Electronic Journal of Mathematics
www.shahindp.com/locate/ejm

Electron. J. Math. **10** (2025) 104–110
DOI: 10.47443/ejm.2025.071

Research Article

Maximizing the Sombor index of unicyclic graphs of fixed order with k pendant vertices

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(Received: 17 November 2025. Received in revised form: 27 December 2025. Accepted: 30 December 2025. Published online: 31 December 2025.)

Abstract

The Sombor index of a graph G is defined as $SO(G) = \sum_{uv\in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$, where $d_G(u)$ represents the degree of vertex u. In this paper, we establish a sharp upper bound for the Sombor index of unicyclic graphs with n vertices and k pendant vertices, and characterize the extremal graph attaining this bound. Using a case analysis based on the graph structure and an inductive argument, we demonstrate that the maximum Sombor index is achieved by the graph formed by attaching k pendant vertices to a single vertex of an $(n-k)$-cycle.

Keywords: Sombor index; unicyclic graph; pendant vertex; extremal graph.

2020 Mathematics Subject Classification: 05C09, 05C35, 05C92.

1. Introduction

Let G be a finite, simple, and connected graph with vertex set $V(G)$ and edge set $E(G)$. The order of G is the number of vertices in $V(G)$, denoted by n. Two vertices are said to be neighbors of each other if they are adjacent. The degree of the vertex $v \in V(G)$, denoted by $d_G(v)$, is equal to the number of neighbors of v in G. A vertex of degree one is called a pendant vertex. A unicyclic graph is a connected graph with exactly one cycle. For $p \geq 3$ and $k \geq 0$, let $C_{p,k}$ be the unicyclic graph formed by attaching k pendant vertices to a single vertex of a p-cycle C_p. For any vertex $u \in V(G)$, $G-u$ is the graph obtained from G by deleting u and its incident edges.

The Sombor index, proposed by Gutman [3], is a vertex-degree-based topological index. It is defined by treating the edges of a graph as points in a two-dimensional coordinate system and calculating their Euclidean distance from the origin, offering a new perspective and tool in chemical graph theory. The Sombor index of a graph G is defined by

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

The extremal values of the Sombor index for unicyclic graphs and trees with given parameters have been extensively studied. Liu [6] established the maximum Sombor index for unicyclic graphs with a prescribed diameter, whereas Alidadi, Parsian and Arianpoor [1] derived the corresponding minimum Sombor index under the same constraint. Senthilkumar et al. [9] determined the maximum Sombor index for unicyclic graphs with fixed girth, a result complemented by Chen and Zhu [2], who characterized extremal Sombor indices for both general and chemical unicyclic graphs under girth restrictions. Additionally, Zhou, Lin and Miao [13] studied the Sombor index of trees and unicyclic graphs with fixed maximum degree. The problem of determining the maximum Sombor index of trees and unicyclic graphs with a given matching number was considered in [7] and completed in [14].

The extremal problem for graphs with a given number of pendant vertices has been explored for various topological indices. Vetrík and Balachandran [11] determined the extremal general Randić indices of unicyclic graphs with fixed pendant vertices. Extremal values of the sum-connectivity index and its generalizations for graphs with k pendant vertices were studied for unicyclic graphs in [10] and trees in [12]. Pandey and Patra [8] determined the connected graphs with a prescribed number of pendant vertices that attain the maximum and minimum Wiener indices. Extremal values of the Zagreb indices and the signless Laplacian index for cacti with given pendant vertices were investigated in [4] and [5].

The main objective of this paper is to establish an upper bound for the Sombor index of unicyclic graphs with a given number of pendant vertices.

