

Extremal problems on Sombor indices of bicyclic graphs with a given diameter

Linlin Cui¹ and Xianya Geng²

¹School of Mathematics and Big Data,
 Anhui University of Science & Technology, Huainan , China
 1150396216@qq.com

²School of Mathematics and Big Data,
 Anhui University of Science & Technology, Huainan , China
 gengxianya@sina.com

ABSTRACT

Sombor index is a novel topological index, which was introduced by Gutman and defined for a graph G as $S(G) = \sum_{uv \in E_G} \sqrt{d_u^2 + d_v^2}$, where $d_u = d_G(u)$ and $d_v = d_G(v)$ denote the degree of vertex u and v in G . Liu et al. investigated extremal problems concerning the Sombor indices of unicyclic graphs under diameter constraints. Extending their findings, we apply inductive reasoning to derive the extremal Sombor indices for bicyclic graphs with prescribed order and diameter.

Keywords: Sombor index, bicyclic graph, extremal value, diameter.

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1 Introduction

Graph invariants are widely used to analyze molecular graph properties and characterize their structures.

Consider a graph $G = (V_G, E_G)$ with $|V_G| = m$ vertices and $|E_G| = m'$ edges. For a vertex u , let $N_G(u)$ denote its neighbor set, and $d_G(u) = |N_G(u)|$ its degree. A vertex u is *pendent* if $d_G(u) = 1$, and PV_G represents the set of all pendent vertices in G . The distance $d_G(u, v)$ between vertices u and v is the shortest path length between them, and the *diameter* of G is defined as $d = \max_{u, v \in V_G} \{d(u, v)\}$.

Bicyclic graphs can be classified into three structural types (see Figure 1):

- $\mathcal{B}_0$: Graphs with two independent cycles.
- $\mathcal{B}_1$: Graphs with two cycles connected by a path of length $l \geq 1$.
- $\mathcal{B}_2$: Graphs with two cycles sharing a common path, where $l \geq 1$ is the length of the connecting path, and $|V_C| + |V_{C'}| = m + 1 - l$ (Cruz and Rada, 2021).

In the 1970s, the first and second Zagreb indices were introduced (Gutman and Trinajstić, 1972) (Gutman and Trinajstić, 1972)

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{uv \in E(G)} (d_G(u) + d_G(v)),$$

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v),$$

where $d_G(\cdot)$ denotes vertex degree.

Several related vertex-degree-based indices were subsequently developed:

- Forgotten index (Furtula and Gutman, 2015): $F(G) = \sum_{uv \in E(G)} (d_G(u)^2 + d_G(v)^2)$
- Reciprocal sum-connectivity index (Ali, Furtula, Redžepović and Gutman, 2022): $\chi_{1/2}(G) = \sum_{uv \in E(G)} \sqrt{d_G(u) + d_G(v)}$

Building on these concepts, Gutman recently introduced the Sombor indices (Gutman, 2021):

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

$$SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_G(u) - 1)^2 + (d_G(v) - 1)^2}.$$

For comprehensive studies on Sombor indices, see (Alikhani and Ghanbari, 2021) (Cruz, Gutman and Rada, 2021) (Došlić, Réti and Ali, 2021) (Deng, Tang and Wu, 2021) (Fang, You and Liu, 2021) (Li and Wang, 2021) (Liu, Chen, Xiao, Fang and Tang, 2021) (Liu, You and Huang, 2021) (Liu, You, Huang and Fang, 2021) (Liu, You, Tang and Liu, 2021) (Redžepović, 2021) (Zhang, You, Liu and Huang, 2021).

Here, $\mathcal{B}_0(m)$ denotes the class of $\mathcal{B}_0$ -type graphs with m vertices, while $\mathcal{B}_1(m, l)$ and $\mathcal{B}_2(m, l)$ represent the corresponding classes for $\mathcal{B}_1$ and $\mathcal{B}_2$, respectively.

Our paper investigates the extremal problem for bicyclic graphs with a given diameter. This work extends previous studies on Sombor indices of graphs with specific parameters.

The foundation for our research comes from several key works:

- (Chen, Li and Wang, 2022) established fundamental results for Sombor indices of trees with given parameters including diameter and pendent vertices
- (Li, Wang and Zhang, 2022) determined extremal Sombor indices for n -vertex trees with diameter $d \geq 4$
- (Alfuraidan, Das, Vetrík and Balachandran, 2022) (Alfuraidan, Das, Vetrík and Balachandran, 2021) solved the extremal problem for general Randić index of unicyclic graphs with prescribed diameter
- (Cruz and Rada, 2021) (Li et al., 2022) (Liu, 2022) investigated extremal values for unicyclic and bicyclic graphs

Building upon these results, we employ inductive methods to:

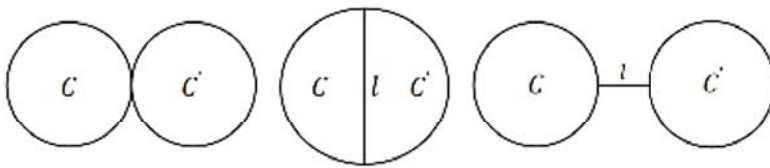


Figure 1: The graphs $\mathcal{B}_0$ (left), $\mathcal{B}_1$ (middle) and $\mathcal{B}_2$ (right)

- Characterize the maximum Sombor indices for bicyclic graphs with fixed order and given diameter
- Completely determine these extremal values for all relevant cases

We establish tight upper bounds for the Sombor indices of diameter-constrained bicyclic graphs.

2 Preliminaries

Let $\mathcal{B}_{m,d} = \{G \mid G \text{ is a bicyclic graph of order } m \text{ and diameter } d\}$. $\mathcal{B}_m^d \in \mathcal{B}_{m,d}$ ($d \geq 4$) in Figure.2.

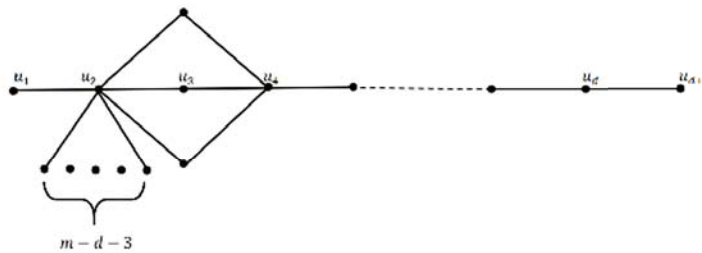


Figure 2: The graphs $\mathcal{B}_m^d$.

For $4 \leq d \leq m - 3$

$$S(\mathcal{B}_m^d) = (m - d - 2)\sqrt{(m - d + 1)^2 + 1} + 3\sqrt{(m - d + 1)^2 + 4} + F_1 \quad (2.1)$$

where $F_1 = 6\sqrt{5} + \sqrt{17}$ if $d = 4$; $F_1 = 8\sqrt{5} + 2(d - 5)\sqrt{2} + \sqrt{5}$ if $d \geq 5$.

