MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **90** (2023) 513–532
ISSN: 0340–6253
doi: 10.46793/match.90-2.513M

Extreme Sombor Spectral Radius of Unicyclic Graphs

Yinzhen Mei[a,*], **Huifeng Fu**[a], **Hongli Miao**[a], **Yubin Gao**[a]

[a] *School of Mathematics, North University of China, Taiyuan, Shanxi, 030051, P. R. China*

myzmath@nuc.edu.cn

(Received March 24, 2023)

Abstract

Let G be a graph, the Sombor matrix $S(G)$ of G was recently introduced by Wang et al. It is a new matrix based on Sombor index, where the (i, j) entry $S_{ij} = \sqrt{d_i^2 + d_j^2}$ if vertices i and vertices j are adjacent in G, and $S_{ij} = 0$ for other cases. Xueliang Li and Junming Wang solved the conjecture for the upper and lower bounds of the ABC spectral radius for unicyclic graphs by Ghorbani et all. Inspired by this, we investigate the spectral radius on Sombor matrix of unicyclic graphs. In the paper, we use the method of classified discussion and Cauchy-Schwartz inequality to determine the external Sombor spectral radius of unicyclic graphs and provide the conditions for the equality.

1 Introduction

Let $G = (V, E)$ be a simple connected graph of order n, where vertex set $V = \{v_1, v_2, \cdots, v_n\}$ and edge set $E = \{e_1, e_2, \cdots, e_m\}$. A graph G is called unicyclic graph if $m = n$. We denote by d_i the degree of vertex v_i, by δ the minimum degree of G, and by $A = (A_{ij})_{n\times n}$ the adjacency matrix

*Corresponding author.

of a graph G. The eigenvalues of the adjacency matrx A are denoted by $\lambda_1(G), \lambda_2(G), \cdots, \lambda_n(G)$, and $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$. The spectral radius of G is the largest eigenvalue of the adjacency matrix, which is denoted by $\lambda_1(G)$. For more definitions, the reader can refer to [1,2].

The Sombor matrix $S = S(G) = (s_{ij})_{n\times n}$ of G is defined as

$$S_{ij} = \begin{cases} \sqrt{d_i^2 + d_j^2}, & if \quad v_i v_j \in E(G), \\ 0, & otherwise. \end{cases}$$

The eigenvalues of the Sombor matrx $S(G)$ are denoted by $\mu_1(G)$, $\mu_2(G)$, $\cdots, \mu_n(G)$, and $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$. The Sombor spectral radius of G is the largest eigenvalue of the Sombor matrix, which is denoted by $\mu_1(G)$. This matrix was recently introduced by Wang et al [3] based on the concept of Sombor index by Gutman [4] in the chemical graph theory. This new matrix is related to the forgotten index [5] that is a well-known degree-based topological index. Up to date, the study of the Sombor matrix of graphs mainly focuses on the Sombor index of chemical graphs [6–8] and graph operators [9]. For more related results, the reader can refer to [10,13,14,17,18].

In 2020, Ghorbani et al posed a conjecture for the upper and lower bouns of the ABC spectral for unicyclic graphs [11], and Xueliang Li et al solved the conjecture [15]. In this paper, for unicyclic graphs we investigate the Sombor matrix and calculate the largest and smallest Sombor spectral radius and characterize the corresponding extremal graphs.

2 Preliminary

Lemma 1. *[12] [16] Let $T \geq 0$ be an irreducible matrix. Then $\overline{R} \leq \mu_1(T) \leq R_{\max}$, where $\overline{R}$ is the average value of row sums of T and $R_{\max}$ is the value of the largest row sum. Either equality holds if and only if the row sums are equal.*

Lemma 2. *(Perron-Frobenius Theory) Let $T \geq 0$ be an irreducible matrix with an eigenvalue θ_0. Suppose $t \in R, x \in R^n$, $x \geq 0, x \neq 0$. If $Tx \leq tx$,* *then* $t \geq \theta_0$.

