} \\
& +((x+y-2)^p+2^p)^{\frac{1}{p}}-(x^p+y^p)^{\frac{1}{p}}.
\end{aligned}
$$

Let the function $l(x,y)=(x+y-2)^p-x^p$, since $l_x=p[(x+y-2)^{p-1}-x^{p-1}]>0$, the function $l(x,y)$ is monotonically increasing with respect to x . So $(x+y-2)^p-x^p>y^p-2^p, (x+y-2)^p+2^p>x^p+y^p$. We have $((x+y-2)^p+2^p)^{\frac{1}{p}}>(x^p+y^p)^{\frac{1}{p}}$. By lemma 2.3, we know $\left(2^p+d_{G'}^p(u_3)\right)^{\frac{1}{p}}-\left(y^p+d_G^p(u_3)\right)^{\frac{1}{p}}>(2^p+2^p)^{\frac{1}{p}}-(y^p+2^p)^{\frac{1}{p}}$.

$$
\begin{aligned}
S(G')-S(G) &> ((x+y-2)^p+1^p)^{\frac{1}{p}}-(x^p+1^p)^{\frac{1}{p}}+(2^p+2^p)^{\frac{1}{p}}-(y^p+2^p)^{\frac{1}{p}} \\
&= f(x+y-2,1)-f(x,1)-[f(y,2)-f(2,2)] \quad = f_x(\mathbf{C}_1,1)-f_x(\mathbf{C},2).
\end{aligned}
$$

By lemma 2.1 and $x+y-2>\mathbf{C}_1>x\geq y>\mathbf{C}_2>2$, we have $S(G')>S(G)$.

Case 2. When $\kappa>2$, then $d_G(u_2)=\cdots=d_G(u_{\kappa-1})=2$, by lemma 2.3 we have $\left(2^p+d_{G'}^p(u_{\kappa+1})\right)^{\frac{1}{p}}-\left(y^p+d_G^p(u_{\kappa+1})\right)^{\frac{1}{p}}>(2^p+2^p)^{\frac{1}{p}}-(y+2^p)^{\frac{1}{p}}$.

$$S(G') - S(G) = \sum_{\omega \in N_G(u_1)\setminus\{u_2,u_g\}} \left[\left(d_{G'}^p(u_1) + d_{G'}^p(\omega)\right)^{\frac{1}{p}} - \left(d_G^p(u_1) + d_G^p(\omega)\right)^{\frac{1}{p}} \right]$$
$$+ \sum_{\omega \in N_G(u_\kappa)\setminus\{u_{\kappa-1},u_{\kappa+1}\}} \left[\left(d_{G'}^p(u_1) + d_{G'}^p(\omega)\right)^{\frac{1}{p}} - \left(d_G^p(u_\kappa) + d_G^p(\omega)\right)^{\frac{1}{p}} \right]$$
$$+ \left(d_{G'}^p(u_1) + d_{G'}^p(u_2)\right)^{\frac{1}{p}} - \left(d_G^p(u_1) + d_G^p(u_2)\right)^{\frac{1}{p}} + \left(d_{G'}^p(u_1) + d_{G'}^p(u_g)\right)^{\frac{1}{p}}$$
$$- \left(d_G^p(u_1) + d_G^p(u_g)\right)^{\frac{1}{p}} + \left(d_{G'}^p(u_\kappa) + d_{G'}^p(u_{\kappa-1})\right)^{\frac{1}{p}} - \left(d_G^p(u_\kappa) + d_G^p(u_{\kappa-1})\right)^{\frac{1}{p}}$$
$$+ \left(d_{G'}^p(u_\kappa) + d_{G'}^p(u_{\kappa+1})\right)^{\frac{1}{p}} - \left(d_G^p(u_\kappa) + d_G^p(u_{\kappa+1})\right)^{\frac{1}{p}}$$
$$= (x-2)\left[((x+y-2)^p + 1^p)^{\frac{1}{p}} - (x^p + 1^p)^{\frac{1}{p}} \right]$$
$$+ (y-2)\left[((x+y-2)^p + 1^p)^{\frac{1}{p}} - (y^p + 1^p)^{\frac{1}{p}} \right] + ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}}$$
$$+ \left((x+y-2)^p + d_{G'}^p(u_g)\right)^{\frac{1}{p}} - \left(x^p + d_G^p(u_g)\right)^{\frac{1}{p}} + (2^p + 2^p)^{\frac{1}{p}} - (y^p + 2^p)^{\frac{1}{p}}$$
$$+ \left(2^p + d_{G'}^p(u_{\kappa+1})\right)^{\frac{1}{p}} - \left(y^p + d_G^p(u_{\kappa+1})\right)^{\frac{1}{p}}$$
$$> ((x+y-2)^p + 1^p)^{\frac{1}{p}} - (x^p + 1^p)^{\frac{1}{p}} + ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} + (2^p + 2^p)^{\frac{1}{p}}$$
$$- (y^p + 2^p)^{\frac{1}{p}} + (2^p + 2^p)^{\frac{1}{p}} - (y^p + 2^p)^{\frac{1}{p}}$$
$$= f(x+y-2,1) - f(x,1) - [f(y,2) - f(2,2)] + f(x+y-2,2) - f(x,2)$$
$$- [f(y,2) - f(2,2)] = f_x(\mathbf{C}_1, 1) - f_x(\mathbf{C}_2, 2) + f_x(\mathbf{C}_3, 2) - f_x(\mathbf{C}_4, 2)$$
$$> f_x(\mathbf{C}_1, 2) - f_x(\mathbf{C}_2, 2) + f_x(\mathbf{C}_3, 2) - f_x(\mathbf{C}_4, 2).$$

Since $x + y - 2 > \mathbf{C}_1 > x \geq y > \mathbf{C}_2 > 2, x + y - 2 > \mathbf{C}_3 > x \geq y > \mathbf{C}_4 > 2$. then $f_x(\mathbf{C}_1, 2) - f_x(\mathbf{C}_2, 2) + f_x(\mathbf{C}_3, 2) - f_x(\mathbf{C}_4, 2) > 0. S(G') > S(G)$.

