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THE FIRST TWO MAXIMUM SOMBOR SPECTRAL RADII OF BICYCLIC GRAPHS

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Abstract. The Sombor matrix $S(G)$ of a graph G was introduced by Gutman in 2021, in which the (i,j)-entry is equal to $\sqrt{\deg^2(u_i)+\deg^2(u_j)}$ if the vertices u_i and u_j are adjacent in G, and zero otherwise, where $\deg(u_i)$ denotes the degree of vertex u_i in G. In this paper, we obtain the extremal graphs with the first two maximum Sombor spectral radii in bicyclic graphs.

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1. Introduction

In this work, we will use notations and terminologies from [1]. Let G be a simple graph with vertex set $V(G)=\{u_1,u_2,\ldots,u_n\}$ and edge set $E(G)$. The *order* of G is the number $|V(G)|$ of its vertices and its *size* is the number $|E(G)|$ of its edges. A graph is said to be bicyclic if the graph is connected and $|E(G)|=|V(G)|+1$. For $u_i\in V(G)$, the *neighbour set* of vertex u_i is defined as $N_G(u_i)=\{u_j\in V(G)\mid u_iu_j\in E(G)\}$ and the number $\deg(u_i)=|N_G(u_i)|$ is the *degree* of vertex u_i. Let $N_G[u_i]=N_G(u_i)\cup\{u_i\}$. Let Δ_1 and Δ_2 be the *maximum degree* and the *second maximum degree* of the graph G, respectively.

In 2021, the *Sombor index* of a graph G was proposed by Gutman [4]. Based on the concept of Sombor index, Gutman [5] introduced the *Sombor matrix* of graphs. The Sombor matrix of a graph G is defined as $S(G)=(s_{ij})_{n\times n}$, where

$$s_{ij}=\begin{cases}\sqrt{\deg^2(u_i)+\deg^2(u_j)}, & u_iu_j\in E(G),\\ 0, & \text{otherwise.}\end{cases}$$

Let $\phi(G,x)=|xI-S(G)|$ be the *Sombor characteristic polynomial* of a graph G, where I is the identity matrix of order n. Obviously, the Sombor matrix of a graph is real symmetric, so its eigenvalues are all real. The eigenvalues of the Sombor matrix of a graph G are called the *Sombor eigenvalues* of G, and the largest Sombor eigenvalue of G is called the *Sombor spectral radius* of G, denoted by $\rho(G)$.

Sombor matrix of a graph have been paid a serious attention by the researchers in the recent years. Li *et al.* [6] identified the unique trees that minimize and maximize the Sombor spectral radius. In 2021, Lin [7] derived

Keywords. Sombor matrix, Sombor spectral radius, bicyclic graphs, maximum degree.

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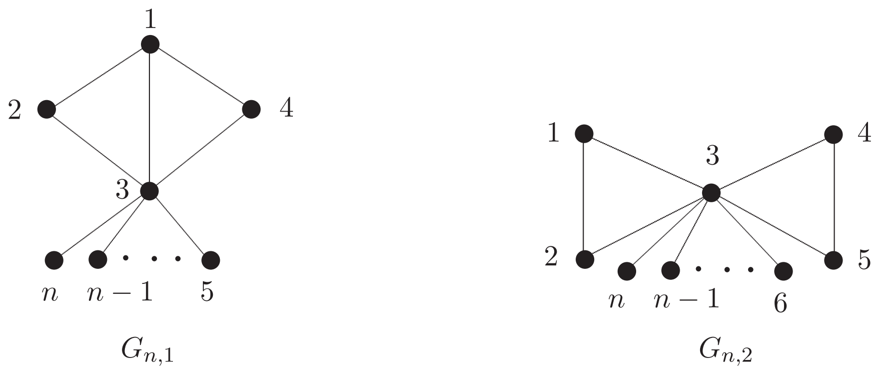

FIGURE 1. $\mathcal{B}_n^1$.

bounds for the Sombor spectral radius of connected graphs and characterized the corresponding extremal graphs. In 2023, Mei [8] determined the unique unicyclic graphs that achieve the minimum and maximum values of the Sombor spectral radius. In 2025, Pirzada *et al.* [9] obtained some bounds for Sombor spectral radius and Sombor energy of the connected graphs, and determined corresponding extremal graphs.

There is an extensive body of literature focusing on the spectrum of matrices associated with graph invariants across various classes of graphs, as seen in [3, 5, 10–14, 16, 18].

Be inspired by the above works, in this paper, we obtain the extremal graphs with the first two maximum Sombor spectral radii in bicyclic graphs, which are exactly the unique two bicyclic graphs of order n with maximum degree $n-1$ when $n \geq 6$ (see Fig. 1). Our main goal is to show that $G_{n,1}$ and $G_{n,2}$ are unique graphs with the largest and second largest Sombor spectral radii, respectively. Therefore, firstly, we prove $\rho(G_{n,1}) > \rho(G_{n,2})$. And then we show that the Sombor spectral radius of $G_{n,2}$ is larger than that of any bicyclic graph of order n with $\Delta_1 \leq n-2$.

2. MAIN RESULTS

Let $\mathcal{B}_n$ be the set of all the bicyclic graphs of order n. According to the maximum degree Δ_1, $\mathcal{B}_n$ can be partitioned into four parts, that is $\mathcal{B}_n = \mathcal{B}_n^1 \cup \mathcal{B}_n^2 \cup \mathcal{B}_n^3 \cup \mathcal{B}_n^4$, where

(i) $\mathcal{B}_n^1$ is the subset of $\mathcal{B}_n$ with $\Delta_1 = n-1$;
(ii) $\mathcal{B}_n^2$ is the subset of $\mathcal{B}_n$ with $\Delta_1 = n-2$;
(iii) $\mathcal{B}_n^3$ is the subset of $\mathcal{B}_n$ with $\Delta_1 = n-3$;
(iv) $\mathcal{B}_n^4$ is the subset of $\mathcal{B}_n$ with $\Delta_1 \leq n-4$.

We will give a lemma, which will be useful for proving our main result.