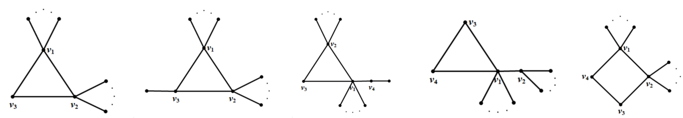
Lemma 3. *(Cauchy-Schwarz Inequality) Let* $(a_1, a_2, \cdots, a_n)$ *and* $(b_1, b_2, \cdots, b_n)$ *be positive real numbers. Then*

$$\sum_{i=1}^{n} a_i b_i \leq \sqrt{\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2},$$

where the equality holds if and only if $a_i = kb_i, 1 \leq i \leq n$.

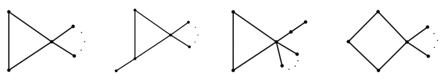
3 Extrend Sombor spectral radius

For convenience's sake, we denote the star graph, cycle graph of order n by S_n and C_n respectively. Let S_3^+ denote a unicyclic graph obtained by attaching $n-3$ vertices to some fixed vertex of C_3 . Let $\mathcal{U}_i (1 \leq i \leq 5)$ and $G_i (1 \leq i \leq 4)$ denote some special graphs in Figure 1 and Figure 2.



(a) $\mathcal{U}_1$ (b) $\mathcal{U}_2$ (c) $\mathcal{U}_3$ (d) $\mathcal{U}_4$ (e) $\mathcal{U}_5$

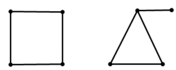
Figure 1. $\mathcal{U}_i (1 \leq i \leq 5)$



(a) G_1 (b) G_2 (c) G_3 (d) G_4

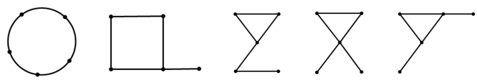
Figure 2. $G_i (1 \leq i \leq 4)$

It is well known that there is only one type C_3 of unicyclic graph for $n = 3$, and its Sombor spectral radius is $\mu_1(C_3) = 4\sqrt{2}$. Then we calculate Sombor spectral radius of unicyclic graphs for $4 \leq n \leq 6$(see Figure 3, Figure 4 and Figure 5), and display the computed result in Tab.1. In the following section, we consider the case of unicyclic graphs for $n \geq 7$.



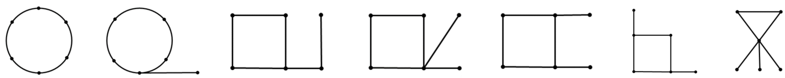
(a) a (b) b

Figure 3. Unicyclic graphs with $n = 4$

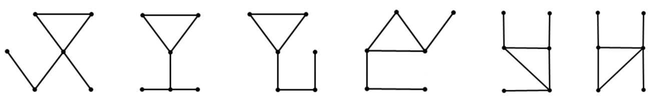


(a) B_1 (b) B_2 (c) B_3 (d) B_4 (e) B_5

Figure 4. Unicyclic graphs with $n = 5$



(a) D_1 (b) D_2 (c) D_3 (d) D_4 (e) D_5 (f) D_6 (g) D_7



(h) D_8 (i) D_9 (j) D_{10} (k) D_{11} (l) D_{12} (m) D_{13}

Figure 5. Unicyclic graphs with $n = 6$

Table 1. Sombor spectral radius of the unicyclic graphs for $4 \leq n \leq 6$.

$n = 4$	a	b					
μ_1	$4\sqrt{2}$	7.2538					
$n = 5$	B_1	B_2	B_3	B_4	B_5		
μ_1	$4\sqrt{2}$	6.9797	7.4872	9.5328	8.4853		
$n = 6$	D_1	D_2	D_3	D_4	D_5	D_6	D_7
μ_1	$4\sqrt{2}$	6.8356	7.2079	9.1369	8.0039	7.8740	12.3766
$n = 6$	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	
μ_1	9.7225	8.1108	7.5467	8.6409	9.5341	10.4129	

3.1 The lower bound for the Sombor spectrial radius

Theorem 1. *If G is the unicyclic graph with n vertices, then*

$$\mu_1(G) \geq \mu_1(C_n) = 4\sqrt{2},$$

where the equality holds if and only if $G \cong C_n$.