Thus, the proof is complete.

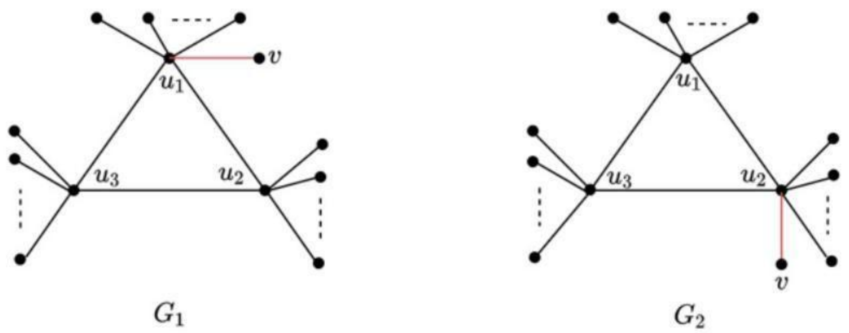

Figure 3: Graphs G_1, G_2

Lemma 2.7. Let G be a graph consisting of a cycle of length 3 and some pendant edges, where u_1, u_2, u_3 are the vertices of the cycle of length 3. Suppose $d_T(u_1) = \Delta$, where $d_T(u_1) > \max\{d_T(u_2), d_T(u_3)\}$. Let v be a pendant vertex. $G_1 = G + \{u_1 v\}, G_2 = G + \{u_2 v\}$, then $S(G_1) > S(G_2)$.

Proof: For convenience, let $d_T(u_1) = x, d_T(u_2) = y, d_T(u_3) = z$, where $x > y, x > z$, since $(x+1)^p - x^p$ is monotonically increasing with respect to x , then $(x+1)^p + y^p - x^p - (y+1)^p > 0, (x+1)^p + y^p > x^p + (y+1)^p$.

$$S(G_1)-S(G_2)=\sum_{\omega\in N_G(u_1)\setminus\{u_2,u_3\}}\left[\left(d_{G_1}^p(u_1)+d_{G_1}^p(\omega)\right)^{\frac{1}{p}}-\left(d_{G_2}^p(u_1)+d_{G_2}^p(\omega)\right)^{\frac{1}{p}}\right]$$
$$+\sum_{\omega\in N_G(u_2)\setminus\{u_1,u_3\}}\left[\left(d_{G_1}^p(u_2)+d_{G_1}^p(\omega)\right)^{\frac{1}{p}}-\left(d_{G_2}^p(u_2)+d_{G_2}^p(\omega)\right)^{\frac{1}{p}}\right]+\left(d_{G_1}^p(u_1)+d_{G_1}^p(v)\right)^{\frac{1}{p}}$$
$$-\left(d_{G_2}^p(u_2)+d_{G_2}^p(v)\right)^{\frac{1}{p}}+\left(d_{G_1}^p(u_1)+d_{G_1}^p(u_2)\right)^{\frac{1}{p}}-\left(d_{G_2}^p(u_1)+d_{G_2}^p(u_2)\right)^{\frac{1}{p}}$$
$$+\left(d_{G_1}^p(u_1)+d_{G_1}^p(u_3)\right)^{\frac{1}{p}}-\left(d_{G_2}^p(u_1)+d_{G_2}^p(u_3)\right)^{\frac{1}{p}}+\left(d_{G_1}^p(u_2)+d_{G_1}^p(u_3)\right)^{\frac{1}{p}}$$
$$-\left(d_{G_2}^p(u_2)+d_{G_2}^p(u_3)\right)^{\frac{1}{p}}$$
$$=(x-2)\left[((x+1)^p+1^p)^{\frac{1}{p}}-(x^p+1^p)^{\frac{1}{p}}\right]+(y-2)\left[(y^p+1^p)^{\frac{1}{p}}-((y+1)^p+1^p)^{\frac{1}{p}}\right]$$
$$+((x+1)^p+1^p)^{\frac{1}{p}}-((y+1)^p+1^p)^{\frac{1}{p}}+((x+1)^p+y^p)^{\frac{1}{p}}-(x^p+(y+1)^p)^{\frac{1}{p}}$$
$$+((x+1)^p+z^p)^{\frac{1}{p}}-(x^p+z^p)^{\frac{1}{p}}+(y^p+z^p)^{\frac{1}{p}}-((y+1)^p+z^p)^{\frac{1}{p}}$$
$$>(y-2)[f(x+1,1)-f(x,1)-(f(y+1,1)-f(y,1))]$$
$$+[f(x+1,z)-f(x,z)-(f(y+1,z)-f(y,z))]$$
$$=(y-2)[f_x(\mathbf{C}_1,1)-f_x(\mathbf{C}_2,1)]+f_x(\mathbf{C}_3,z)-f_x(\mathbf{C}_4,z)>0.$$

Thus, the proof is complete.

Lemma 2.8. Let G be a unicyclic graph with girth 3, and the vertices on the cycle are denoted as u_1,u_2,u_3 . Suppose $d_T(u_1)=\Delta\geq 2, d_T(u_2)\geq 2, d_T(u_3)\geq 2$. If $G'=G-\{u_2\omega:\omega\in N_G(u_2)\setminus\{u_1,u_3\}\}+\{u_1\omega:\omega\in N_G(u_2)\setminus\{u_1,u_3\}\}$, then $S(G')>S(G)$.