Lemma 2.1 ([17]). *If M is a real symmetric $n \times n$ matrix with the largest eigenvalue λ_1, then for any $X \in R^n$ such that $X \neq 0$,*

$$\frac{X^\top M X}{X^\top X} \leq \lambda_1,$$

equality holds if and only if X is an eigenvector of M corresponding to λ_1.

2.1. The bound of the maximum Sombor spectral radius in $\mathcal{B}_n^1$

Let $G_{n,1}$ and $G_{n,2}$ be two bicyclic graphs, which are depicted in Figure 1. Clearly,

$$\mathcal{B}_n^1 = \{G_{n,1}, G_{n,2}\}.$$

It is worth mentioning that $G_{n,1}$ occurs when $n \geq 4$ and $G_{n,2}$ occurs when $n \geq 5$.

Now, we present estimates about the maximum Somber spectra radius in $\mathcal{B}_n^1$ below.

Theorem 2.1. *Let $G_{n,1}$ and $G_{n,2}$ be the two bicyclic graphs in $\mathcal{B}_n^1$. Then for $n \geq 8$,*

$$\rho(G_{n,1}) > \rho(G_{n,2}) > \sqrt{n^3 - 3n^2 + 4n - 2}.$$

Proof. By the structure of $G_{n,1}$ and $G_{n,2}$ and the definition of the Somber matrix of a graph, we have $\phi(G_{n,1}, x) = x^{n-4} f_{n,1}(x)$, where

$$f_{n,1}(x) = x^4 - \big(n^3 - 3n^2 + 4n + 38\big)x^2 - 4\sqrt{13(n^2 - 2n + 5)(n^2 - 2n + 10)}x + 26\big(n^3 - 6n^2 + 10n - 8\big),$$

and $\phi(G_{n,2}, x) = x^{n-6}(x^2 - 8) f_{n,2}(x)$, where

$$f_{n,2}(x) = x^4 - \big(n^3 - 3n^2 + 4n + 18\big)x^2 - 4\sqrt{8}\big(n^2 - 2n + 5\big)x + 8\big(n^3 - 7n^2 + 12n - 10\big).$$

Denote by $x_1 \geq x_2 \geq x_3 \geq x_4$ the four roots of $f_{n,1}(x) = 0$, and $y_1 \geq y_2 \geq y_3 \geq y_4$ the four roots of $f_{n,2}(x) = 0$. Obviously, $\rho(G_{n,1}) = x_1$, and since

$$f_{n,2}\left(\sqrt{8}\right) = -10n^3 - 112n^2 + 192n - 32 < 0,$$

we have $\sqrt{8} < y_1 = \rho(G_{n,2})$. Thus our desired inequalities

$$\rho(G_{n,1}) > \rho(G_{n,2}) > \sqrt{n^3 - 3n^2 + 4n - 2}$$

are equivalent to

$$x_1 > y_1 > \sqrt{n^3 - 3n^2 + 4n - 2}.$$

Because

$$\begin{aligned} f_{n,1}\left(\sqrt{n^3 - 3n^2 + 4n - 2}\right) &= -14n^3 - 36n^2 + 100n - 128 \\ &\quad - 4\sqrt{13(n-1)(n^2 - 2n + 2)(n^2 - 2n + 5)(n^2 - 2n + 10)} < 0, \end{aligned}$$

and

$$f_{n,2}\left(\sqrt{n^3 - 3n^2 + 4n - 2}\right) = -12n^3 + 4n^2 + 16n - 40 - 4\big(n^2 - 2n + 5\big)\sqrt{8(n-1)(n^2 - 2n + 2)} < 0,$$

we deduce that $x_1 > \sqrt{n^3 - 3n^2 + 4n - 2}$ and $y_1 > \sqrt{n^3 - 3n^2 + 4n - 2}$, for $n \geq 8$.

Next, we prove $x_1 > y_1$. Let $W = (w_1, w_2, \ldots, w_n)$ be an unit eigenvector corresponding to y_1. Then we can get $y_1 = W^\top S(G_{n,2})W$ and $x_1 \geq W^\top S(G_{n,1})W$ from Lemma 2.1, which implies that

$$\begin{aligned} x_1 - y_1 &\geq W^\top S(G_{n,1})W - W^\top S(G_{n,2})W \\ &= W^\top [S(G_{n,1}) - S(G_{n,2})]W \\ &= 2\left(\sqrt{13} - \sqrt{8}\right)w_1 w_2 + 2\left(\sqrt{n^2 - 2n + 10} - \sqrt{n^2 - 2n + 5}\right)w_1 w_3 \\ &\quad + 2\sqrt{13}w_1 w_4 + 2\left(\sqrt{n^2 - 2n + 2} - \sqrt{n^2 - 2n + 5}\right)w_3 w_5 - 2\sqrt{8}w_4 w_5 \\ &= 4\left(\sqrt{13} - \sqrt{8}\right)w_1 w_2 + 2\left(\sqrt{n^2 - 2n + 10} - 2\sqrt{n^2 - 2n + 5} + \sqrt{n^2 - 2n + 2}\right)w_1 w_3. \end{aligned}$$

Considering the components of the vector W, since w_1, w_2, w_4 and w_5 are equal, we obtain $x_1 - y_1 > 0$.