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2. Preliminaries

Lemma 2.1. *For $x \geq 2$, the function $f(x) = \sqrt{x^2+a^2} - \sqrt{(x-1)^2+a^2}$ is strictly increasing on x, where a is a positive integer.*

Proof. We have

$$f'(x) = \frac{x}{\sqrt{x^2+a^2}} - \frac{x-1}{\sqrt{(x-1)^2+a^2}}.$$

Let

$$A(x) = \frac{x}{\sqrt{x^2+a^2}}.$$

Since $x \geq 2$ and $a \geq 1$, we have

$$A'(x) = \frac{a^2}{(x^2+a^2)^{\frac{3}{2}}} > 0.$$

Thus, $A(x)$ is a strictly increasing function for $x \geq 2$, which implies $A(x) > A(x-1)$. Therefore, for $x \geq 2$, it follows that $f'(x) > 0$. Hence, the lemma holds. □

Lemma 2.2. *Let $g(x) = (x-b)\sqrt{1+x^2} - (x-b-1)\sqrt{1+(x-1)^2}$. When $b = 1$ or $b = 2$, the function $g(x)$ is strictly increasing on the domain $x \geq 2$.*

Proof. The derivative of $g(x)$ is computed as follows:

$$g'(x) = \left(\sqrt{1+x^2} + \frac{x(x-b)}{\sqrt{1+x^2}}\right) - \left(\sqrt{1+(x-1)^2} + \frac{(x-1)(x-b-1)}{\sqrt{1+(x-1)^2}}\right)$$

$$= \sqrt{1+x^2} - \sqrt{1+(x-1)^2} + \frac{x(x-b)}{\sqrt{1+x^2}} - \frac{(x-1)(x-b-1)}{\sqrt{1+(x-1)^2}}.$$

For $b = 1$, the derivative expression simplifies to

$$g'(x) = \sqrt{1+x^2} - \sqrt{1+(x-1)^2} + \frac{x(x-1)}{\sqrt{1+x^2}} - \frac{(x-1)(x-2)}{\sqrt{1+(x-1)^2}}$$

$$= \left(\sqrt{1+x^2} - \sqrt{1+(x-1)^2}\right) + (x-1)\left(\frac{x}{\sqrt{1+x^2}} - \frac{x-2}{\sqrt{1+(x-1)^2}}\right).$$

The first term $\sqrt{1+x^2} - \sqrt{1+(x-1)^2}$ is positive for all $x \geq 2$. To analyze the second term, consider the function

$$B(x) = \frac{x}{\sqrt{1+x^2}},$$

which is strictly increasing by Lemma 2.1. For $x \geq 2$, we have

$$B(x) > B(x-1) > \frac{x-2}{x-1}B(x-1),$$

which implies

$$\frac{x}{\sqrt{1+x^2}} - \frac{x-2}{\sqrt{1+(x-1)^2}} > 0.$$

Therefore, $g'(x) > 0$, which means $g(x)$ is strictly increasing for $x \geq 2$.

For $b = 2$, the derivative becomes

$$g'(x) = \sqrt{1+x^2} - \sqrt{1+(x-1)^2} + \frac{x(x-2)}{\sqrt{1+x^2}} - \frac{(x-1)(x-3)}{\sqrt{1+(x-1)^2}}$$

$$= \frac{2x^2-2x+1}{\sqrt{1+x^2}} - \frac{2x^2-6x+5}{\sqrt{1+(x-1)^2}}.$$

To prove that $g'(x) > 0$, we introduce the following two auxiliary functions:

$$A(x) = \frac{2x^2-2x+1}{2x^2-6x+5}, \qquad B(x) = \sqrt{\frac{1+x^2}{1+(x-1)^2}}.$$