Proof: For convenience, let $d_G(u_1)=x, d_G(u_2)=y, d_G(u_3)=z, d_G(\omega)=d_{G'}(\omega)\geq 1$.

$$S(G')-S(G)=\sum_{\omega\in N_G(u_2)\setminus\{u_1,u_3\}}\left[d_{G'}^p(u_1)+d_{G'}^p(\omega)^{\frac{1}{p}}-\left(d_G^p(u_2)+d_G^p(\omega)\right)^{\frac{1}{p}}\right]$$
$$+\sum_{\omega\in N_G(u_1)\setminus\{u_2,u_3\}}\left[d_{G'}^p(u_1)+d_{G'}^p(\omega)^{\frac{1}{p}}-\left(d_G^p(u_1)+d_G^p(\omega)\right)^{\frac{1}{p}}\right]+\left(d_{G'}^p(u_1)+d_{G'}^p(u_2)\right)^{\frac{1}{p}}$$
$$-\left(d_G^p(u_1)+d_G^p(u_2)\right)^{\frac{1}{p}}+\left(d_{G'}^p(u_1)+d_{G'}^p(u_3)\right)^{\frac{1}{p}}-\left(d_G^p(u_1)+d_G^p(u_3)\right)^{\frac{1}{p}}$$
$$+\left(d_{G'}^p(u_2)+d_{G'}^p(u_3)\right)^{\frac{1}{p}}-\left(d_G^p(u_2)+d_G^p(u_3)\right)^{\frac{1}{p}}$$
$$=(y-2)\left[((x+y-2)^p+\omega^p)^{\frac{1}{p}}-(y^p+\omega^p)^{\frac{1}{p}}\right]$$
$$+(x-2)\left[((x+y-2)^p+\omega^p)^{\frac{1}{p}}-(x^p+\omega^p)^{\frac{1}{p}}\right]+((x+y-2)^p+2^p)^{\frac{1}{p}}$$
$$-(x^p+y^p)^{\frac{1}{p}}+((x+y-2)^p+z^p)^{\frac{1}{p}}-(x^p+z^p)^{\frac{1}{p}}+(2^p+z^p)^{\frac{1}{p}}$$
$$-(y^p+z^p)^{\frac{1}{p}}\geq((x+y-2)^p+z^p)^{\frac{1}{p}}-(x^p+z^p)^{\frac{1}{p}}+(2^p+z^p)^{\frac{1}{p}}-(y^p+z^p)^{\frac{1}{p}}$$
$$=f(x+y-2,z)-f(x,z)-[f(y,z)-f(2,z)]=f_x(\mathbf{C}_1,z)-f_x(\mathbf{C}_2,z)>0.$$

Thus, the proof is complete.

Lemma 2.9. Let G be a unicyclic graph with girth 3, and the vertices on the cycle are denoted as u_1,u_2,u_3 . Assume that $d_G(u_1)=\Delta>2, d_G(u_2)=d_G(u_3)=2$. In the tree connected to u_1 , there exists a vertex v , such that $d_G(v)\geq 3$, Let v_1 and v_2 be two neighbors of v , and there is a path $P=vv_2\ldots v_iu$. If $G'=G-\{v\omega:\omega\in N_T(v)\setminus\{v_1,v_2\}\}+\{u_1\omega:\omega\in N_T(v)\setminus\{v_1,v_2\}\}$. then$S(G')>S(G)\}$.

Proof: For convenience, let $d_G(u_1) = x, d_G(v) = y, d_G(v_1) = z \geq 1, d_G(\omega) = d_{G'}(\omega) = \omega \geq 1$. Case 1. when $u_1 v \in G$, then $v_2 = u$.

$$\begin{aligned}
S(G') - S(G) = &\sum_{\omega \in N_G(v)\setminus\{v_2,v_1\}} \left[\left(d_{G'}^p(u_1) + d_{G'}^p(\omega)\right)^{\frac{1}{p}} - \left(d_G^p(v) + d_G^p(\omega)\right)^{\frac{1}{p}}\right] \\
&+ \sum_{\omega \in N_G(u_1)\setminus\{u_2,u_3,v\}} \left[\left(d_{G'}^p(u_1) + d_{G'}^p(\omega)\right)^{\frac{1}{p}} - \left(d_G^p(u_1) + d_G^p(\omega)\right)^{\frac{1}{p}}\right] + \left(d_{G'}^p(u_1) + d_{G'}^p(u_2)\right)^{\frac{1}{p}} \\
&- \left(d_G^p(u_1) + d_G^p(u_2)\right)^{\frac{1}{p}} + \left(d_{G'}^p(u_1) + d_{G'}^p(u_3)\right)^{\frac{1}{p}} - \left(d_G^p(u_1) + d_G^p(u_3)\right)^{\frac{1}{p}} \\
&+ \left(d_{G'}^p(u_1) + d_{G'}^p(v)\right)^{\frac{1}{p}} - \left(d_G^p(u_1) + d_G^p(v)\right)^{\frac{1}{p}} + \left(d_{G'}^p(v) + d_{G'}^p(v_1)\right)^{\frac{1}{p}} \\
&- \left(d_G^p(v) + d_G^p(v_1)\right)^{\frac{1}{p}} \\
&= (y-2)\left[((x+y-2)^p + \omega^p)^{\frac{1}{p}} - (y^p + \omega^p)^{\frac{1}{p}}\right] \\
&+ (x-3)\left[((x+y-2)^p + \omega^p)^{\frac{1}{p}} - (x^p + \omega^p)^{\frac{1}{p}}\right] \quad + ((x+y-2)^p + 2^p)^{\frac{1}{p}} \\
&- (x^p + 2^p)^{\frac{1}{p}} \quad + ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} \\
&+ ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + y^p)^{\frac{1}{p}} + (2^p + z^p)^{\frac{1}{p}} - (y^p + z^p)^{\frac{1}{p}} \\
&> ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} - \left[(y^p + z^p)^{\frac{1}{p}} - (2^p + z^p)^{\frac{1}{p}}\right] \\
&> ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} - \left[(y^p + 1^p)^{\frac{1}{p}} - (2^p + 1^p)^{\frac{1}{p}}\right] \\
&> ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} - \left[(y^p + 2^p)^{\frac{1}{p}} - (2^p + 1^p)^{\frac{1}{p}}\right].
\end{aligned}$$

If $x \geq y$, then

$$S(G') - S(G) > ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} - \left[(y^p + 2^p)^{\frac{1}{p}} - (2^p + 1^p)^{\frac{1}{p}}\right] = f_x(\mathbf{C}_1, 2) - f_x(\mathbf{C}_2, 2).$$

Since $1 < \mathbf{C_2} < y \leq x < \mathbf{C_1} < x + y - 2$, then $S(G') > S(G)$.