Hence, we have the desired result $\rho(G_{n,1}) > \rho(G_{n,2}) > \sqrt{n^3 - 3n^2 + 4n - 2}$, for $n \geq 8$. $\square$

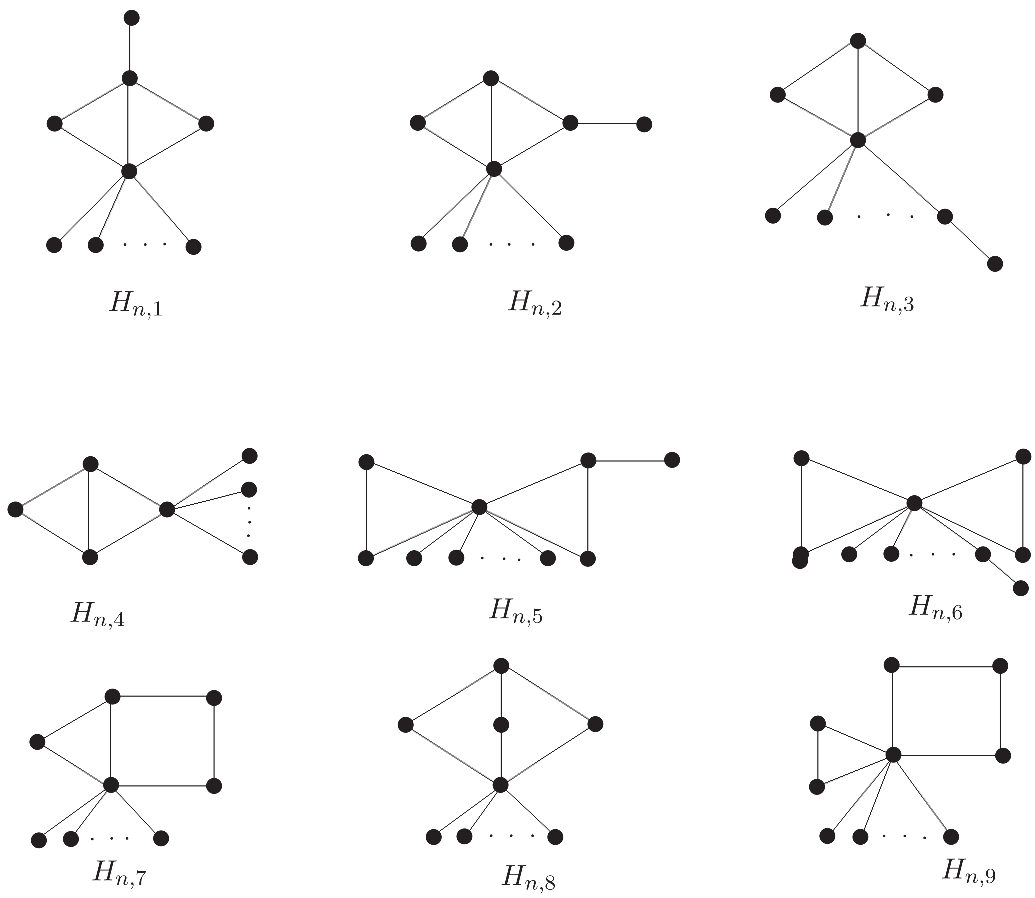

FIGURE 2. $\mathcal{B}_n^2$.

2.2. The bound of the maximum Sombor spectral radius in $\mathcal{B}_n^2$

Recall that $\mathcal{B}_n^2$ is the set of all the bicyclic graphs of order n with $\Delta_1 = n-2$. Let $H_{n,i}, 1 \leq i \leq 9$ be the bicyclic graphs which depicted in Figure 2. From Lemma 2.2 in [15], we have

$$\mathcal{B}_n^2 = \{H_{n,i}, 1 \leq i \leq 9\}. \tag{1}$$

In what follows, when $n \geq 8$, we can infer that the Sombor spectral radii of all such graphs are less than $\sqrt{n^3 - 3n^2 + 4n - 2}$.

Theorem 2.2. *Let G be a bicyclic graph on $n \geq 8$ vertices in $\mathcal{B}_n^2$. Then*

$$\rho(G) < \sqrt{n^3 - 3n^2 + 4n - 2}.$$

Proof. From equation (1), we know that $G \cong H_{n,i}$ for some $1 \leq i \leq 9$. We just need to prove $\rho(H_{n,i}) < \sqrt{n^3 - 3n^2 + 4n - 2}$ for each $1 \leq i \leq 9$.

For the graph $H_{n,1}$, by simple calculation, we can get that $\phi(H_{n,1}, x) = x^{n-4} f_n(x)$, where

$$f_n(x) = x^4 - \big(n^3 - 6n^2 + 13n + 68\big)x^2 - 8\sqrt{5(n^2 - 4n + 8)(n^2 - 4n + 20)}x + \big(57n^3 - 479n^2 + 1289n - 1153\big).$$

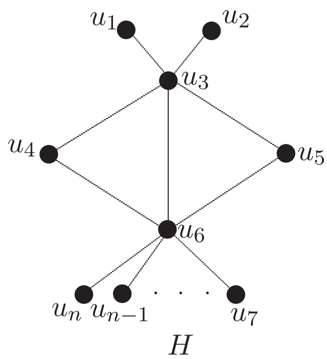

FIGURE 3. $\mathcal{B}_n^{31}$.

Denote by $x_4 \leq x_3 \leq x_2 \leq x_1$ the four roots of $f_n(x) = 0$. Obviously, $\rho(H_{n,1}) = x_1$. From $x_1 > 0, x_4 < 0$ and for $n \geq 8$, we know that

$$f_n(0) = 57n^3 - 479n^2 + 1289n - 1153 > 0.$$

Thus, we see $x_3 < 0 < x_2$.

In addition, by direct calculation, when $n \geq 8$, we have

$$f_n(n-1) = -n^5 + 9n^4 + 27n^3 - 509n^2 + 1408n - 1220 - 8(n-1)\sqrt{5(n^2-4n+8)(n^2-4n+20)} < 0$$

and

$$f_n\left(\sqrt{n^3-3n^2+4n-2}\right) = 3n^5 - 18n^4 + 26n^3 - 311n^2 + 1027n - 1013 - 8\sqrt{5(n-1)(n^2-2n+2)(n^2-4n+8)(n^2-4n+20)} > 0,$$

which implies that $x_1 < \sqrt{n^3-3n^2+4n-2}$, that is $\rho(H_{n,1}) < \sqrt{n^3-3n^2+4n-2}$.