Theorem 2.1. For any $G \in \mathcal{B}(m, d)$, we have

$$S(G) \leq S(\mathcal{B}_m^d),$$

with equality holding precisely when $G \cong \mathcal{B}_m^d$ (see Figure 2).

3 Manin Results

Theorem 3.1. For any $G \in \mathcal{B}_m$ ($m \geq 6$),

$$S(G) \geq 2\sqrt{2}m - 5\sqrt{2} + 4\sqrt{13} = S(G'),$$

where equality holds if and only if $G \cong G' \in \mathcal{B}_1(m, 1) \cup \mathcal{B}_2(m, 1)$ (Figure 3).

Let $C = v_1v_2 \cdots v_{|V_C|}$ and $C' = v'_1v'_2 \cdots v'_{|V_{C'}|}$ be the two cycles in a bicyclic graph G , and $P = u_1u_2 \cdots u_du_{d+1}$ its diametral path. Denote by PV_G the set of pendant vertices of G .

The extremal graph $\mathcal{B}_{m,d}^{\max} \in \mathcal{B}_{m,d}$ with maximal Sombor index must satisfy:

- Contains at least one pendant vertex
- Has order $m \geq d + 3$

Theorem 3.2. For any $G \in \mathcal{B}_{d+3,d}$,

$$S(G) \leq S(\mathcal{B}_{d+3}^d),$$

with equality if and only if $G \cong \mathcal{B}_{d+3}^d$.

Proof. Let $G^* \in \mathcal{B}_{d+3,d}^{\max}$. Since $m = d + 3$, there exist two vertices w and w' not on the diametral path $P = u_1u_2 \cdots u_du_{d+1}$. The cycles in G^* must be one of the following forms:

1. $C = u_iu_{i+1}wu_i$ and $C' = u_iu_{i+1}w'u_i$ (two 3-cycles)
2. $C = u_iu_{i+1}u_{i+2}wu_i$ and $C' = u_iu_{i+1}u_{i+2}w'u_i$ (two 4-cycles)
3. $C = u_iu_{i+1}u_{i+2}wu_i$ and $C' = u_iu_{i+1}w'u_i$ (one 4-cycle and one 3-cycle)

□

Claim 1. We have $u_1 \notin V_C \cup V_{C'}$ and $u_{d+1} \notin V_C \cup V_{C'}$.

If $u_1 \in V_C \cup V_{C'}$, then the cycles must be one of the following cases:

1. $C = u_1u_2wu_1$ and $C' = u_1u_2w'u_1$ (both 3-cycles)
2. $C = u_1u_2u_3wu_1$ and $C' = u_1u_2u_3w'u_1$ (both 4-cycles)

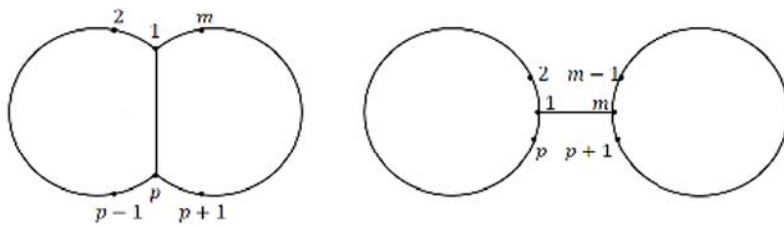


Figure 3: $\mathcal{B}_1(m, 1)$ (left) and $\mathcal{B}_2(m, 1)$ (right)

3. $C = u_1u_2u_3wu_1$ (4-cycle) and $C' = u_2u_3w'u_2$ (3-cycle)

Case 1. $C = u_1u_2wu_1$ and $C' = u_1u_2w'u_1$

Let $G^{***} = G^* - \{u_1w\} - \{u_1w'\} + \{u_3w\} + \{u_3w'\}$, then $G^{***} \in \mathcal{B}_{d+3,d}$, and

$$\begin{aligned} S(G^*) - S(G^{***}) &= 2\sqrt{3^2 + 2^2} + \sqrt{3^2 + 4^2} + \sqrt{2^2 + 2^2} - \sqrt{1^2 + 4^2} - 2\sqrt{2^2 + 4^2} - \sqrt{4^2 + 4^2} \\ &= 2\sqrt{13} + 5 + 2\sqrt{2} - \sqrt{17} - 4\sqrt{5} - 4\sqrt{2} \\ &< 0. \end{aligned} \tag{3.1}$$

Case 2. $C = u_1u_2u_3wu_1$ and $C' = u_1u_2u_3w'u_1$

Let $G^{***} = G^* - \{u_1w\} - \{u_1w'\} + \{u_2w\} + \{u_2w'\}$, then $G^{***} \in \mathcal{B}_{d+3,d}$, and

$$\begin{aligned} S(G^*) - S(G^{***}) &= 3\sqrt{3^2 + 2^2} + \sqrt{2^2 + 4^2} - \sqrt{1^2 + 4^2} - 2\sqrt{2^2 + 4^2} - \sqrt{4^2 + 4^2} \\ &= 3\sqrt{13} - 2\sqrt{5} - 4\sqrt{2} \\ &< 0, \end{aligned} \tag{3.2}$$

Case 3. $C = u_1u_2u_3wu_1$ and $C' = u_2u_3w'u_2$

Let $G^{***} = G^* - \{u_1w\} + \{u_2w\}$, then $G^{***} \in \mathcal{B}_{d+3,d}$,

$$\begin{aligned} S(G^*) - S(G^{***}) &= \sqrt{2^2 + 2^2} + 2\sqrt{2^2 + 3^2} + \sqrt{4^2 + 3^2} - \sqrt{1^2 + 4^2} - 2\sqrt{2^2 + 4^2} - \sqrt{4^2 + 4^2} \\ &= 2\sqrt{2} + 2\sqrt{13} + 5 - \sqrt{17} - 4\sqrt{5} - 4\sqrt{2} \\ &< 0, \end{aligned} \tag{3.3}$$

This contradicts the maximality of G^* . Therefore, we must have:

$$\begin{aligned} u_1 &\notin V_C \cup V_{C'} \\ u_{d+1} &\notin V_C \cup V_{C'} \end{aligned}$$

Claim 2. $|E_C| = 4$ and $|E_{C'}| = 4$.

Proof. If $|E_C| \geq 5$ or $|E_{C'}| \geq 5$, this would contradict the choice of the diametral path $P = u_1u_2 \cdots u_du_{d+1}$. The remaining possibilities are:

- $|E_C| = 3$ and $|E_{C'}| = 3$
- $|E_C| = 3$ and $|E_{C'}| = 4$
- $|E_C| = 4$ and $|E_{C'}| = 4$

Case 1. $|E_C| = 3$ and $|E_{C'}| = 3$.