If $y \geq x$, then

$$\begin{aligned}
S(G') - S(G) &> ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} - \left[(y^p + 2^p)^{\frac{1}{p}} - (2^p + 1^p)^{\frac{1}{p}}\right] \\
&= ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (y^p + 2^p)^{\frac{1}{p}} - \left[(x^p + 2^p)^{\frac{1}{p}} - (2^p + 1^p)^{\frac{1}{p}}\right] \\
&= f_x(\mathbf{C}_1, 2) - f_x(\mathbf{C}_2, 2).
\end{aligned}$$

Since $1 < \mathbf{C_2} < x \leq y < \mathbf{C_1} < x + y - 2$, then $S(G') > S(G)$.

Case 2. When $u_1 v \notin G$, then at this time $d_G(v_2) = \cdots = d_G(v_i) = 2$.

$$S(G') - S(G) = \sum_{\omega \in N_G(v)\setminus\{v_2,v_1\}} \left[\left(d_{G'}^p(u_1) + d_{G'}^p(\omega)\right)^{\frac{1}{p}} - \left(d_G^p(v) + d_G^p(\omega)\right)^{\frac{1}{p}}\right]$$
$$+ \sum_{\omega \in N_G(u_1)\setminus\{u_2,u_3,v_i\}} \left[\left(d_{G'}^p(u_1) + d_{G'}^p(\omega)\right)^{\frac{1}{p}} - \left(d_G^p(u_1) + d_G^p(\omega)\right)^{\frac{1}{p}}\right] + \left(d_{G'}^p(u_1) + d_{G'}^p(u_2)\right)^{\frac{1}{p}}$$
$$- \left(d_G^p(u_1) + d_G^p(u_2)\right)^{\frac{1}{p}} + \left(d_{G'}^p(u_1) + d_{G'}^p(u_3)\right)^{\frac{1}{p}} - \left(d_G^p(u_1) + d_G^p(u_3)\right)^{\frac{1}{p}}$$
$$+ \left(d_{G'}^p(u_1) + d_{G'}^p(v_i)\right)^{\frac{1}{p}} - \left(d_G^p(u_1) + d_G^p(v_i)\right)^{\frac{1}{p}} + \left(d_{G'}^p(v) + d_{G'}^p(v_2)\right)^{\frac{1}{p}}$$
$$- \left(d_G^p(v) + d_G^p(v_2)\right)^{\frac{1}{p}} + \left(d_{G'}^p(v) + d_{G'}^p(v_1)\right)^{\frac{1}{p}} - \left(d_G^p(v) + d_G^p(v_1)\right)^{\frac{1}{p}}$$
$$= (y-2)\left[((x+y-2)^p + \omega^p)^{\frac{1}{p}} - (y^p + \omega^p)^{\frac{1}{p}}\right]$$
$$+ (x-3)\left[((x+y-2)^p + \omega^p)^{\frac{1}{p}} - (x^p + \omega^p)^{\frac{1}{p}}\right] + ((x+y-2)^p + 2^p)^{\frac{1}{p}}$$
$$- (x^p + 2^p)^{\frac{1}{p}} + ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}}$$
$$+ ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} + (2^p + z^p)^{\frac{1}{p}} - (y^p + z^p)^{\frac{1}{p}}$$
$$+ (2^p + 2^p)^{\frac{1}{p}} - (y^p + 2^p)^{\frac{1}{p}}$$
$$> ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} + (2^p + 1^p)^{\frac{1}{p}} - (y^p + 1^p)^{\frac{1}{p}} + ((x+y-2)^p + 2^p)^{\frac{1}{p}}$$
$$- (x^p + 2^p)^{\frac{1}{p}} - (2^p + 2^p)^{\frac{1}{p}} - (y^p + 2^p)^{\frac{1}{p}}$$
$$> ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} - (2^p + 2^p)^{\frac{1}{p}} - (y^p + 2^p)^{\frac{1}{p}}.$$

Similarly, if $x \geq y$, then

$$S(G') - S(G) > ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (x^p + 2^p)^{\frac{1}{p}} - \left[(y^p + 2^p)^{\frac{1}{p}} - (2^p + 2^p)^{\frac{1}{p}}\right] = f_x(\mathbf{C}_1, 2) - f_x(\mathbf{C}_2, 2).$$

Since $2 < \mathbf{C_2} < y \leq x < \mathbf{C_1} < x + y - 2$, then $S(G') > S(G)$.

If $y \geq x$, then

$$S(G') - S(G) > ((x+y-2)^p + 2^p)^{\frac{1}{p}} - (y^p + 2^p)^{\frac{1}{p}} - \left[(x^p + 2^p)^{\frac{1}{p}} - (2^p + 2^p)^{\frac{1}{p}}\right] = f_x(\mathbf{C}_1, 2) - f_x(\mathbf{C}_2, 2).$$

Since $2 < \mathbf{C_2} < x \leq y < \mathbf{C_1} < x + y - 2$, then $S(G') > S(G)$.

Thus, the proof is complete.

III. Main Results

3.1 Graphs with the Top Three p -Sombor Indices among Unicyclic Graphs

The graph $\mathcal{U}_{n,\kappa}^{n-\kappa}$ is called a unicyclic graph, It contains n vertices and has a girth of κ , where $3 \leq \kappa \leq n$. As can be seen in Figure 4, this graph is constructed by connecting some pendant edges to a cycle $\mathbf{C}_\kappa$ The number of pendant edges is $n - \kappa$.

Theorem 3.1.1 For $G \in \mathbb{U}_{n,\kappa}$, with $3 \leq \kappa \leq n$, the following inequality holds for graph G

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

Figure 4: Graphs $\mathcal{U}_{n,3}^{n-3}, \mathcal{U}_{n,k}^{n-k}$

The equality holds if and only if $G \cong \mathcal{U}_{n,3}^{n-3}$.

Proof: Assume that G is the graph with the maximum p -Sombor index among unicyclic graphs. Since G is a unicyclic graph, let its cycle be $\mathbf{C} := u_1 u_2 u_3 \dots u_\kappa u_1$.