For other graphs $H_{n,i}$ with $2 \leq i \leq 9$, by using a similar analysis, we can obtain $\rho(H_{n,i}) < \sqrt{n^3-3n^2+4n-2}$. Therefore, it completes the proof. □

2.3. The bound of the maximum Sombor spectral radius in $\mathcal{B}_n^3$

In the subsection, we consider the bound of the maximum Sombor spectral radius in $\mathcal{B}_n^3$. By means of the structure of the bicyclic graph and $\Delta_1 = n-3$, we deduce that the second maximum degree of all graphs is no more than 5 in $\mathcal{B}_n^3$. Therefore, by virtue of the second maximum degree, we partition $\mathcal{B}_n^3$ into three parts $\mathcal{B}_n^{31}$, $\mathcal{B}_n^{32}$ and $\mathcal{B}_n^{33}$, where

(a) $\mathcal{B}_n^{31}$ is the subset of $\mathcal{B}_n^3$ with $\Delta_2 = 5$;
(b) $\mathcal{B}_n^{32}$ is the subset of $\mathcal{B}_n^3$ with $\Delta_2 = 4$;
(c) $\mathcal{B}_n^{33}$ is the subset of $\mathcal{B}_n^3$ with $\Delta_2 \leq 3$.

Lemma 2.2 ([2]). *Let M be an irreducible nonnegative matrix with the largest eigenvalue $\rho(M)$. Suppose $k \in R$, $X \in R^n$, $X \geq 0, X \neq 0$. If $MX \leq kX$, then $\rho(M) \leq k$.*

In the following, by using the properties of graphs in $\mathcal{B}_n^3$, we obtain the bounds of the maximum Sombor spectral radius in $\mathcal{B}_n^{31}$, $\mathcal{B}_n^{32}$ and $\mathcal{B}_n^{33}$, respectively. Now, let H be a bicyclic graph, which is depicted in Figure 3. In fact, $\mathcal{B}_n^{31} = \{H\}$.

Lemma 2.3. *Let G be a bicyclic graph of order $n \geq 8$ in $\mathcal{B}_n^{31}$. Then*

$$\rho(G) \leq \sqrt{n^3-3n^2+4n-2}.$$

Proof. Since $\mathcal{B}_n^{31} = \{H\}$, we have $G \cong H$. Suppose $V(H) = \{u_1, u_2, \ldots, u_n\}$, the matrix $M = S(H)$ and $\rho(M) = \rho(H)$. Let $X = \left(\sqrt{\deg(u_1)}, \sqrt{\deg(u_2)}, \ldots, \sqrt{\deg(u_n)}\right)^\top$. Then in order to complete this proof from Lemma 2.2, we need to show that

$$(MX)_{u_i} \leq \sqrt{n^3 - 3n^2 + 4n - 2}\sqrt{\deg(u_i)}$$

for all $u_i \in V(H)$.

Next, for all $u_i \in V(H)$, we calculate $(MX)_{u_i}$ in light of the label of the vertex in the Figure 3.

$$\begin{aligned}(MX)_{u_i} &= \sum_{u_j \in N_G(u_i)} \sqrt{\deg^2(u_i) + \deg^2(u_j)}\sqrt{\deg(u_j)} \\ &= \sqrt{\deg^2(u_i) + \deg^2(u_3)}\sqrt{\deg(u_3)} \\ &= \sqrt{1^2 + 5^2}\sqrt{5} \\ &\leq \sqrt{n^3 - 3n^2 + 4n - 2}\sqrt{\deg(u_i)}, \text{ holds for } n \geq 7,\ i = 1, 2.\end{aligned} \tag{2}$$

$$\begin{aligned}(MX)_{u_3} &= \sum_{u_j \in N_G(u_3)} \sqrt{\deg^2(u_3) + \deg^2(u_j)}\sqrt{\deg(u_j)} \\ &= \sqrt{\deg^2(u_3) + \deg^2(u_1)}\sqrt{\deg(u_1)} + \sqrt{\deg^2(u_3) + \deg^2(u_2)}\sqrt{\deg(u_2)} \\ &\quad + \sqrt{\deg^2(u_3) + \deg^2(u_4)}\sqrt{\deg(u_4)} + \sqrt{\deg^2(u_3) + \deg^2(u_5)}\sqrt{\deg(u_5)} \\ &\quad + \sqrt{\deg^2(u_3) + \deg^2(u_6)}\sqrt{\deg(u_6)} \\ &= 2\sqrt{1^2 + 5^2}\sqrt{1} + 2\sqrt{2^2 + 5^2}\sqrt{2} + \sqrt{(n-3)^2 + 5^2}\sqrt{n-3} \\ &\leq \sqrt{n^3 - 3n^2 + 4n - 2}\sqrt{\deg(u_3)}, \text{ holds for } n \geq 8.\end{aligned} \tag{3}$$

$$\begin{aligned}(MX)_{u_i} &= \sum_{u_j \in N_G(u_i)} \sqrt{\deg^2(u_i) + \deg^2(u_j)}\sqrt{\deg(u_j)} \\ &= \sqrt{\deg^2(u_i) + \deg^2(u_3)}\sqrt{\deg(u_3)} + \sqrt{\deg^2(u_i) + \deg^2(u_6)}\sqrt{\deg(u_6)} \\ &= \sqrt{2^2 + 5^2}\sqrt{5} + \sqrt{(n-3)^2 + 2^2}\sqrt{n-3} \\ &\leq \sqrt{n^3 - 3n^2 + 4n - 2}\sqrt{\deg(u_i)}, \text{ holds for } n \geq 7,\ i = 4, 5.\end{aligned} \tag{4}$$

$$\begin{aligned}(MX)_{u_6} &= \sum_{u_j \in N_G(u_6)} \sqrt{\deg^2(u_6) + \deg^2(u_j)}\sqrt{\deg(u_j)} \\ &= (n-6)\sqrt{\deg^2(u_6) + \deg^2(u_7)}\sqrt{\deg(u_7)} + 2\sqrt{\deg^2(u_6) + \deg^2(u_4)}\sqrt{\deg(u_4)} \\ &\quad + \sqrt{\deg^2(u_6) + \deg^2(u_3)}\sqrt{\deg(u_3)} \\ &= (n-6)\sqrt{n^2 - 6n + 10}\sqrt{1} + \sqrt{n^2 - 6n + 34}\sqrt{5} + 2\sqrt{n^2 - 6n + 13}\sqrt{2} \\ &\leq \sqrt{n^3 - 3n^2 + 4n - 2}\sqrt{\deg(u_6)}, \text{ holds for } n \geq 8.\end{aligned} \tag{5}$$

$$\begin{aligned}(MX)_{u_i} &= \sum_{u_j \in N_G(u_i)} \sqrt{\deg^2(u_i) + \deg^2(u_j)}\sqrt{\deg(u_j)} \\ &= \sqrt{\deg^2(u_i) + \deg^2(u_6)}\sqrt{\deg(u_6)} \\ &= \sqrt{1^2 + (n-3)^2}\sqrt{n-3}\end{aligned} \tag{6}$$

$$\leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_i)},\ \text{holds for } n\geq 7,\ i=7,8,\ldots,n.$$