In this configuration, we have:

$$\begin{aligned} C &= u_iu_{i+1}wu_i \\ C' &= u_iu_{i+1}w'u_i \end{aligned}$$

Since $d \geq 4$, either $u_{i-1} \notin PV_{G^*}$ or $u_{i+2} \notin PV_{G^*}$.

Assuming $u_{i-1} \notin PV_{G^*}$, we have $d_{G^*}(u_{i-2}) \in \{1, 2\}$. Define the graph modification:

$$G^{**} = G^* - \{u_i w\} - \{u_i w'\} + \{u_{i-1} w\} + \{u_{i-1} w'\}$$

Then $G^{**} \in \mathcal{B}_{d+3,d}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i-2}) + 2^2} - \sqrt{d_{G^*}^2(u_{i-2}) + 4^2} + \sqrt{4^2 + 4^2} \\ &\quad - \sqrt{2^2 + 4^2} (d_{G^*}(u_{i-2}) = 2) \\ &\leq \sqrt{2^2 + 2^2} - \sqrt{2^2 + 4^2} + \sqrt{4^2 + 4^2} - \sqrt{2^2 + 4^2} \\ &= 2\sqrt{2} - 2\sqrt{5} + 4\sqrt{2} - 2\sqrt{5} \\ &= 6\sqrt{2} - 4\sqrt{5} \\ &< 0, \end{aligned} \tag{3.4}$$

□

Case 2. $|E_C| = 3$ and $|E_{C'}| = 4$

In this configuration, the cycles must be:

$$\begin{aligned} C &= u_i u_{i+1} w u_i, \\ C' &= u_{i-1} u_i u_{i+1} w' u_{i-1}, \end{aligned}$$

where $2 \leq i \leq d-1$. Since $d \geq 4$, we have either $u_{i-1} \notin PV_{G^*}$ or $u_{i+2} \notin PV_{G^*}$.

Assuming $u_{i-1} \notin PV_{G^*}$, the vertex u_{i-2} satisfies $d_{G^*}(u_{i-2}) \in \{1, 2\}$. Performing the edge modification:

$$G^{**} = G^* - \{u_i w\} + \{u_{i-1} w\},$$

we obtain $G^{**} \in \mathcal{B}_{d+3,d}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i-2}) + 3^2} - \sqrt{d_{G^*}^2(u_{i-2}) + 4^2} + \sqrt{3^2 + 3^2} + 2\sqrt{2^2 + 3^2} \\ &\quad + \sqrt{4^2 + 3^2} - 4\sqrt{4^2 + 2^2} \\ &\leq \sqrt{2^2 + 3^2} - \sqrt{2^2 + 4^2} + \sqrt{3^2 + 3^2} \\ &\quad + 2\sqrt{2^2 + 3^2} + \sqrt{4^2 + 3^2} - 4\sqrt{4^2 + 2^2} (d_{G^*}(u_{i-2}) = 2) \\ &= \sqrt{13} - 2\sqrt{5} + 3\sqrt{2} + 2\sqrt{13} + 5 - 8\sqrt{5} < 0, \end{aligned} \tag{3.5}$$

This configuration contradicts the maximality of G^* . Similarly, the case $|E_C| = 4$ and $|E_{C'}| = 3$ also leads to a contradiction with G^* being maximal. Therefore, the only remaining possibility is:

$$|E_C| = 4 \quad \text{and} \quad |E_{C'}| = 4.$$

Furthermore, we have the position constraint $2 \leq i \leq d-2$.

$$\begin{aligned} S(G^*) - S(\mathcal{B}_{d+3}^d) &= \sqrt{1^2 + 2^2} + \sqrt{2^2 + 3^2} - \sqrt{1^2 + 4^2} - \sqrt{2^2 + 2^2} \\ &= \sqrt{5} + \sqrt{13} - \sqrt{17} - 2\sqrt{2} \\ &< 0. \end{aligned} \tag{3.6}$$

Next $m \geq d+4$.

Lemma 3.3. Let $G^* \in \mathcal{B}_{m,d}^{\max}$ be with $3 \leq d \leq m - 4$. Consider a pendant vertex $u \in PV_{G^*}$ adjacent to u_2 or u_d on the diametral path $P = u_1 u_2 \cdots u_d u_{d+1}$. Then cycles C and C' satisfy:

$$|V_C \cap V_P| \geq 2 \quad \text{and} \quad |V_{C'} \cap V_P| \geq 2.$$

Proof. Assume to the contrary that

$$|V_C \cap V_P| \leq 1 \quad \text{and} \quad |V_{C'} \cap V_P| \leq 1.$$

This leads to the following cases: □

- **Case 1:** Both cycles intersect P at exactly one vertex
- **Case 2:** One cycle intersects P at one vertex while the other is disjoint from P

Case 1. $|V_C \cap V_P| = 0$ and $|V_{C'} \cap V_P| = 0$

We construct $G^{**} \in \mathcal{B}_{m,d}$ through the following operation:

1. **Case $k \geq 2$:**

$$G^{**} = G^* - \{z_1 z_2\} - \{z'_1 z'_2\} + \{u_i z_2\} + \{u'_i z'_2\}$$

2. **Case $k = 1$:** Perform these steps:

- Delete edges $u_i z_1$ and $u_i z'_1$
- Identify u_i with z_1 and u_i with z'_1
- Add two new pendant edges to u_i

In both cases, the resulting graph G^{**} maintains the required bicyclic structure with order m and diameter d .

Subcase 1.1: $k = 1$

$$\begin{aligned} S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 8^2} \right) \\ &\quad + \left(\sqrt{d_{G^*}^2(u_{i+1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i+1}) + 8^2} \right) \\ &\quad + 2\sqrt{3^2 + 4^2} + 4\sqrt{3^2 + 2^2} - 4\sqrt{8^2 + 2^2} - 2\sqrt{8^2 + 1^2} \\ &< 0. \end{aligned} \tag{3.7}$$

Subcase 1.2: $k = 2$

$$\begin{aligned} S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 6^2} \right) \\ &\quad + \left(\sqrt{d_{G^*}^2(u_{i+1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i+1}) + 6^2} \right) \\ &\quad + 2\sqrt{2^2 + 4^2} + 2\sqrt{3^2 + 2^2} - 2\sqrt{1^2 + 6^2} - 2\sqrt{3^2 + 6^2} \\ &< 0. \end{aligned} \tag{3.8}$$

Subcase 1.3: $k \geq 3$

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 6^2} \right) \\
 &\quad + \left(\sqrt{d_{G^*}^2(u_{i+1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i+1}) + 6^2} \right) \\
 &\quad + 2\sqrt{2^2 + 4^2} + 2\sqrt{2^2 + 2^2} - 2\sqrt{2^2 + 6^2} - 2\sqrt{1^2 + 6^2} \\
 &< 0.
 \end{aligned} \tag{3.9}$$