Proof. Since G is the unicyclic graph with n vertices, we have

$$d_1 + d_2 + \cdots + d_n = 2n.$$

According to Lemma 1, we have

$$\mu_1(G) \geq \frac{2}{n} \sum_{v_i v_j \in E(G)} \sqrt{d_i^2 + d_j^2} = \frac{\sqrt{2}}{n} \sum_{v_i v_j \in E(G)} \sqrt{2}\sqrt{d_i^2 + d_j^2}.$$

By Cauchy-Schwarz Inequality,

$$\sqrt{2}\sqrt{d_i^2 + d_j^2} \geq d_i + d_j,$$

$$n \sum_{i=1}^{n} d_i^2 \geq \left(\sum_{i=1}^{n} d_i \right)^2 = 4n^2. \tag{1}$$

Then

$$\mu_1(G) \geq \frac{\sqrt{2}}{n} \sum_{v_i v_j \in E(G)} (d_i + d_j) = \frac{\sqrt{2}}{n} \sum_{i=1}^{n} d_i^2 \geq 4\sqrt{2}.$$

It is easy to check that $\mu_1(C_n) = 4\sqrt{2}$. So

$$\mu_1(G) \geq \mu_1(C_n) = 4\sqrt{2}. \tag{2}$$

If the equation in (2) holds, then all the above inequalities must be equalities. By Lemma 3, the equality in (1) holds if and only if $d_i = d_j$ for any $1 \leq i, j \leq n$. Since G is a unicyclic graph, it implies that $G \cong C_n$.

Conversely, if $G \cong C_n$, then $d_i = 2$ for $1 \leq i \leq n$, and so $\mu_1(C_n) = 4\sqrt{2}$. ■

3.2 The upper bound for the Sombor spectrial radius

Let $\Delta_{adj}(G) = \max\{d_v + d_u | uv \in E(G)\}, X = (\sqrt{d_1}, \sqrt{d_2}, \cdots, \sqrt{d_n})^T$.

Lemma 4. *Let G be an unicyclic graph with n vertices. If $\Delta_{adj}(G) \leq n-1$, then $\mu_1(G) \leq \sqrt{n+1}\sqrt{n^2-6n+13}$.*

Proof. Since $\Delta_{adj}(G) \leq n-1$, we have $1 \leq d_i \leq n-3, i = 1, 2, \cdots, n$, and $d_{j_1} + d_{j_2} + \cdots + d_{j_{d_i}} \leq n+1$, where $v_{j_1}, v_{j_2}, \cdots, v_{j_{d_i}}$ denote the adjacent vertices to the vertice v_i.

$$(SX)_i = \sum_{v_iv_j \in E(G)} \sqrt{d_i^2 + d_j^2}\sqrt{d_j} \leq \sqrt{d_i^2 + (n-1-d_i)^2} \sum_{v_iv_j \in E(G)} \sqrt{d_j}.$$

By Cauchy-Schwarz Inequality,

$$\sum_{v_iv_j \in E(G)} \sqrt{d_j} \leq \sqrt{\sum_{v_iv_j \in E(G)} d_j}\sqrt{d_i} \leq \sqrt{n+1}\sqrt{d_i},$$

So

$$\begin{aligned}(SX)_i &\leq \sqrt{2d_i^2 - 2(n-1)d_i + (n-1)^2}\sqrt{n+1}\sqrt{d_i} \\ &\leq \sqrt{n^2-6n+13}\sqrt{n+1}\sqrt{d_i}.\end{aligned}$$

Namely, $SX \leq \sqrt{n+1}\sqrt{n^2-6n+13}X$.