By using equations (2)–(6), we know that $MX \leq \sqrt{n^3-3n^2+4n-2}X$. It implies that $\rho(G) \leq \sqrt{n^3-3n^2+4n-2}$ from Lemma 2.2, for all $n\geq 8$. □

Before giving the bound of the maximum Sombor radius of graphs in $\mathcal{B}_n^{32}$, we present the following lemma, which plays an important role later.

Lemma 2.4. *Let G be a bicyclic graph on $n\geq 8$ vertices in $\mathcal{B}_n^{32}$. Then $G\cong K_{n,i}$, for some $1\leq i\leq 11$, where $K_{n,i}$, $1\leq i\leq 11$, are depicted in Figure 4.*

In fact, by Lemma 2.4, we know that

$$\mathcal{B}_n^{32}=\{K_{n,i}, 1\leq i\leq 11\}.$$

Lemma 2.5. *Let G be a bicyclic graph on $n\geq 8$ vertices in $\mathcal{B}_n^{32}$. Then*

$$\rho(G)\leq\sqrt{n^3-3n^2+4n-2}.$$

Proof. Since $\mathcal{B}_n^{32}=\{K_{n,i}, 1\leq i\leq 11\}$, we get that $G\cong K_{n,i}$ for some $1\leq i\leq 11$. For the sake of having the desired result, we need to prove that $\rho(K_{n,i})\leq\sqrt{n^3-3n^2+4n-2}$ for each $1\leq i\leq 11$.

For the graph $K_{n,1}$, we suppose that $V(K_{n,1})=\{u_1,u_2,\ldots,u_n\}$ and the vertices of $V(K_{n,1})$ are labelled in the Figure 5. Let $M=S(K_{n,1})$, $\rho(M)=\rho(K_{n,1})$ and $X=(\sqrt{\deg(u_1)},\sqrt{\deg(u_2)},\ldots,\sqrt{\deg(u_n)})^\top$. If we obtain that

$$(MX)_{u_i}\leq\sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_i)}$$

for all $u_i\in V(K_{n,1})$, then the result follows immediately.

So, we consider the following cases.

$$\begin{aligned}(MX)_{u_1} &= \sum_{u_j\in N_G(u_1)}\sqrt{\deg^2(u_1)+\deg^2(u_j)}\sqrt{\deg(u_j)} \qquad (7)\\ &= \sqrt{\deg^2(u_1)+\deg^2(u_2)}\sqrt{\deg(u_2)}+\sqrt{\deg^2(u_1)+\deg^2(u_3)}\sqrt{\deg(u_3)}\\ &\quad+\sqrt{\deg^2(u_1)+\deg^2(u_6)}\sqrt{\deg(u_6)}\\ &= \sqrt{3^2+2^2}\sqrt{2}+\sqrt{3^2+4^2}\sqrt{4}+\sqrt{3^2+(n-3)^2}\sqrt{n-3}\\ &\leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_1)},\ \text{holds for } n\geq 7.\end{aligned}$$

$$\begin{aligned}(MX)_{u_2} &= \sum_{u_j\in N_G(u_2)}\sqrt{\deg^2(u_2)+\deg^2(u_j)}\sqrt{\deg(u_j)} \qquad (8)\\ &= \sqrt{\deg^2(u_2)+\deg^2(u_1)}\sqrt{\deg(u_1)}+\sqrt{\deg^2(u_2)+\deg^2(u_6)}\sqrt{\deg(u_6)}\\ &= \sqrt{2^2+3^2}\sqrt{3}+\sqrt{2^2+(n-3)^2}\sqrt{n-3}\\ &\leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_2)},\ \text{holds for } n\geq 7.\end{aligned}$$

$$\begin{aligned}(MX)_{u_3} &= \sum_{u_j\in N_G(u_3)}\sqrt{\deg^2(u_3)+\deg^2(u_j)}\sqrt{\deg(u_j)} \qquad (9)\\ &= \sqrt{\deg^2(u_3)+\deg^2(u_1)}\sqrt{\deg(u_1)}+\sqrt{\deg^2(u_3)+\deg^2(u_6)}\sqrt{\deg(u_6)}\\ &\quad+\sqrt{\deg^2(u_3)+\deg^2(u_4)}\sqrt{\deg(u_4)}+\sqrt{\deg^2(u_3)+\deg^2(u_5)}\sqrt{\deg(u_5)}\end{aligned}$$