Case 2. $|V_C \cap V_P| = 1$ and $|V_{C'} \cap V_P| = 1$

Given $|V_C \cap V_P| = 1$ and $|V_{C'} \cap V_P| = 1$, we may assume:

$$C = v_1 v_2 v_3 \cdots v_{|V_C|} v_1$$

$$C' = v_1 v'_2 v'_3 \cdots v'_{|V_{C'}|} v_1$$

where v_1 is the unique intersection point:

$$u_i(v_1) = |V_C \cap V_{C'} \cap V_P| = 1$$

Subcase 2.1: $|V_C| = 3$ and $|V_{C'}| = 3$

Let $G^{**} = G^* - \{v_2 v_3\} - \{v'_2 v'_3\} + \{v_2 u_{i+1}\} + \{v'_2 u'_{i+1}\}$, then $G^{**} \in \mathcal{B}_{m,d}$, $d_{G^*}(u_i) \geq 6$,

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= 2\sqrt{2^2 + 2^2} - 2\sqrt{(d_{G^*}(u_{i+1}) + 2)^2 + 2^2} \\
 &\quad + 2\sqrt{d_{G^*}^2(u_i) + 2^2} - 2\sqrt{d_{G^*}^2(u_i) + 1^2} \\
 &\quad + \left(\sqrt{d_{G^*}^2(u_i) + d_{G^*}^2(u_{i+1})} - \sqrt{d_{G^*}^2(u_i) + (d_{G^*}(u_i) + 2)^2} \right) \\
 &\quad + \left(\sqrt{d_{G^*}^2(u_{i+1}) + d_{G^*}^2(u_i)} - \sqrt{(d_{G^*}(u_{i+1}) + 2)^2 + d_{G^*}^2(u_{i+2})} \right) \\
 &< 4\sqrt{2} - \sqrt{(d_{G^*}(u_{i+1}) + 2)^2 + 2^2} + 2\sqrt{d_{G^*}^2(u_i) + 2^2} \\
 &\quad - 2\sqrt{d_{G^*}^2(u_i) + 1^2} (d_{G^*}(u_{i+1}) = 2, d_{G^*}(u_i) = 6) \\
 &\leq 4\sqrt{2} - 4\sqrt{5} + 2\sqrt{6^2 + 2^2} - 2\sqrt{6^2 + 1^2} \\
 &< 0.
 \end{aligned} \tag{3.10}$$

Subcase 2.2: $|V_C| \geq 4$ and $|V_{C'}| \geq 4$

Given $|V_C| \geq 4$ and $|V_{C'}| \geq 4$, the intersection index satisfies $3 \leq i \leq d - 1$.

Construct the modified graph:

$$G^{**} = G^* - \{v_2 v_3\} - \{v'_2 v'_3\} + \{u_i v_3\} + \{u_i v'_3\}$$

This operation preserves the bicyclic structure, so $G^{**} \in \mathcal{B}_{m,d}$. Moreover, since $d_{G^*}(u_{i+1}) \geq 2$, we have

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 6^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 8^2} \right) \\
 &\quad + \left(\sqrt{d_{G^*}^2(u_{i+1}) + 6^2} - \sqrt{d_{G^*}^2(u_{i+1}) + 8^2} \right) \\
 &\quad + 4\sqrt{2^2 + 6^2} + 2\sqrt{2^2 + 2^2} - 4\sqrt{2^2 + 8^2} - 2\sqrt{1^2 + 8^2} \\
 &\quad < 4\sqrt{2^2 + 6^2} + 2\sqrt{2^2 + 2^2} - 4\sqrt{2^2 + 8^2} - 2\sqrt{1^2 + 8^2} \\
 &\quad < 0.
 \end{aligned} \tag{3.11}$$

Case 3. $|V_C \cap V_P| = 1$ and $|V_{C'} \cap V_P| = 0$

Given the cycle $C = v_1 v_2 v_3 \cdots v_{|V_C|} v_1$ with intersection $u_i(v_1) = |V_C \cap V_P|$, we define G^{**} through case analysis:

1. **For** $|V_C| = 3$:

$$G^{**} = G^* - \{v_2 v_3\} + \{v_2 u_{i+1}\}$$

2. **For** $|V_C| \geq 4$:

$$G^{**} = G^* - \{v_2 v_3\} + \{v_2 v_3\}$$

3. **For** $k \geq 2$:

$$G^{**} = G^* - \{z_1 z_2\} + \{u_i z_2\}$$

4. **For** $k = 1$: Perform the sequence:

- Delete edge $u_i z_1$
- Identify vertices u_i and z_1
- Attach two new pendant edges to u_i

In all cases, the resulting graph satisfies $G^{**} \in \mathcal{B}_{m,d}$.

Subcase 3.1: $|V_C| = 3$ and $k = 1$

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 5^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 7^2} \right) \\
 &\quad + \left(\sqrt{d_{G^*}^2(u_{i+1}) + 5^2} - \sqrt{(d_{G^*}(u_{i+1}) + 1)^2 + 7^2} \right) \\
 &\quad + \left(\sqrt{d_{G^*}^2(u_{i+1}) + d_{G^*}^2(u_{i+2})} - \sqrt{(d_{G^*}(u_{i+1}) + 1)^2 + d_{G^*}^2(u_{i+2})} \right) \\
 &\quad + 2\sqrt{2^2 + 5^2} + \sqrt{2^2 + 2^2} + \sqrt{3^2 + 5^2} \\
 &\quad + 2\sqrt{2^2 + 3^2} - \sqrt{(d_{G^*}(u_{i+1}) + 1)^2 + 2^2} \\
 &\quad - 3\sqrt{2^2 + 7^2} - 2\sqrt{1^2 + 7^2} \\
 &\quad < 0.
 \end{aligned} \tag{3.12}$$

Subcase 3.2: $|V_C| = 3$ and $k = 2$

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 5^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 6^2} \right) \\
 &+ \left(\sqrt{d_{G^*}^2(u_{i+1}) + 5^2} - \sqrt{(d_{G^*}(u_{i+1}) + 1)^2 + 6^2} \right) \\
 &+ \left(\sqrt{d_{G^*}^2(u_{i+1}) + d_{G^*}^2(u_{i+2})} - \sqrt{(d_{G^*}(u_{i+1}) + 1)^2 + d_{G^*}^2(u_{i+2})} \right) \\
 &+ 3\sqrt{2^2 + 5^2} + \sqrt{2^2 + 2^2} + \sqrt{2^2 + 3^2} - \sqrt{(d_{G^*}(u_{i+1}) + 1)^2 + 2^2} \\
 &- \sqrt{2^2 + 7^2} - 2\sqrt{1^2 + 7^2} - \sqrt{6^2 + 3^2} \\
 &< 0.
 \end{aligned} \tag{3.13}$$