Claim 1: Except for the vertices on the cycle of the unicyclic graph G the degree of each remaining vertex is 1 .

Proof: Suppose there is at least one vertex $v \notin \{u_1, u_2, \dots, u_\kappa\}$, such that $d(v) \geq 2$, Let u_i be the vertex on the cycle adjacent to v , Then there exists a graph G' , where $G' = G - \{v\omega : \omega \in N_G(v) \setminus \{u_i\}\} + \{u_i\omega : \omega \in N_G(v) \setminus \{u_i\}\}$, By Lemma 2.5, we have $\mathrm{SOp}(G') > \mathrm{SOp}(G)$, which contradicts the assumption.

Claim 2: The girth of the unicyclic graph G is 3 .

Proof: Assume that the girth of G is greater than 3. Let $\{u_i, u_{i+1}\} \in \{u_1, \dots, u_\kappa\}$, Then there exists a graph G' ,, where $G' = G - \{u_{i+1}\omega : \omega \in N_G(u_{i+1}) \setminus \{u_i\}\} + \{u_i\omega : \omega \in N_G(u_{i+1}) \setminus \{u_i\}\}$. By Lemma 2.5, we have $\mathrm{SOp}(G') > \mathrm{SOp}(G)$. which contradicts the assumption.

Claim 3: There is only one vertex with degree greater than 2 in the unicyclic graph G .

Proof: At this time, G is composed of a cycle of girth 3 and some pendant edges. We use $G(k_1, k_2, k_3)$ to represent the number of pendant vertices of vertices u_1, u_2, u_3 on the cycle of G , where $k_1 \geq \max\{k_2, k_3\}$. By Lemma 2.7, we have $G(k_1, k_2, k_3) < G(k_1 + 1, k_2 - 1, k_3) < \cdots < G(k_1 + k_2, 0, k_3) < G(k_1 + k_2 + 1, 0, k_3 - 1) < \ \dots < G(k_1 + k_2 + k_3, 0, 0)$. This completes the proof of the claim.

By Claims 1,2 and 3, we obtain that $\mathcal{U}_{n,3}^{n-3}$ is the graph with the maximum p -Sombor index among unicyclic graphs.

By Theorem 3.1.1, we know that the graph $\mathcal{U}_{n,3}^{n-3}$ is the graph with the maximum p -Sombor index among unicyclic graphs. In this case, we continue to find the graph with the second largest p-Sombor index among unicyclic graphs.

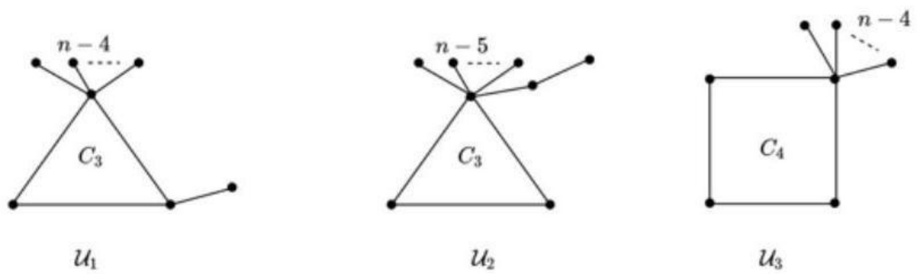

Figure 5: Graphs $\mathcal{U}_1, \mathcal{U}_2, \mathcal{U}_3$

Lemma 3.1.1 Considering that $G \in \{\mathcal{U}_1, \mathcal{U}_2, \mathcal{U}_3\}$, the following inequalities hold for these graphs:

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

The equality holds if and only if $G \cong \mathcal{U}_1$.

Proof:

$$SOp(\mathcal{U}_1) = (n-4)((n-2)^p+1^p)^{\frac{1}{p}} + ((n-2)^p+2^p)^{\frac{1}{p}} + ((n-2)^p+3^p)^{\frac{1}{p}} + (3^p+1^p)^{\frac{1}{p}} + (2^p+3^p)^{\frac{1}{p}}.$$

$$\mathrm{SOp}(\mathcal{U}_2) = (n-5)((n-2)^p+1^p)^{\frac{1}{p}} + 3((n-2)^p+2^p)^{\frac{1}{p}} + (2^p+1^p)^{\frac{1}{p}} + (2^p+2^p)^{\frac{1}{p}}.$$

$$\mathrm{SOp}(\mathcal{U}_3) = (n-4)((n-2)^p+1^p)^{\frac{1}{p}} + 2((n-2)^p+2^p)^{\frac{1}{p}} + 2(2^p+2^p)^{\frac{1}{p}}.$$

$$\begin{aligned}\mathrm{SOp}(\mathcal{U}_1) - \mathrm{SOp}(\mathcal{U}_3) &= (n-4)((n-2)^p+1^p)^{\frac{1}{p}} + ((n-2)^p+2^p)^{\frac{1}{p}} + ((n-2)^p+3^p)^{\frac{1}{p}} + (3^p + 1^p)^{\frac{1}{p}} + (2^p + 3^p)^{\frac{1}{p}} \\ &\quad - [(n-5)((n-2)^p + 1^p)^{\frac{1}{p}} + 3((n-2)^p + 2^p)^{\frac{1}{p}} + (2^p + 1^p)^{\frac{1}{p}} + (2^p + 2^p)^{\frac{1}{p}}] \\ &= ((n-2)^p + 3^p)^{\frac{1}{p}} - ((n-2)^p + 2^p)^{\frac{1}{p}} + (3^p + 2^p)^{\frac{1}{p}} - (2^p + 2^p)^{\frac{1}{p}} + (3^p + 1^p)^{\frac{1}{p}} \\ &\quad - (2^p + 2^p)^{\frac{1}{p}} > (3^p + 1^p)^{\frac{1}{p}} - (2^p + 2^p)^{\frac{1}{p}}.\end{aligned}$$

Since $x^p - (x-1)^p$ is monotonically increasing with respect to x , then $\mathrm{SOp}(\mathcal{U}_1) - \mathrm{SOp}(\mathcal{U}_3) > 0$.