The desired inequality $g'(x) > 0$ is equivalent to $A(x) > B(x)$. Squaring both sides yields

$$\frac{(2x^2-2x+1)^2}{(2x^2-6x+5)^2} \geq \frac{x^2+1}{x^2-2x+2}.$$

Define the polynomial difference:

$$G(x) = (2x^2-2x+1)^2(x^2-2x+2) - (x^2+1)(2x^2-6x+5)^2.$$

Expanding and simplifying gives

$$G(x) = 8x^5 - 28x^4 + 48x^3 - 56x^2 + 50x - 23.$$

The derivatives of $G(x)$ are computed to analyze its behavior:

$$\begin{aligned} G'(x) &= 40x^4 - 112x^3 + 144x^2 - 112x + 50, \\ G''(x) &= 160x^3 - 336x^2 + 288x - 112, \\ G'''(x) &= 480x^2 - 672x + 288. \end{aligned} \tag{1}$$

The third derivative $G'''(x)$ is positive for all x, as seen from its discriminant $\triangle = (-672)^2 - 4 \times 480 \times 288 < 0$ and leading coefficient $480 > 0$. This implies $G''(x)$ is strictly increasing. Evaluating at $x = 2$ gives $G''(2) = 280 > 0$, ensuring $G''(x) > 0$ for all $x \geq 2$. Consequently, $G'(x)$ is strictly increasing with $G'(2) = 146 > 0$, guaranteeing $G'(x) > 0$ on the domain. Therefore, $G(x)$ itself is strictly increasing, and since $G(2) = 45 > 0$, we conclude $G(x) > 0$ for all $x \geq 2$ and the lemma follows. □

Lemma 2.3. *For $x \geq 1$, the function $h(x) = \sqrt{x^2+c^2} - \sqrt{x^2+(c-1)^2}$ is strictly decreasing on x, where c is a positive integer.*

Proof. We have

$$h'(x) = \frac{x}{\sqrt{x^2+c^2}} - \frac{x}{\sqrt{x^2+(c-1)^2}} = x\left(\frac{1}{\sqrt{x^2+c^2}} - \frac{1}{\sqrt{x^2+(c-1)^2}}\right).$$

Since

$$\frac{1}{\sqrt{x^2+c^2}} < \frac{1}{\sqrt{x^2+(c-1)^2}}$$

for all $c \geq 1$ and $x \geq 1$, it follows that

$$h'(x) = x\left(\frac{1}{\sqrt{x^2+c^2}} - \frac{1}{\sqrt{x^2+(c-1)^2}}\right) < 0.$$

Therefore, $h(x)$ is strictly decreasing for $x \geq 1$. □

Lemma 2.4. *For $x \geq 2$, the function*

$$p(x) = x\sqrt{1+(x+2)^2} - (2x-1)\sqrt{1+(x+1)^2} + (x-1)\sqrt{1+x^2} + 2\sqrt{4+(x+2)^2} - 3\sqrt{4+(x+1)^2} + \sqrt{4+x^2}$$

is positive, i.e., $p(x) > 0$.

Proof. To establish the positivity of $p(x)$, we decompose it into two components

$$p(x) = \phi(x) + \varphi(x).$$

where

$$\phi(x) = x\sqrt{1+(x+2)^2} - (2x-1)\sqrt{1+(x+1)^2} + (x-1)\sqrt{1+x^2}$$

and

$$\varphi(x) = 2\sqrt{4+(x+2)^2} - 3\sqrt{4+(x+1)^2} + \sqrt{4+x^2}.$$

We first rewrite $\phi(x)$ as:

$$\begin{aligned} \phi(x) &= x\sqrt{1+(x+2)^2} - x\sqrt{1+(x+1)^2} + (1-x)\sqrt{1+(x+1)^2} + (x-1)\sqrt{1+x^2} \\ &= x\left(\sqrt{1+(x+2)^2} - \sqrt{1+(x+1)^2}\right) - (x-1)\left(\sqrt{1+(x+1)^2} - \sqrt{1+x^2}\right). \end{aligned} \tag{2}$$