Subcase 3.3: $|V_C| = 3$ and $k \geq 3$

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 5^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 6^2} \right) \\
 &+ \left(\sqrt{d_{G^*}^2(u_{i+1}) + 5^2} - \sqrt{(d_{G^*}(u_{i+1}) + 1)^2 + 6^2} \right) \\
 &+ \left(\sqrt{d_{G^*}^2(u_{i+1}) + d_{G^*}^2(u_{i+2})} - \sqrt{(d_{G^*}(u_{i+1}) + 1)^2 + d_{G^*}^2(u_{i+2})} \right) \\
 &+ 3\sqrt{2^2 + 5^2} + 2\sqrt{2^2 + 2^2} - \sqrt{(d_{G^*}(u_{i+1}) + 1)^2 + 2^2} \\
 &- 2\sqrt{2^2 + 6^2} - 2\sqrt{1^2 + 6^2} \\
 &< 0.
 \end{aligned} \tag{3.14}$$

Subcase 3.4: $|V_C| \geq 4$ and $k = 1$

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 5^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 8^2} \right) \\
 &+ \left(\sqrt{d_{G^*}^2(u_{i+1}) + 5^2} - \sqrt{d_{G^*}^2(u_{i+1}) + 8^2} \right) \\
 &+ 2\sqrt{2^2 + 5^2} + \sqrt{2^2 + 2^2} + \sqrt{3^2 + 5^2} + 2\sqrt{3^2 + 2^2} \\
 &- 2\sqrt{2^2 + 8^2} - 4\sqrt{1^2 + 8^2} \\
 &< 0.
 \end{aligned} \tag{3.15}$$

Subcase 3.5: $|V_C| \geq 4$ and $k = 2$

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 5^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 7^2} \right) \\
 &+ \left(\sqrt{d_{G^*}^2(u_{i+1}) + 5^2} - \sqrt{d_{G^*}^2(u_{i+1}) + 7^2} \right) \\
 &+ 2\sqrt{2^2 + 5^2} + \sqrt{2^2 + 2^2} + \sqrt{2^2 + 5^2} + \sqrt{3^2 + 2^2} \\
 &- 2\sqrt{2^2 + 7^2} - 2\sqrt{1^2 + 7^2} - \sqrt{3^2 + 7^2} \\
 &< 0.
 \end{aligned} \tag{3.16}$$

Subcase 3.6: $|V_C| \geq 4$ and $k \geq 3$

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 5^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 7^2} \right) \\
 &\quad + \left(\sqrt{d_{G^*}^2(u_{i+1}) + 5^2} - \sqrt{d_{G^*}^2(u_{i+1}) + 7^2} \right) \\
 &\quad + 3\sqrt{2^2 + 5^2} + 2\sqrt{2^2 + 2^2} - 3\sqrt{2^2 + 7^2} - 2\sqrt{1^2 + 7^2} \\
 &< 0.
 \end{aligned} \tag{3.17}$$

We know $|V_C \cap V_P| \geq 2$ and $|V_{C'} \cap V_P| \geq 2$.

Lemma 3.4. For the extremal graph $G^* \in \mathcal{B}_{m,d}^{\max}$ with $3 \leq d \leq m - 4$, if there exists a pendant vertex $u \in PV_{G^*}$ adjacent to u_2 or u_d on the diametral path $P = u_1 u_2 \cdots u_d u_{d+1}$, then the cycles C and C' must satisfy:

$$|V_C \cap V_{C'}| \geq 2.$$

Proof. Assume that the cycles intersect in at most one vertex:

$$|V_C \cap V_{C'}| \leq 1.$$

Given the established conditions:

$$|V_C \cap V_P| \geq 2$$

$$|V_{C'} \cap V_P| \geq 2$$

Thus, the initial assumption is false, and we must have $|V_C \cap V_{C'}| \geq 2$. $\square$

Case 1. $|V_C \cap V_{C'}| = 0$

Since $|V_C \cap V_{C'}| = 0$, we may assume that $C = u_i u_{i+1} u_{i+2} w u_i$ and $C' = u_{i+3} u_{i+4} u_{i+5} w' u_{i+3}$.

Let $G^{**} = G^* - \{u_{i+3} w'\} - \{u_{i+5} w'\} + \{u_i w'\} + \{u_{i+2} w'\}$, $G^{**} \in \mathcal{B}_{n,d}$, and $d_{G^*}(u_{i+6}) \geq 2$

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 3^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 4^2} \right) \\
 &\quad + \left(\sqrt{d_{G^*}^2(u_{i+6}) + 3^2} - \sqrt{d_{G^*}^2(u_{i+6}) + 2^2} \right) \\
 &\quad + 8\sqrt{2^2 + 3^2} + \sqrt{3^2 + 3^2} - 7\sqrt{2^2 + 4^2} - 2\sqrt{2^2 + 2^2} \\
 &< 0.
 \end{aligned} \tag{3.18}$$

Case 2. $|V_C \cap V_{C'}| = 1$

Since $|V_C \cap V_{C'}| = 1$, we assume $C = u_i u_{i+1} u_{i+2} w u_i$ and $C' = u_{i+2} u_{i+3} u_{i+4} w' u_{i+2}$.

Let $G^{**} = G^* - \{u_{i+2} w'\} - \{u_{i+4} w'\} + \{u_i w'\} + \{u_{i+2} w'\}$, and $d_{G^*}(u_{i+6}) \geq 2$

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \left(\sqrt{d_{G^*}^2(u_{i-1}) + 3^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 4^2} \right) \\
 &\quad + \left(\sqrt{d_{G^*}^2(u_{i+5}) + 3^2} - \sqrt{d_{G^*}^2(u_{i+5}) + 2^2} \right) \\
 &\quad + 4\sqrt{2^2 + 3^2} + 4\sqrt{4^2 + 3^2} - 7\sqrt{2^2 + 4^2} - \sqrt{2^2 + 2^2} \\
 &< \left(\sqrt{d_{G^*}^2(u_{i+5}) + 3^2} - \sqrt{d_{G^*}^2(u_{i+5}) + 2^2} \right) \\
 &\quad + 4\sqrt{2^2 + 3^2} + 4\sqrt{4^2 + 3^2} - 7\sqrt{2^2 + 4^2} - \sqrt{2^2 + 2^2} (d_{G^*}(u_{i+5}) = 2) \\
 &< 0.
 \end{aligned} \tag{3.19}$$

Thus, $|V_C \cap V_{C'}| \geq 2$.