$$\begin{aligned}\mathrm{SOp}(\mathcal{U}_3) - \mathrm{SOp}(\mathcal{U}_2) &= (n-4)((n-2)^p + 1^p)^{\frac{1}{p}} + 2((n-2)^p + 2^p)^{\frac{1}{p}} + 2(2^p + 2^p)^{\frac{1}{p}} \\ &\quad - [(n-5)((n-2)^p + 1^p)^{\frac{1}{p}} + 3((n-2)^p + 2^p)^{\frac{1}{p}} + (2^p + 1^p)^{\frac{1}{p}} + (2^p + 2^p)^{\frac{1}{p}}] \\ &= ((n-2)^p + 1^p)^{\frac{1}{p}} - ((n-2)^p + 2^p)^{\frac{1}{p}} + (2^p + 2^p)^{\frac{1}{p}} - (2^p + 1^p)^{\frac{1}{p}} \\ &= (2^p + 2^p)^{\frac{1}{p}} - (1^p + 2^p)^{\frac{1}{p}} - [(2^p + (n-2)^p)^{\frac{1}{p}} - (1^p + (n-2)^p)^{\frac{1}{p}}].\end{aligned}$$

Note that $(2^p + x^p)^{\frac{1}{p}} - (1^p + x^p)^{\frac{1}{p}}$ is monotonically decreasing with respect to x , then $\mathrm{SOp}(\mathcal{U}_3) > \mathrm{SOp}(\mathcal{U}_2)$. In conclusion, $\mathrm{SOp}(\mathcal{U}_1) > \mathrm{SOp}(\mathcal{U}_3) > \mathrm{SOp}(\mathcal{U}_2)$. Thus, the proof is complete.

Theorem 3.1.2 Considering that $G \in \mathbb{U}_{n,\kappa}$, and $G \ncong \mathcal{U}_{n,3}^{n-3}$, when $3 \le \kappa \le n$, the following inequality holds for the graph G :

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

The equality holds if and only if $G \cong \mathcal{U}_1$.

Proof: Assume that G is the graph with the second largest p -Sombor index among unicyclic graphs. Considering that G is a unicyclic graph, let its cycle be $\mathbf{C} := u_1 u_2 u_3 \dots u_\kappa u_1$.

Claim 1: The girth of the unicyclic graph G is less than or equal to 4 .

Proof: Suppose the girth of G is greater than 4 . Then, by Lemma 2.5 and Lemma 2.7, there exists a G' , such that G' is isomorphic to $\mathcal{U}_1, \mathcal{U}_2, \mathcal{U}_3$, We have $\mathrm{SOp}(G') > \mathrm{SOp}(G)$, which contradicts the assumption.

Claim 2: When the girth of the unicyclic graph G is $4, \mathcal{U}_3$ is the graph with the second largest p -Sombor index.

Proof: Assume that $\mathcal{U}_3$ is not the graph with the second largest p -Sombor index when the girth is 4 . If in the unicyclic graph G, there exists at least one non-pendant vertex other than the vertices on the cycle, then by Lemma 2.5, there exists a G' such that $SOp(G') > SOp(G)$. At this time, G becomes a graph composed of a cycle of girth 4 and some pendant edges. We use $G(k_1, k_2, k_3, k_4)$ to represent the number of pendant vertices of vertices u_1, u_2, u_3, u_4 in G , and $k_1 \ge \max\{k_2, k_3, k_4\}$. By Lemma 2.6, we have $G(k_1, k_2, k_3, k_4) < G(k_1 + k_2, 0, k_3, k_4) < G(k_1 + k_2 + k_3, 0,0, k_4) < G(k_1 + k_2 + k_3 + k_4, 0,0,0)$. Thus, the proof is complete.

Claim 3: When the girth of graph G is 3 and all vertices except those on the cycle are pendant vertices, $\mathcal{U}_1$ is the graph with the second largest p -Sombor index.

Proof: Assume that $\mathcal{U}_1$ is not the graph with the second largest p -Sombor index. At this time, G is composed of a cycle of girth 3 and some pendant edges. We use $G(k_1,k_2,k_3)$ to represent the number of pendant vertices of vertices u_1,u_2,u_3 in G , and $k_1 \geq \max\{k_2,k_3\}$. By Lemma 2.7, we have the p -Sombor index $G(k_1,k_2,k_3) < G(k_1+1,k_2-1,k_3) < \cdots < G(k_1+k_2-1,1,k_3) < \cdots < G(k_1+k_2+k_3-2,1,1) < G(k_1+k_2+k_3-1,1,0) = G(k_1+k_2+k_3-1,0,1)$. Thus, the proof is complete.

Claim 4: When the girth of graph G is 3 and in addition to the vertices on the cycle, there is at least one vertex that is not a pendant vertex, $\mathcal{U}_2$ is the graph with the second largest p -Sombor index.

Proof: Assume that $\mathcal{U}_2$ is not the graph with the second largest p -Sombor index. Then, by Lemma 2.5, 2.8 and 2.9, for any graph G , we have $\mathrm{SOp}(G) < \mathrm{SOp}(\mathcal{U}_2)$.

Through claims 1, 2, 3 and 4, we obtain that there are three cases for the unicyclic graph with the second largest p -Sombor index, which are the graphs $\mathcal{U}_1,\mathcal{U}_2,\mathcal{U}_3$. By Lemma 3.1.1, we have $\mathrm{SOp}(\mathcal{U}_1) > \mathrm{SOp}(\mathcal{U}_3) > SOp(\mathcal{U}_2)$. Then, when $G \cong \mathcal{U}_1$ the unicyclic graph has the second largest p -Sombor index.

Based on Theorem 3.1.2, we can get that $\mathcal{U}_1$ is the graph with the second largest p -Sombor index among unicyclic graphs. Under this assumption, we continue to find the graph with the third largest p -Sombor index among unicyclic graphs.