Define the auxiliary function $A(t) = \sqrt{1+t^2}$. Its first and second derivatives are given as follows:

$$A'(t) = \frac{t}{\sqrt{1+t^2}}, \qquad A''(t) = \frac{1}{(1+t^2)^{3/2}} > 0.$$

Hence, $A(t)$ is strictly convex for all $t \geq 2$. Consequently, the first-order finite difference $\triangle_1(t) = A(t+1) - A(t)$ is strictly increasing on t, implying $\triangle_1(t+1) > \triangle_1(t)$. Thus,

$$\phi(x) = x\,\triangle_1(x+1) - (x-1)\,\triangle_1(x) > (x-1)\,(\triangle_1(x+1) - \triangle_1(x)) > 0.$$

Similarly, we rewrite $\varphi(x)$ as

$$\varphi(x) = 2\left(\sqrt{4+(x+2)^2} - \sqrt{4+(x+1)^2}\right) - \left(\sqrt{4+(x+1)^2} - \sqrt{4+x^2}\right).$$

Define $B(t) = \sqrt{4+t^2}$. Its derivatives are given as follows:

$$B'(t) = \frac{t}{\sqrt{4+t^2}}, \qquad B''(t) = \frac{4}{(4+t^2)^{3/2}} > 0.$$

Thus, $B(t)$ is a strictly convex function for $t \geq 2$. Hence, the first-order finite difference $\triangle_2(t) = B(t+1) - B(t)$ is strictly increasing on t, satisfying $\triangle_2(t+1) > \triangle_2(t)$ for all $t \geq 2$. Since

$$\triangle_2(x) = B(x+1) - B(x) = \sqrt{4+(x+1)^2} - \sqrt{4+x^2} > 0,$$

we obtain

$$\varphi(x) = 2\,\triangle_2(x+1) - \triangle_2(x) > 2\,\triangle_2(x) - \triangle_2(x) = \triangle_2(x) > 0.$$

This completes the proof. □

3. Main result

In this section, we establish an upper bound for the Sombor index of unicyclic graphs with n vertices and k pendant vertices. The extremal graph $C_{n-k,k}$, which is the graph formed by attaching k pendant vertices to exactly one vertex of an $(n-k)$-cycle, is shown in Figure 3.1. Note that for every unicyclic graph with n vertices and k pendent vertices, we have $n \geq 3$ and $0 \leq k \leq n-3$.

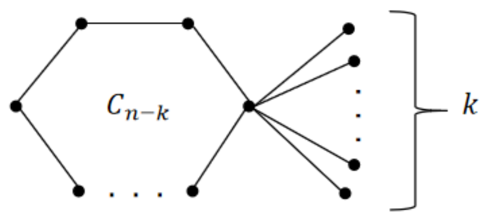

Figure 3.1: The extremal graph $C_{n-k,k}$.

Theorem 3.1. *For any unicyclic graph G with n vertices and k pendant vertices, it holds that*

$$SO(G) \leq k\sqrt{1+(k+2)^2} + 2\sqrt{4+(k+2)^2} + 2\sqrt{2}(n-k-2),$$

where the equality holds if and only if G is $C_{n-k,k}$.

Proof. We proceed by induction on n. The base case for $k=0$ is trivial, as the only unicyclic graph with n vertices and no pendant vertices is $C_n = C_{n,0}$. For the general case where $n \geq k+3$ and $k \geq 1$, assume that the result holds for all unicyclic graphs with at most $n-1$ vertices. Let G be a unicyclic graph with n vertices and k pendant vertices. Let C be the unique cycle in G. Denote by $V(C)$ the vertex set of the cycle C. Select a pendant vertex u whose distance to C is maximized, and let v be its unique neighbor with degree $d_G(v) = m$.

Define $G' = G - u$. We analyze the following cases.