Lemma 3.5. *For any extremal graph $G^* \in \mathcal{B}_{m,d}^{\max}$ where $3 \leq d \leq m-4$, there exists a pendant vertex $u_0 \in PV_{G^*}$ whose removal yields:*

$$G^* - u_0 \in \mathcal{B}_{m-1,d}$$

Proof. For the cycles C and C' with shared path segment $u_i \cdots u_{i+l}$ ($1 \leq l \leq k$):

$$C = u_i \cdots u_{i+l} v_k \cdots v_1 u_i$$

$$C' = u_i \cdots u_{i+l} v'_k \cdots v'_1 u_i$$

When $m \geq d+4$, the following hold:

- Minimum tail length: $k \geq 3$

- Vertex degrees:

$$d(u_{i-1}) \geq 1, d(u_i) = 3 \text{ (branch point)}$$

$$d(v_j) = d(v'_j) = 2 \text{ for } j \in \{2, 3\}$$

□

Case 1. $C: k = l; C': k = l$

We have $k = l \geq 3$. Let $G^{**} = G^* - \{u_i v_2\} - \{u_i v'_2\} - \{v_2 v_3\} - \{v'_2 v'_3\} + \{u_{i+1} v_2\} + \{u_{i+1} v'_2\} + \{u_{i+1} v_3\} + \{u_{i+1} v'_3\}$,

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 2^2} \\ &\quad + 3\sqrt{2^2 + 4^2} + 3\sqrt{2^2 + 2^2} - 4\sqrt{2^2 + 6^2} - 2\sqrt{1^2 + 6^2} (d_{G^*}(u_{i-1}) = 1) \\ &< \sqrt{17} - \sqrt{5} + 6\sqrt{5} + 6\sqrt{2} - 8\sqrt{10} - 2\sqrt{37} \\ &< 0. \end{aligned} \quad (3.20)$$

Case 2. $C: k > l; C': k > l$

Let $G^{**} = G^* - \{v_2 v_3\} - \{v'_2 v'_3\} + \{u_i v_3\} + \{u_i v'_3\}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 6^2} + \sqrt{d_{G^*}^2(u_{i+1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i+1}) + 6^2} \\ &\quad + 2\sqrt{2^2 + 4^2} + 2\sqrt{2^2 + 2^2} - 2\sqrt{2^2 + 6^2} - 2\sqrt{1^2 + 6^2} \\ &< 2\sqrt{2^2 + 4^2} + 2\sqrt{2^2 + 2^2} - 2\sqrt{2^2 + 6^2} - 2\sqrt{1^2 + 6^2} \\ &< 0. \end{aligned} \quad (3.21)$$

Case 3. $C: k = l; C': k > l$

Let $G^{**} = G^* - \{u_i v_2\} - \{v_2 v_3\} - \{v'_2 v'_3\} + \{u_{i+1} v_2\} + \{u_{i+1} v_3\} + \{u_i v'_3\}$.

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i+1}) + 4^2} - \sqrt{(d_{G^*}(u_{i+1}) + 2)^2 + 4^2} \\
 &\quad + \sqrt{d_{G^*}^2(u_{i+1}) + d_{G^*}^2(u_{i+2})^2} - \sqrt{(d_{G^*}(u_i) + 2)^2 + d_{G^*}^2(u_{i+1})} \\
 &\quad + 2\sqrt{2^2 + 4^2} + 2\sqrt{2^2 + 2^2} - \sqrt{(d_{G^*}(u_i) + 2)^2 + 1^2} - \sqrt{(d_{G^*}(u_i) + 2)^2 + 2^2} \\
 &\quad - \sqrt{1^2 + 4^2} - \sqrt{2^2 + 4^2} \\
 &< 0.
 \end{aligned} \tag{3.22}$$

Thus the conclusion holds.

Claim 1. $B^* \subseteq N_{G^*}(u_2) \cup N_{G^*}(u_d)$

Let $G^{**} = G^* - \bigcup_{1 \leq i \leq t} \{x_i w\} + \bigcup_{1 \leq i \leq t} \{x_i v\}$, then $G^{**} \in \mathcal{B}_{m,d}$, we have

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \sum_{i=1}^t \left(\sqrt{(t+1)^2 + d_{G^*}^2(x_i)} - \sqrt{(d_{G^*}(v) + 1)^2 + d_{G^*}^2(x_i)} \right) \\
 &\quad + (d_{G^*}(v) - 1) \left(\sqrt{d_{G^*}^2(v) + 1^2} - \sqrt{(d_{G^*}(v) + 1)^2 + 1^2} \right) \\
 &\quad + \left(\sqrt{(t+2)^2 + d_{G^*}^2(v)} - \sqrt{(d_{G^*}(v) + t)^2 + 1^2} \right) \\
 &< 0.
 \end{aligned} \tag{3.23}$$

Claim 2. $|V_C \setminus V_P| = 1$ and $|V_{C'} \setminus V_P| = 1$

Case 1. $|V_C \setminus V_P| \geq 2$ and $|V_{C'} \setminus V_P| \geq 2$

Let $C = u_i u_{i+1} \cdots u_{i+l} v_k v_{k-1} \cdots v_3 v_2 v_1(u_i)$ and $C' = u_i u_{i+1} \cdots u_{i+l} v'_k v'_{k-1} \cdots v'_3 v'_2 v'_1(u_i)$ ($l \geq 1$), it is obvious that $l \leq k$.

Subcase 1.1: $C: k = l; C': k = l$

Let $G^{**} = G^* - \{u_i v_2\} - \{u_i v'_2\} - \{v_2 v_3\} - \{v'_2 v'_3\} + \{u_{i+1} v_2\} + \{u_{i+1} v'_2\} + \{u_{i+1} v_3\} + \{u_{i+1} v'_3\}$.

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 2^2} \\
 &\quad + 3\sqrt{2^2 + 4^2} + 3\sqrt{2^2 + 2^2} - 4\sqrt{2^2 + 6^2} - 2\sqrt{1^2 + 6^2} (d_{G^*}(u_{i-1}) = 2) \\
 &\leq \sqrt{2^2 + 4^2} - \sqrt{2^2 + 2^2} + 6\sqrt{5} + 6\sqrt{2} - 8\sqrt{10} - 2\sqrt{37} \\
 &< 0.
 \end{aligned} \tag{3.24}$$

Subcase 1.2: $C: k > l; C': k > l$

Let $G^{**} = G^* - \{v_2 v_3\} - \{v'_2 v'_3\} + \{u_i v_3\} + \{u_i v'_3\}$.

$$\begin{aligned}
 S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 6^2} + \sqrt{d_{G^*}^2(u_{i+1}) + 4^2} \\
 &\quad - \sqrt{d_{G^*}^2(u_{i+1}) + 6^2} \\
 &\quad + 2\sqrt{2^2 + 4^2} + 2\sqrt{2^2 + 2^2} - 2\sqrt{2^2 + 6^2} - 2\sqrt{1^2 + 6^2} \\
 &< 2\sqrt{2^2 + 4^2} + 2\sqrt{2^2 + 2^2} - 2\sqrt{2^2 + 6^2} - 2\sqrt{1^2 + 6^2} \\
 &< 0.
 \end{aligned} \tag{3.25}$$

Subcase 1.3: $C: k = l; C': k > l$

Let $G^{**} = G^* - \{u_i v_2\} - \{v_2 v_3\} - \{v'_2 v'_3\} + \{u_{i+1} v_2\} + \{u_{i+1} v_3\} + \{u_i v'_3\}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i+1}) + 4^2} - \sqrt{(d_{G^*}(u_{i+1}) + 2)^2 + 4^2} \\ &\quad + \sqrt{d_{G^*}^2(u_{i+1}) + d_{G^*}^2(u_{i+2})^2} - \sqrt{(d_{G^*}(u_i) + 2)^2 + d_{G^*}^2(u_i)} \\ &\quad + 2\sqrt{2^2 + 4^2} + 2\sqrt{2^2 + 2^2} - \sqrt{(d_{G^*}(u_i) + 2)^2 + 1^2} \\ &\quad - \sqrt{(d_{G^*}(u_i) + 2)^2 + 2^2} - \sqrt{1^2 + 4^2} - \sqrt{2^2 + 4^2} \\ &< 0. \end{aligned} \quad (3.26)$$

Case 2. $|V_C \setminus V_P| \geq 2$ and $|V_{C'} \setminus V_P| = 1$

Let $C = u_i u_{i+1} \cdots u_{i+l} v_k v_{k-1} \cdots v_3 v_2 v_1(u_i)$ and $C' = u_i u_{i+1} w' u_i$, it is obvious that $l \leq k$.