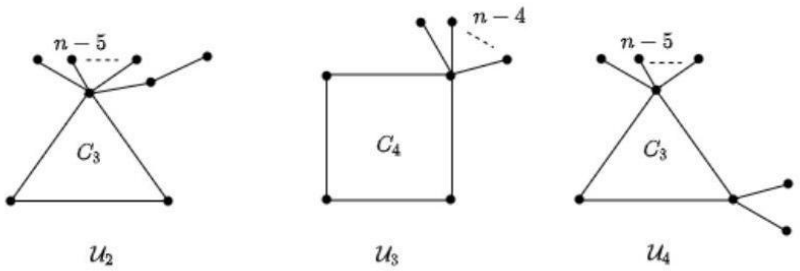

Figure 6: Graphs $\mathcal{U}_2,\mathcal{U}_3,\mathcal{U}_4$

Lemma3.1.2 Considering $G \in \{\mathcal{U}_2,\mathcal{U}_3,\mathcal{U}_4\}$, when $n \geq 7$, then G satisfies the following inequality:

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

The equality holds if and only if $G \cong \mathcal{U}_3$.

Proof: By the lemma 3.1.1, we know that $\mathrm{SOp}(\mathcal{U}_3) > \mathrm{SOp}(\mathcal{U}_2)$.

$$\begin{aligned}\mathrm{SOp}(\mathcal{U}_3) - \mathrm{SOp}(\mathcal{U}_4) = {} & (n-4)((n-2)^p+1^p)^{\frac{1}{p}} + 2((n-2)^p+2^p)^{\frac{1}{p}} + 2(2^p+2^p)^{\frac{1}{p}} \\ & - [(n-5)((n-3)^p+1^p)^{\frac{1}{p}} + 2(4^p+1^p)^{\frac{1}{p}} \\ & + ((n-3)^p+2^p)^{\frac{1}{p}} + ((n-3)^p+4^p)^{\frac{1}{p}} + (4^p+2^p)^{\frac{1}{p}}].\end{aligned}$$

We calculate the minimum value of $\mathrm{SOp}(\mathcal{U}_3) - \mathrm{SOp}(\mathcal{U}_4)$ in the software Lingo, and get that this value is 0 when $n \geq 7, p \geq 1$. Then $\mathrm{SOp}(\mathcal{U}_3) \geq \mathrm{SOp}(\mathcal{U}_4)$.

In conclusion, among $\mathcal{U}_2,\mathcal{U}_3,\mathcal{U}_4,\mathcal{U}_3$ has the largest p -Sombor index.

Theorem 3.1.3 Considering $G \in \mathbb{U}_{n,\kappa}$ and $G \ncong \mathcal{U}_{n,3}^{n-3}, G \ncong \mathcal{U}_1$, when $3 \leq \kappa \leq n, n \geq 7$, the following inequality exists:

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

The equality holds if and only if $G \cong \mathcal{U}_3$.

Proof: Assume that G is the graph with the third largest p -Sombor index among unicyclic graphs. Considering that G is a unicyclic graph, let its cycle be $\mathbf{C} := u_1 u_2 u_3 \dots u_\kappa u_1$.

Claim 1: The girth of G is less than or equal to 4 .

Proof: Suppose the girth of G is greater than 4. Then, by Lemma 2.5 and Lemma 2.7, there exists a G' such that G' is isomorphic to $\mathcal{U}_2, \mathcal{U}_3, \mathcal{U}_4$. We have $\mathrm{SOp}(G') > \mathrm{SOp}(G)$, which contradicts the assumption.

Claim 2: When the girth of G is 4, $\mathcal{U}_3$ is the graph with the third largest p -Sombor index.

Proof: Assume that $\mathcal{U}_3$ is not the graph with the third largest p -Sombor index when the girth is 4 . If in the unicyclic graph G , there exists at least one non-pendant vertex other than the vertices on the cycle, then by Lemma 2.5, there exists a G' such that $\mathrm{SOp}(G') > \mathrm{SOp}(G)$. At this time, G becomes a graph composed of a cycle of girth 4 and some pendant edges. We use $G(k_1, k_2, k_3, k_4)$ to represent the number of pendant vertices of vertices u_1, u_2, u_3, u_4 in G , and $k_1 \geq \max\{k_2, k_3, k_4\}$. By Lemma 2.6, we have $G(k_1, k_2, k_3, k_4) < G(k_1 + k_2, 0, k_3, k_4) < G(k_1 + k_2 + k_3, 0,0, k_4) < G(k_1 + k_2 + k_3 + k_4, 0,0,0)$.

Claim 3: When the girth of graph G is 3 and all vertices except those on the cycle are pendant vertices, $\mathcal{U}_4$ is the graph with the third largest p -Sombor index.

Proof: Assume that $\mathcal{U}_4$ is not the graph with the third largest p -Sombor index. At this time, G is composed of a cycle of girth 3 and some pendant edges. We use $G(k_1, k_2, k_3)$ to represent the number of pendant vertices of vertices u_1, u_2, u_3 in G , and $k_1 \geq \max\{k_2, k_3\}$. By Lemma 2.7, we have the p -Sombor index $G(k_1, k_2, k_3) < G(k_1 + 1, k_2 - 1, k_3) < \cdots < G(k_1 + k_2 - 1,1, k_3) < \cdots < G(k_1 + k_2 + k_3 - 2,1,1) < G(k_1 + k_2 + k_3 - 2,2,0) = G(k_1 + k_2 + k_3 - 2,0,2)$. Thus, the proof is complete.

Claim 4: When the girth of graph G is 3 and in addition to the vertices on the cycle, there is at least one vertex that is not a pendant vertex, $\mathcal{U}_2$ is the graph with the third largest p -Sombor index.

Proof: Suppose $\mathcal{U}_2$ is not the graph with the third largest p -Sombor. Then, by Lemmas 2.5,2.8 and 2.9, we have $\mathrm{SOp}(G) < \mathrm{SOp}(\mathcal{U}_2)$, which completes the proof.