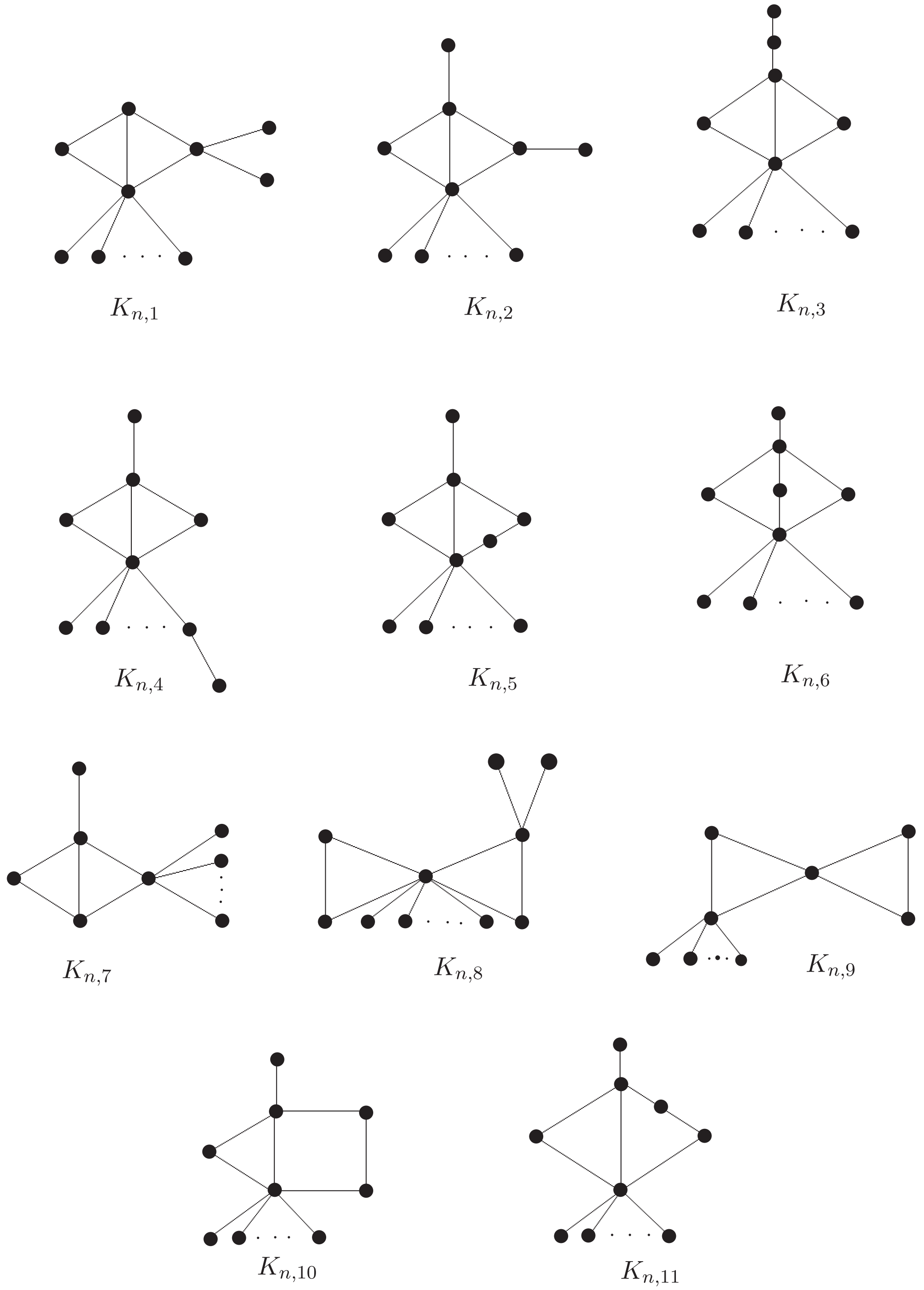

FIGURE 4. $\mathcal{B}_n^{32}$.

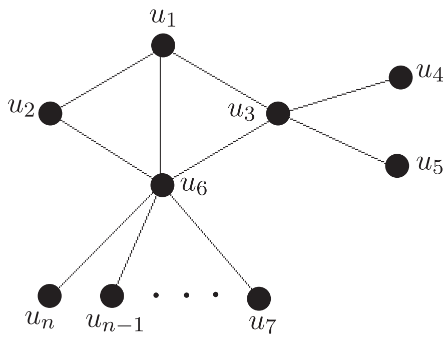

FIGURE 5. $K_{n,1}$.

$$
\begin{aligned}
&= \sqrt{4^2+3^2}\sqrt{3}+\sqrt{(n-3)^2+4^2}\sqrt{n-3}+2\sqrt{4^2+1^2}\sqrt{1}\\
&\leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_3)},\ \text{holds for } n\geq 7.
\end{aligned}
$$

$$
\begin{aligned}
(MX)_{u_i} &= \sum_{u_j\in N_G(u_i)} \sqrt{\deg^2(u_i)+\deg^2(u_j)}\sqrt{\deg(u_j)} \qquad (10)\\
&= \sqrt{\deg^2(u_i)+\deg^2(u_3)}\sqrt{\deg(u_3)}\\
&= \sqrt{4^2+1^2}\sqrt{4}\\
&\leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_i)},\ \text{holds for } n\geq 7,\ i=4,5.
\end{aligned}
$$

$$
\begin{aligned}
(MX)_{u_6} &= \sum_{u_j\in N_G(u_6)} \sqrt{\deg^2(u_6)+\deg^2(u_j)}\sqrt{\deg(u_j)} \qquad (11)\\
&= \sqrt{\deg^2(u_6)+\deg^2(u_1)}\sqrt{\deg(u_1)}+\sqrt{\deg^2(u_6)+\deg^2(u_2)}\sqrt{\deg(u_2)}\\
&\quad+\sqrt{\deg^2(u_6)+\deg^2(u_3)}\sqrt{\deg(u_3)}+(n-6)\sqrt{\deg^2(u_6)+\deg^2(u_7)}\sqrt{\deg(u_7)}\\
&= \sqrt{n^2-6n+13}\sqrt{2}+\sqrt{n^2-6n+18}\sqrt{3}+\sqrt{n^2-6n+25}\sqrt{4}\\
&\quad+(n-6)\sqrt{n^2-6n+10}\sqrt{1}\\
&\leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_6)},\ \text{holds for } n\geq 8.
\end{aligned}
$$

$$
\begin{aligned}
(MX)_{u_i} &= \sum_{u_j\in N_G(u_i)} \sqrt{\deg^2(u_i)+\deg^2(u_j)}\sqrt{\deg(u_j)} \qquad (12)\\
&= \sqrt{\deg^2(u_i)+\deg^2(u_6)}\sqrt{\deg(u_6)}\\
&= \sqrt{1^2+(n-3)^2}\sqrt{n-3}\\
&\leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_i)},\ \text{holds for } n\geq 7,\ i=7,8,\ldots n.
\end{aligned}
$$

By equations (7)–(12), we get $MX \leq \sqrt{n^3-3n^2+4n-2}X$. So, from Lemma 2.2, we have $\rho(K_{n,1}) \leq \sqrt{n^3-3n^2+4n-2}$, for all $n\geq 8$.