Subcase 2.1: $C: k = l$

Let $G^{**} = G^* - \{u_i v_2\} - \{v_2 v_3\} + \{u_{i+1} v_2\} + \{u_{i+1} v_3\}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 3^2} + \sqrt{d_{G^*}^2(u_{i+2}) + 3^2} - \sqrt{d_{G^*}^2(u_{i+2}) + 5^2} \\ &\quad + 2\sqrt{2^2 + 4^2} + \sqrt{3^2 + 2^2} + \sqrt{2^2 + 2^2} + \sqrt{3^2 + 4^2} - 2\sqrt{5^2 + 2^2} - \sqrt{5^2 + 3^2} \\ &\quad - \sqrt{3^2 + 2^2} - \sqrt{5^2 + 1^2} \\ &< \sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 3^2} + 2\sqrt{2^2 + 4^2} + \sqrt{3^2 + 2^2} \\ &\quad + \sqrt{2^2 + 2^2} + \sqrt{3^2 + 4^2} \\ &\quad - 2\sqrt{5^2 + 2^2} - \sqrt{5^2 + 3^2} - \sqrt{3^2 + 2^2} - \sqrt{5^2 + 1^2} \\ &< 0. \end{aligned} \quad (3.27)$$

Subcase 2.2: $C: k > l$

Let $G^{**} = G^* - \{v_2 v_3\} + \{u_i v_3\}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_{i-1}) + 4^2} - \sqrt{d_{G^*}^2(u_{i-1}) + 5^2} + \sqrt{3^2 + 4^2} + 2\sqrt{2^2 + 4^2} + \sqrt{2^2 + 2^2} \\ &\quad - \sqrt{5^2 + 3^2} - 2\sqrt{5^2 + 2^2} - \sqrt{5^2 + 1^2} \\ &< \sqrt{3^2 + 4^2} + 2\sqrt{2^2 + 4^2} + \sqrt{2^2 + 2^2} - \sqrt{5^2 + 3^2} - 2\sqrt{5^2 + 2^2} - \sqrt{5^2 + 1^2} \\ &< 0. \end{aligned} \quad (3.28)$$

Claim 3. $d_{G^*}(u_{d+1}) = 1$

Case 1. $|E_C| = 3$ and $|E_{C'}| = 3$

There are two cycles $C = u_d u_{d+1} w u_d$ and $C' = u_d u_{d+1} w' u_d$. Let $G^{**} = G^* - \{u_{d+1} w\} - \{u_{d+1} w'\} + \{u_{d-1} w\} + \{u_{d-1} w'\}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_d) + 2^2} - \sqrt{d_{G^*}^2(u_{d-2}) + 4^2} + \sqrt{2^2 + 4^2} + 2\sqrt{3^2 + 2^2} + \sqrt{4^2 + 3^2} \\ &\quad - \sqrt{4^2 + 4^2} - 2\sqrt{2^2 + 4^2} - \sqrt{4^2 + 1^2} \\ &< 2\sqrt{5} + 5 + 2\sqrt{13} + 5 - 4\sqrt{2} - 4\sqrt{5} - \sqrt{17} \\ &< 0. \end{aligned} \quad (3.29)$$

Case 2. $|E_C| = 4$ and $|E_{C'}| = 4$

There are two cycles $C = u_{d-1}u_du_{d+1}wu_{d-1}$ and $C' = u_{d-1}u_du_{d+1}w'u_{d-1}$. Let $G^{**} = G^* - \{u_{d+1}w\} - \{u_{d+1}w'\} + \{u_dw\} + \{u_dw'\}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{4^2 + 2^2} + 3\sqrt{2^2 + 3^2} - \sqrt{4^2 + 4^2} - \sqrt{1^2 + 4^2} - 2\sqrt{4^2 + 4^2} \\ &= 2\sqrt{5} + 3\sqrt{13} - 4\sqrt{2} - \sqrt{17} - 4\sqrt{5} \\ &< 0, \end{aligned} \quad (3.30)$$

Case 3. $|E_C| = 3$ and $|E_{C'}| = 4$

There are two cycles $C = u_du_{d+1}wu_d$ and $C' = u_{d-1}u_du_{d+1}w'u_{d-1}$. Let $G^{**} = G^* - \{u_{d+1}w\} - \{u_{d+1}w'\} + \{u_{d-1}w\} + \{u_dw'\}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= \sqrt{d_{G^*}^2(u_d) + 3^2} - \sqrt{d_{G^*}^2(u_{d-2}) + 4^2} \\ &\quad + 4\sqrt{3^2 + 2^2} + 2\sqrt{3^2 + 3^2} - 4\sqrt{4^2 + 2^2} - \sqrt{4^2 + 4^2} - \sqrt{4^2 + 1^2} \\ &< 4\sqrt{13} + 6\sqrt{2} - 8\sqrt{5} - 4\sqrt{2} - \sqrt{17} \\ &< 0, \end{aligned} \quad (3.31)$$

Claim 4. $|E_C| = 4$ and $|E_{C'}| = 4$

We suppose $|E_C| = 3$ and $|E_{C'}| = 3$, There are two cycles $C = u_iu_{i+1}wu_i$ and $C' = u_iu_{i+1}w'u_i$ ($3 \leq i \leq d-1$). Since $\mathcal{B}^* = \{u \in PV_{G^*} | G^* - u \in \mathcal{B}_{m-1,d} \neq \emptyset\}$. We know $|V_C \cap V_{C'}| \geq 2$.