Case 1: $v \in V(C)$.
Here, v is adjacent to two vertices $v_1, v_2 \in V(C)$ and $m-2$ pendant vertices in G, where $3 \leq m \leq k+2$. Let $d_G(v_1) = t_1 \geq 2$ and $d_G(v_2) = t_2 \geq 2$. Then,

$$\begin{aligned} SO(G) = SO(G') &+ \sqrt{t_1^2 + m^2} - \sqrt{t_1^2 + (m-1)^2} + \sqrt{t_2^2 + m^2} \\ &- \sqrt{t_2^2 + (m-1)^2} + (m-2)\sqrt{1+m^2} - (m-3)\sqrt{1+(m-1)^2}. \end{aligned} \tag{3}$$

By Lemmas 2.1 and 2.2, for $3 \leq m \leq k+2$, the following inequality holds:

$$\begin{aligned} &\sqrt{t_1^2 + m^2} - \sqrt{t_1^2 + (m-1)^2} + \sqrt{t_2^2 + m^2} - \sqrt{t_2^2 + (m-1)^2} \\ &+ (m-2)\sqrt{1+m^2} - (m-3)\sqrt{1+(m-1)^2} \\ &\leq \sqrt{t_1^2 + (k+2)^2} - \sqrt{t_1^2 + (k+1)^2} + \sqrt{t_2^2 + (k+2)^2} - \sqrt{t_2^2 + (k+1)^2} \\ &+ k\sqrt{1+(k+2)^2} - (k-1)\sqrt{1+(k+1)^2}, \end{aligned} \tag{4}$$

with equality if and only if $m = k+2$. By Lemma 2.3, for $t_1, t_2 \geq 2$, we have

$$\begin{aligned} h(t_1) &= \sqrt{t_1^2 + (k+2)^2} - \sqrt{t_1^2 + (k+1)^2} \\ &\leq \sqrt{2^2 + (k+2)^2} - \sqrt{2^2 + (k+1)^2} = h(2) \end{aligned} \tag{5}$$

and

$$\begin{aligned} h(t_2) &= \sqrt{t_2^2 + (k+2)^2} - \sqrt{t_2^2 + (k+1)^2} \\ &\leq \sqrt{2^2 + (k+2)^2} - \sqrt{2^2 + (k+1)^2} = h(2). \end{aligned} \tag{6}$$

with equalities if and only if $t_1 = t_2 = 2$. Combining these results, we obtain

$$SO(G) \leq SO(G') + 2\sqrt{4+(k+2)^2} - 2\sqrt{4+(k+1)^2} + k\sqrt{1+(k+2)^2} - (k-1)\sqrt{1+(k+1)^2}. \tag{7}$$

Since G' has $n-1$ vertices and $k-1$ pendant vertices, the induction hypothesis yields

$$SO(G') \leq (k-1)\sqrt{1+(k+1)^2} + 2\sqrt{4+(k+1)^2} + 2\sqrt{2}\,(n-k-2),$$

with equality if and only if G' is $C_{n-k,k-1}$. Therefore, we conclude

$$SO(G) \leq k\sqrt{1+(k+2)^2} + 2\sqrt{4+(k+2)^2} + 2\sqrt{2}\,(n-k-2).$$

Case 2: $v \notin V(C)$.
Since u is a pendant vertex furthest from the cycle C in G and $v \notin V(C)$, there is exactly one non-pendant vertex adjacent to v in G. We denote this vertex by w, where $d_G(w) = s \geq 2$. The remaining $m-1$ neighbors of v in G are pendant vertices. Note that $2 \leq m \leq k+1$.

Case 2.1: $m \geq 3$.
The Sombor index $SO(G)$, in this case, is given by

$$SO(G) = SO(G') + (m-1)\sqrt{1+m^2} - (m-2)\sqrt{1+(m-1)^2} + \sqrt{s^2+m^2} - \sqrt{s^2+(m-1)^2}. \tag{8}$$