For other graphs $K_{n,i}$ with $2\leq i\leq 11$, by using a similar analysis, we can obtain

$$\rho(K_{n,i})\leq\sqrt{n^3-3n^2+4n-2}.$$

Therefore, it completes the proof. □

Now, we investigate the bound of the maximum Sombor radius of graphs in $\mathcal{B}_n^{33}$.

Lemma 2.6. *Let G be a bicyclic graph of order $n \geq 14$ in $\mathcal{B}_n^{33}$. Then*

$$\rho(G) \leq \sqrt{n^3 - 3n^2 + 4n - 2}.$$

Proof. Let G be a bicyclic graph of order $n \geq 14$ in $\mathcal{B}_n^{33}$. Suppose $V(G) = \{u_1, u_2, \dots, u_n\}$, $M = S(G)$ and $\rho(M) = \rho(G)$. Let $X = \left(\sqrt{\deg(u_1)}, \sqrt{\deg(u_2)}, \dots, \sqrt{\deg(u_n)}\right)^\top$. Then for any $u_i \in V(G)$, we have

$$(MX)_{u_i} = \sum_{u_j \in N_G(u_i)} \sqrt{\deg^2(u_i) + \deg^2(u_j)}\sqrt{\deg(u_j)}. \tag{13}$$

Recall that $\sum_{u_i \in V_G} \deg(u_i) = 2|E(G)|$. As a consequence, it is easy to check that

$$\begin{aligned}\sum_{u_j \in N_G(u_i)} \deg(u_j) &= 2(n+1) - \deg(u_i) - \sum_{u_k \notin N_G[u_i]} \deg(u_k) \\ &\leq 2n + 2 - \deg(u_i) - \sum_{u_k \notin N_G[u_i]} 1 \\ &= 2n + 2 - \deg(u_i) - (n - 1 - \deg(u_i)) \\ &= n + 3.\end{aligned} \tag{14}$$

By means of the degree of u_i, let us analyze the next two cases.

Case 1. Suppose now that $\deg(u_i) = 1$ and denote by u_j the unique neighbor of u_i in G. Then by equation (13), we have

$$\begin{aligned}(MX)_{u_i} &= \sqrt{1 + \deg^2(u_j)}\sqrt{\deg(u_j)} \\ &\leq \sqrt{(n-3)(n^2 - 6n + 10)} \\ &< \sqrt{n^3 - 3n^2 + 4n - 2}.\end{aligned} \tag{15}$$

Case 2. Suppose that $2 \leq \deg(u_i) \leq \Delta_1 \leq n - 3, \Delta_2 \leq 3$. Then from equation (14), we know

$$\begin{aligned}(MX)_{u_i} &= \sum_{u_j \in N_G(u_i)} \sqrt{\deg^2(u_i) + \deg^2(u_j)}\sqrt{\deg(u_j)} \\ &\leq \sqrt{(n-3)^2 + 9} \sum_{u_j \in N_G(u_i)} \sqrt{\deg(u_j)} \\ &= \sqrt{(n-3)^2 + 9} \sum_{u_j \in N_G(u_i)} 1 \cdot \sqrt{\deg(u_j)} \\ &\leq \sqrt{(n-3)^2 + 9} \sqrt{\sum_{u_j \in N_G(u_i)} \deg(u_j)\sqrt{\deg(u_i)}} \\ &\leq \sqrt{(n-3)^2 + 9}\sqrt{n+3}\sqrt{\deg(u_i)}.\end{aligned} \tag{16}$$

On the other hand, for $n \geq 14$, we get

$$f(n) = (n+3)\big((n-3)^2 + 9\big) - (n-1)\big(n^2 - 2n + 2\big) = -4n + 56 \leq 0,$$

which implies that

$$\sqrt{(n-3)^2 + 9}\sqrt{n+3} \leq \sqrt{n^3 - 3n^2 + 4n - 2}.$$

Hence, by equation (16), for any $2 \leq \deg(u_i) \leq n-3$, we see

$$(MX)_{u_i} \leq \sqrt{(n-3)^2+9}\sqrt{n+3}\sqrt{\deg(u_i)} \leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_i)}.$$

Combining equation (15) with equation (16), for $1 \leq \deg(u_i) \leq n-3$, we have

$$(MX)_{u_i} \leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_i)}.$$

Therefore, by Lemma 2.2, we have

$$\rho(G) \leq \sqrt{n^3-3n^2+4n-2},$$

which is the desired result. □

Theorem 2.3. *Let G be a bicyclic graph of order $n \geq 8$ in $\mathcal{B}_n^3$. Then*

$$\rho(G_{n,2}) > \rho(G).$$

Proof. If G is a bicyclic graph of order $8 \leq n \leq 13$ in $\mathcal{B}_n^{33}$, then applying Matlab, we can obtain $\rho(G_{n,2}) > \rho(G)$. Therefore, when G is a bicyclic graph of order $n \geq 8$ in $\mathcal{B}_n^3$, together with Theorem 2.1, and Lemmas 2.3, 2.5 and 2.6, we get

$$\rho(G_{n,2}) > \rho(G).$$

The result follows. □

2.4. The bound of the maximum Sombor spectral radius in $\mathcal{B}_n^4$

Next, we deal with all the graphs of order n with maximum degree $\Delta_1 \leq n-4$ in a unified way.