Through assertions 1, 2, 3, and 4, we conclude that there are three cases for unicyclic graphs with the second largest p -Sombor, namely the graphs $\mathcal{U}_2, \mathcal{U}_3$, and $\mathcal{U}_4$. By Lemmas 3.1.1 and 3.1.2, we have $\mathrm{SOp}(\mathcal{U}_3) > SOp(\mathcal{U}_4), SOp(\mathcal{U}_3) > SOp(\mathcal{U}_2)$. Therefore, when $G \cong \mathcal{U}_3$, the unicyclic graph attains the third largest p -Sombor.

3.2 Unicyclic graphs with fixed girth p -Sombor

Theorem 3.2.1 Consider $G \in \mathbb{U}_{n,\kappa}$, when $3 \leq \kappa \leq n$, the following inequality holds for the graph G:

$$SOp(G) \leq (n-\kappa)((n-\kappa+2)^p + 1^p)^{\frac{1}{p}} + 2((n-\kappa+2)^p + 2^p)^{\frac{1}{p}} + (\kappa-2)(2^p + 2^p)^{\frac{1}{p}}.$$

The equality holds if and only if $G \cong \mathcal{U}_{n,\kappa}^{n-\kappa}$.

Proof: According to Lemma 2.5, the graph G can be transformed into a cycle with girth κ by attaching some pendant vertices. Then, by Lemma 2.6, it follows that $\mathcal{U}_{n,k}^{n-k}$ is the graph with the fixed girth κ that attains the maximum p -Sombor.

$$\mathrm{SOp}\big(\mathcal{U}_{n,\kappa}^{n-\kappa}\big) = (n-\kappa)((n-\kappa+2)^p + 1^p)^{\frac{1}{p}} + 2((n-\kappa+2)^p + 2^p)^{\frac{1}{p}} + (\kappa-2)(2^p + 2^p)^{\frac{1}{p}}$$

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

References

[1] Tamás Réti, Tomislav Došlić, and Akbar Ali. On the sombor index of graphs. Contributions to Mathematics, 3:11-18, 2021.
[2] Xiaona Fang, Lihua You, and Hechao Liu. The expected values of sombor indices in random hexagonal chains, phenylene chains and sombor indices of some chemical graphs. International Journal of Quantum Chemistry, 121(17):e26740, 2021.
[3] Hechao Liu, Ivan Gutman, Lihua You, and Yufei Huang. Sombor index: review of extremal results and bounds. Journal of Mathematical Chemistry, 60(5):771-798, 2022.

[4] Igor Milovanovic, Emina Milovanovic, Akbar Ali, and Marjan Matejic. Some results on the sombor indices of graphs. Contrib. Math, 3:59-67, 2021.
[5] Hanyuan Deng, Zikai Tang, and Renfang Wu. Molecular trees with extremal values of sombor indices. International Journal of Quantum Chemistry, 121(11):e26622, 2021.
[6] 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.
[7] Wanping Zhang, Jixiang Meng, and Na Wang. Extremal graphs for sombor index with given parameters. Axioms, 12(2):203, 2023.
[8] Ting Zhou, Zhen Lin, and Lianying Miao. The extremal sombor index of trees and unicyclic graphs with given matching number. Journal of Discrete Mathematical Sciences and Cryptography, 26(8):2205-2216, 2022.
[9] Akbar Ali, Igor Ž. Milovanović, Abeer M. Albalahi, Abdulaziz M. Alanazi, and Amjad E. Hamza. Solutions to some open problems about four sombor-index-like graph invariants. MATCH Commun. Math. Comput. Chem, 90(2):505-512, 2023.
[10] Roberto Cruz, Ivan Gutman, and Juan Rada. Sombor index of chemical graphs. Applied Mathematics and Computation, 399:126018, 2021.
[11] Roberto Cruz, Juan Rada, and José M. Sigarreta. Sombor index of trees with at most three branch vertices. Applied Mathematics and Computation, 409:126414, 2021.
[12] Amjad E. Hamza and Akbar Ali. On a conjecture regarding the exponential reduced sombor index of chemical trees. Discrete Mathematics Letters, 9:107-110, 2022.
[13] 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.
[14] Juan Rada, José M Rodríguez, and José M Sigarreta. General properties on sombor indices. Discrete Applied Mathematics, 299:87-97, 2021.
[15] Kinkar Chandra Das and Yilun Shang. Some extremal graphs with respect to sombor index. Mathematics, 9(11):1202, 2021.
[16] Hanyuan Deng, Zikai Tang, and Renfang Wu. Molecular trees with extremal values of sombor indices. International Journal of Quantum Chemistry, 121(11):e26622, 2021.
[17] Kinkar Chandra Das and Ivan Gutman. On sombor index of trees. Applied Mathematics and Computation, 412:126575, 2022.
[18] Xiaoling Sun and Jianwei Du. On sombor index of trees with fixed domination number. Applied Mathematics and Computation, 421:126946, 2022.
[19] Fangxia Wang and Baoyindureng Wu. The k-sombor index of trees. Asia-Pacific Journal of Operational Research, 41(01):2350002, 2024.
[20] Ting Zhou, Zhen Lin, and Lianying Miao. The extremal sombor index of trees and unicyclic graphs with given matching number. Journal of Interdisciplinary Mathematics, 25(7):2205-2216, 2022.
[21] Ting Zhou, Zhen Lin, and Lianying Miao. The sombor index of trees and unicyclic graphs with given maximum degree. Discrete Mathematics Letters, 7:24-29, 2021.
[22] Hechao Liu, Lihua You, and Yufei Huang. Extremal sombor indices of tetracyclic (chemical) graphs. MATCH Commun. Math. Comput. Chem, 88(3):573-581, 2022.
[23] Kinkar Chandra Das, Ahmet Sinan Cevik, Ismail Naci Cangul, and Yilun Shang. On sombor index. Symmetry, 13(1):140, 2021.
[24] Hechao Liu, Lihua You, and Yufei Huang. Ordering chemical graphs by sombor indices and its applications. MATCH Commun. Math. Comput. Chem, 87(1):5-22, 2022.
[25] 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.
[26] 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.
[27] Shuchao Li, Zheng Wang, and Minjie Zhang. On the extremal sombor index of trees with a given diameter. Applied Mathematics and Computation, 416:126731, 2022.