Case 1. $i = 3$

Let $G^{**} = G^* - \{u_3w\} - \{u_3w'\} + \{u_2w\} + \{u_2w'\}$, then $G^{**} \in \mathcal{B}_{m,d}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= (d_{G^*}(u_2) - 1) \left(\sqrt{d_{G^*}^2(u_2) + 1^2} - \sqrt{(d_{G^*}(u_2) + 2)^2 + 1^2} \right) \\ &\quad + \sqrt{d_{G^*}^2(u_2) + 4^2} - 3\sqrt{(d_{G^*}(u_2) + 2)^2 + 2^2} + \sqrt{4^2 + 4^2} \\ &\quad + 2\sqrt{2^2 + 4^2} - \sqrt{2^2 + 4^2} \\ &< 0, \end{aligned} \quad (3.32)$$

Case 2. $i \geq 4$

Let $G^{**} = G^* - \{u_iw\} - \{u_iw'\} - \{u_{i+1}w\} - \{u_{i+1}w'\} + \{u_2w\} + \{u_2w'\} + \{u_3w\} + \{u_3w'\}$, then $G^{**} \in \mathcal{B}_{m,d}$.

$$\begin{aligned} S(G^*) - S(G^{**}) &= (d_{G^*}(u_2) - 1) \left(\sqrt{d_{G^*}^2(u_2) + 1^2} - \sqrt{(d_{G^*}(u_2) + 2)^2 + 1^2} \right) \\ &\quad + \sqrt{d_{G^*}^2(u_2) + 2^2} - 2\sqrt{(d_{G^*}(u_2) + 2)^2 + 2^2} + \sqrt{4^2 + 4^2} \\ &\quad + \sqrt{d_{G^*}^2(u_{i+2}) + 4^2} - \sqrt{d_{G^*}^2(u_{i+2}) + 2^2} - \sqrt{(d_{G^*}(u_2) + 2)^2 + 4^2} \\ &\quad + 2\sqrt{2^2 + 4^2} - \sqrt{2^2 + 2^2} \\ &< 0, \end{aligned} \quad (3.33)$$

Thus, there are two cycles $C = u_iu_{i+1}u_{i+2}wu_i$ and $C' = u_iu_{i+1}u_{i+2}w'u_i$.

Case 1. $i = 3$

$$\begin{aligned}
 S(G^*) - S(\mathcal{B}_m^d) &= (d_{G^*}(u_2) - 1) \left(\sqrt{d_{G^*}^2(u_2) + 1^2} - \sqrt{(d_{G^*}(u_2) + 2)^2 + 1^2} \right) \\
 &\quad + \sqrt{d_{G^*}^2(u_2) + 4^2} + \sqrt{d_{G^*}^2(u_6) + 4^2} - \sqrt{d_{G^*}^2(u_6) + 2^2} \\
 &\quad - 3\sqrt{(d_{G^*}(u_2) + 2)^2 + 2^2} + 2\sqrt{2^2 + 4^2} \\
 &< 0,
 \end{aligned} \tag{3.34}$$

Case 2. $4 \leq i \leq d - 2$

$$\begin{aligned}
 S(G^*) - S(\mathcal{B}_m^d) &= (d_{G^*}(u_2) - 1) \left(\sqrt{d_{G^*}^2(u_2) + 1^2} - \sqrt{(d_{G^*}(u_2) + 2)^2 + 1^2} \right) \\
 &\quad - 3\sqrt{(d_{G^*}(u_2) + 2)^2 + 2^2} + \sqrt{d_{G^*}^2(u_2) + 2^2} + \sqrt{d_{G^*}^2(u_{i+3}) + 4^2} \\
 &\quad - \sqrt{d_{G^*}^2(u_{i+3}) + 2^2} + 3\sqrt{2^2 + 4^2} - \sqrt{2^2 + 2^2} \\
 &< 0,
 \end{aligned} \tag{3.35}$$

Thus there must exist a vertex $u_0 \in PV_{G^*}$, $G^* - u_0 \in \mathcal{B}_{m-1,d}$.

Theorem 3.6. For any bicyclic graph $G \in \mathcal{B}(m, d)$

$$S(G) \leq S(\mathcal{B}_m^d),$$

where equality holds precisely when G is isomorphic to the extremal graph $\mathcal{B}_m^d$ (see Figure 2).

Proof. The result holds for $m = d + 3$ by direct verification.

Assume the conclusion holds for all graphs in $\mathcal{B}(m - 1, d)$. For $G \in \mathcal{B}(m, d)$.

For any extremal graph $G^* \in \mathcal{B}_{m,d}^{\max}$ with $m \geq d + 4$, there exists a pendant vertex $u \in PV_{G^*}$ such that:

$$\begin{aligned}
 G^{**} &:= G^* - u \in \mathcal{B}_{m-1,d} \\
 S(G^*) &= S(G^{**}) + \sqrt{k^2 + 1^2} + \sum_{i=1}^{k-1} \left(\sqrt{k^2 + k_i^2} - \sqrt{(k-1)^2 + k_i^2} \right) \\
 &\leq S(\mathcal{B}_{m-1}^d) + \sqrt{k^2 + 1^2} + 3(\sqrt{k^2 + 2^2} - \sqrt{(k)^2 + 2^2}) \\
 &\quad + (k-4)(\sqrt{k^2 + 1^2} - \sqrt{(k-1)^2 + 1^2}) \\
 &= S(\mathcal{B}_m^d)
 \end{aligned} \tag{3.36}$$

Thus $S(G) \leq S(\mathcal{B}_m^d)$, $G \cong \mathcal{B}_m^d$. □

4 Conclusions

Let $\mathcal{B}(m, a, b, c, d)$ denote the class of bicyclic graphs formed by:

- Two 3-cycles sharing an edge (a θ -graph base)
- Attaching a, b, c, d pendant vertices to each base vertex respectively

where $a \geq b \geq c \geq d \geq 0$ and $a + b + c + d = m - 4$.

Among all bicyclic graphs in $\mathcal{B}(m, 2)$ and $\mathcal{B}(m, 3)$, the Sombor index is maximized by:

- $\mathcal{B}(m, m - 4, 0, 0, 0)$ (maximum)
- $\mathcal{B}(m, m - 5, 1, 0, 0)$ (second maximum)

as illustrated in Figure 4.

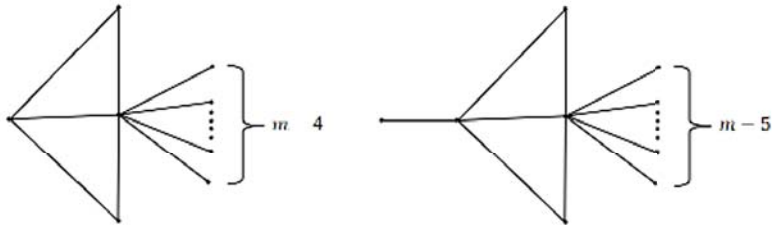


Figure 4: The graphs $\mathcal{B}(m, m - 4, 0, 0, 0)$ (left) and $\mathcal{B}(m, m - 5, 1, 0, 0)$ (right)

This work completely characterizes the maximum Sombor indices for bicyclic graphs with fixed diameter d . Specifically:

- For each $4 \leq d \leq m - 3$, we identify the unique extremal graph $\mathcal{B}_m^d$ maximizing $S(G)$
- The extremal structures exhibit specific patterns of cycle attachments and pendant vertex distributions

- The proof combines structural analysis with careful index comparisons

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