By Lemmas 2.1 and 2.2, for $3 \le m \le k+1$, we derive

$$\begin{aligned} f(m)+g(m) &= (m-1)\sqrt{1+m^2}-(m-2)\sqrt{1+(m-1)^2}+\sqrt{s^2+m^2}-\sqrt{s^2+(m-1)^2} \\ &\le k\sqrt{1+(k+1)^2}-(k-1)\sqrt{1+k^2}+\sqrt{s^2+(k+1)^2}-\sqrt{s^2+k^2} \\ &= f(k+1)+g(k+1). \end{aligned}$$

Equality holds if and only if $m=k+1$. By Lemma 2.3, for $s \ge 2$, we have

$$h(s)=\sqrt{s^2+(k+1)^2}-\sqrt{s^2+k^2} \le \sqrt{2^2+(k+1)^2}-\sqrt{2^2+k^2}=h(2),$$

with equality if and only if $s=2$. Then

$$SO(G) \le SO(G')+k\sqrt{1+(k+1)^2}-(k-1)\sqrt{1+k^2}+\sqrt{4+(k+1)^2}-\sqrt{4+k^2}.$$

From the induction hypothesis and the fact that G' has $n-1$ vertices and $k-1$ pendant vertices, it follows that

$$SO(G') \le (k-1)\sqrt{1+(k+1)^2}+2\sqrt{4+(k+1)^2}+2\sqrt{2}\,(n-k-2).$$

Thus, we have

$$SO(G) \le (2k-1)\sqrt{1+(k+1)^2}-(k-1)\sqrt{1+k^2}+3\sqrt{4+(k+1)^2}-\sqrt{4+k^2}+2\sqrt{2}\,(n-k-2). \tag{9}$$

By Lemma 2.4, we obtain

$$(2k-1)\sqrt{1+(k+1)^2}-(k-1)\sqrt{1+k^2}+3\sqrt{4+(k+1)^2}-\sqrt{4+k^2} \le k\sqrt{1+(k+2)^2}+2\sqrt{4+(k+2)^2}. \tag{10}$$

Combining these results, we obtain

$$SO(G) \le k\sqrt{1+(k+2)^2}+2\sqrt{4+(k+2)^2}+2\sqrt{2}\,(n-k-2).$$

Case 2.2: $m=2$.
For $m=2$, the Sombor index simplifies to

$$SO(G)=SO(G')+\sqrt{s^2+2^2}-\sqrt{s^2+1}+\sqrt{5}.$$

Since G' has $n-1$ vertices and k pendant vertices, the induction hypothesis implies that

$$SO(G) \le k\sqrt{1+(k+2)^2}+2\sqrt{4+(k+2)^2}+2\sqrt{2}\,(n-k-3),$$

with equality if and only if G' is $C_{n-k-1,k}$. By Lemma 2.3, for $s \ge 2$, we have

$$h(s)=\sqrt{s^2+2^2}-\sqrt{s^2+1} \le \sqrt{2^2+2^2}-\sqrt{2^2+1}=\sqrt{8}-\sqrt{5}.$$

with equality if and only if $s=2$. Thus, we have

$$\begin{aligned} SO(G) &\le SO(G')+\sqrt{8}-\sqrt{5}+\sqrt{5}=SO(G')+\sqrt{8} \\ &\le k\sqrt{1+(k+2)^2}+2\sqrt{4+(k+2)^2}+2\sqrt{2}\,(n-k-3)+\sqrt{8} \\ &= k\sqrt{1+(k+2)^2}+2\sqrt{4+(k+2)^2}+2\sqrt{2}\,(n-k-2). \end{aligned}$$

Equality holds if and only if $G'=C_{n-k-1,k}$ and $s=2$, which is impossible as G would then contain an edge $uv \notin C$ with $d_G(v)=2$ and $d_G(w)=2$. Therefore, we have

$$SO(G) < k\sqrt{1+(k+2)^2}+2\sqrt{4+(k+2)^2}+2\sqrt{2}\,(n-k-2).$$

This completes the proof of the theorem. □

Acknowledgment

This work was supported by the Natural Science Foundation of Shanghai (Grant No. 24ZR1415500).

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