Lemma 2.7. *Let G be a bicyclic graph of order $n \geq 17$ in $\mathcal{B}_n^4$. Then*

$$\rho(G) \leq \sqrt{n^3-3n^2+4n-2}.$$

Proof. Let G be a bicyclic graph of order $n \geq 17$ in $\mathcal{B}_n^4$, and $V(G) = \{u_1, u_2, \ldots, u_n\}$, $M = S(G)$, $\rho(M) = \rho(G)$, $X = \left(\sqrt{\deg(u_1)}, \sqrt{\deg(u_2)}, \ldots, \sqrt{\deg(u_n)}\right)^\top$. Then for any $u_i \in V(G)$, we know

$$(MX)_{u_i} = \sum_{u_j \in N_G(u_i)} \sqrt{\deg^2(u_i)+\deg^2(u_j)}\sqrt{\deg(u_j)}. \tag{17}$$

Note that

$$\sum_{u_j \in N_G(u_i)} \deg(u_j) \leq n+3. \tag{18}$$

Case 1. Suppose that $1 \leq \deg(u_i) \leq 5$, denote by u_j the neighbor of u_i in G. Then by (17) and Cauchy–Schwarz inequality, we have

$$\begin{aligned}(MX)_{u_i} &= \sum_{u_j \in N_G(u_i)} \sqrt{\deg^2(u_i)+\deg^2(u_j)}\sqrt{\deg(u_j)} \\ &\leq \sqrt{(n-4)^2+25} \sum_{u_j \in N_G(u_i)} \sqrt{\deg(u_j)} \\ &= \sqrt{(n-4)^2+25} \sum_{u_j \in N_G(u_i)} 1 \cdot \sqrt{\deg(u_j)} \\ &\leq \sqrt{(n-4)^2+25}\sqrt{\sum_{u_j \in N_G(u_i)} \deg(u_j)}\sqrt{\deg(u_i)} \\ &\leq \sqrt{(n-4)^2+25}\sqrt{n+3}\sqrt{\deg(u_i)}.\end{aligned}$$

By direct calculation, for $n \geq 12$, we see

$$((n-4)^2+25)(n+3)-(n-1)(n^2-2n+2)=-2n^2+13n+125<0.$$

It means that $((n-4)^2+25)(n+3) < n^3-3n^2+4n-2$.
So, for $1 \leq \deg(u_i) \leq 5$, we deduce

$$(MX)_{u_i} \leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_i)}.$$

Case 2. Suppose that $6 \leq \deg(u_i) \leq \Delta_1 \leq n-4$.
Since G is a bicyclic graph, we have $\deg(u_i)+\deg(u_j) \leq n+2$ for any edge $u_iu_j \in E(G)$, which implies that $\sqrt{\deg^2(u_i)+\deg^2(u_j)} \leq \sqrt{\deg^2(u_i)+(n+2-\deg(u_i))^2}$. Thus, by equation (18), we have

$$\begin{aligned}(MX)_{u_i} &= \sum_{u_j\in N_G(u_i)} \sqrt{\deg^2(u_i)+\deg^2(u_j)}\sqrt{\deg(u_j)} \\ &\leq \sqrt{\deg^2(u_i)+(n+2-\deg(u_i))^2}\sum_{u_j\in N_G(u_i)}\sqrt{\deg(u_j)} \\ &\leq \sqrt{\deg^2(u_i)+(n+2-\deg(u_i))^2}\sqrt{\deg(u_i)}\sqrt{n+3}.\end{aligned} \tag{19}$$

On the other hand, for $6 \leq x \leq n-4$, suppose

$$f_n(x)=(n+3)(x^2+(n+2-x)^2)-(n-1)(n^2-2n+2).$$

By a simple calculation, for $n \geq 17$, we deduce

$$f_n(x) \leq f_n(n-4) = -2n^2+24n+158<0.$$

So, for $6 \leq \deg(u_i) \leq n-4$, from equation (19), we deduce

$$(MX)_{u_i} \leq \sqrt{n^3-3n^2+4n-2}\sqrt{\deg(u_i)}.$$

Therefore, the result follows from Lemma 2.2. □

Theorem 2.4. *Let G be a bicyclic graph of order $n \geq 8$ in $\mathcal{B}_n^4$. Then*

$$\rho(G_{n,2}) > \rho(G).$$

Proof. Let G be a bicyclic graph of order $8 \leq n \leq 16$ in $\mathcal{B}_n^4$. Then with the aid of Matlab, we obtain $\rho(G_{n,2}) > \rho(G)$. Hence, together with Theorem 2.1 and Lemma 2.7, we have

$$\rho(G_{n,2}) > \rho(G),$$

for all bicyclic graphs on $n \geq 8$ vertices in $\mathcal{B}_n^4$. □

3. The maximum Sombor spectral radius of bicyclic graphs

Since $G_{4,1}$ is the unique bicyclic graph of order 4, we can assume that $n \geq 5$. For $n = 5$, it is straightforward to enumerate all bicyclic graphs of order 5. Subsequently, by employing computational tools such as Matlab, we determine that $G_{5,1}$ and $H_{5,2} \cong H_{5,4}$ are the unique graphs possessing the largest and second largest Sombor spectral radii, which are approximately equal to 11.5181 and 10.4936, respectively. Similarly, for $6 \leq n \leq 7$, we establish that $\rho(G) < \rho(G_{n,2}) < \rho(G_{n,1})$. For $n \geq 8$, by integrating Theorems 2.1–2.4, we conclude that $G_{n,1}$ and $G_{n,2}$ are the unique graphs with the largest and second largest Sombor spectral radii, respectively. Consequently, the following theorem is derived.

Theorem 3.1. *Let G be a bicyclic graph of order $n \geq 5$.*

(i) *If $n = 5$, then $G_{5,1}$ and $H_{5,2} \cong H_{5,4}$ are unique graphs with the largest and second largest Sombor spectral radii, respectively.*
(ii) *If $n \geq 6$, then $G_{n,1}$ and $G_{n,2}$ are unique graphs with the largest and second largest Sombor spectral radii, respectively.*

4. Conclusion

In this paper, we uncover the extremal properties of the Sombor spectral radius for bicyclic graphs. Specifically, we establish that $G_{n,1}$ and $G_{n,2}$ are the unique graphs possessing the largest and second largest Sombor spectral radii among all bicyclic graphs, respectively. Moreover, by employing ideas analogous to those presented in this paper, one can investigate the characterization problem of the bicyclic graph with the minimum Sombor spectral radius. However, the research methods utilized in this article may prove insufficient for this purpose. Consequently, it is necessary to explore novel approaches. This will constitute a key direction for our future research.

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No potential conflict of interest was reported by the author(s).

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No data was used for the research described in the article.

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