Therefore, by Lemma 2, we can get $\mu_1(G) \leq \sqrt{n+1}\sqrt{n^2-6n+13}$. ∎

Lemma 5. *Let $f(x) = x^2 + x + \frac{n^2+2n+3}{x} - 2n - 1, x \in [3, n-3]$ and $n \geq 7$. Then $f(x) \leq n^2 - 6n + 15$.*

Proof. First, for $x \in [3, n-3]$,

$$\begin{aligned}f(x) &\leq x^2 + n - 3 + \frac{n^2+2n+3}{x} - 2n - 1 \\ &= x^2 + \frac{n^2+2n+3}{x} - n - 4 \triangleq g(x).\end{aligned}$$

Second,

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

Let $g'(x) = 0$. Then, we have

$$x = \sqrt[3]{\frac{n^2 + 2n + 3}{2}},$$

$$g\left(\sqrt[3]{\frac{n^2 + 2n + 3}{2}}\right) = 3\left(\frac{n^2 + 2n + 3}{2}\right)^{\frac{2}{3}} - n - 4,$$

$$g(3) = \frac{1}{3}n^2 - \frac{n}{3} + 6,$$

$$g(n-3) = n^2 - 6n + 10 + \frac{18}{n-3} \leq n^2 - 6n + 15.$$

So, for $x \in [3, n-3]$,

$$\max g(x) = g(n-3).$$

Thus, for $x \in [3, n-3]$, $f(x) \leq n^2 - 6n + 15, n \geq 7$. ■

Lemma 6. *[15] Let G be an unicyclic graphs with n vertices. If there exist two adjacent vertices $u, v \in V(G)$ such that $d_u + d_v \geq n$, then $G \in \mathcal{U} = \{\mathcal{U}_1, \mathcal{U}_2, \mathcal{U}_3, \mathcal{U}_4, \mathcal{U}_5\}$, see Figure 1.*

Lemma 7. *If $G \in \mathcal{U}_1 \setminus \{G_1, G_2\}$, then $\mu_1(G) \leq \sqrt{n+1}\sqrt{n^2 - 6n + 15}$.*

Proof. Since $G \in \mathcal{U}_1 \setminus \{G_1, G_2\}$, we have that $d_1 + d_2 = n+1, d_3 = 2, d_4 = \cdots = d_n = 1$, and $4 \leq d_1, d_2 \leq n-3$. Then

$$\begin{aligned}(SX)_1 &= \sum_{v_1 v_j \in E(G)} \sqrt{d_1^2 + d_j^2}\sqrt{d_j} \\ &= \sqrt{d_1^2 + d_2^2}\sqrt{d_2} + \sqrt{d_1^2 + d_3^2}\sqrt{d_3} + (d_1 - 2)\sqrt{d_1^2 + 1}.\end{aligned}$$

By Lemmas 3 and 5, we have

$$\begin{aligned}(SX)_1 &\leq \sqrt{d_1^2 + d_2^2 + d_1^2 + d_3^2 + (d_1 - 2)(d_1^2 + 1)}\sqrt{d_2 + d_3 + d_1 - 2} \\ &= \sqrt{d_1^3 + d_1^2 - (2n+1)d_1 + n^2 + 2n + 3}\sqrt{n+1} \\ &= \sqrt{n+1}\sqrt{d_1^2 + d_1 - 2n - 1 + \frac{n^2 + 2n + 3}{d_1}}\sqrt{d_1} \\ &\leq \sqrt{n+1}\sqrt{n^2 - 6n + 15}\sqrt{d_1}.\end{aligned}$$

Similarly,

$$(SX)_2 \le \sqrt{n+1}\sqrt{n^2-6n+15}\sqrt{d_2}.$$

For $i=3$, we have

$$\begin{aligned}
(SX)_3 &= \sum_{v_3v_j\in E(G)} \sqrt{d_3^2+d_j^2}\sqrt{d_j} \\
&= \sqrt{4+d_1^2}\sqrt{d_1} + \sqrt{4+d_2^2}\sqrt{d_2} \\
&\le \sqrt{8+d_1^2+d_2^2}\sqrt{d_1+d_2} \\
&= \sqrt{n+1}\sqrt{d_1^2-(n+1)d_1+\frac{n^2+2n+9}{2}}\sqrt{d_3} \\
&\le \sqrt{n+1}\sqrt{\frac{1}{2}(n^2-6n+33)}\sqrt{d_3} \\
&\le \sqrt{n+1}\sqrt{n^2-6n+15}\sqrt{d_3}.
\end{aligned}$$

For $4 \le i \le n$, we have

$$\begin{aligned}
(SX)_i &= \sum_{v_iv_j\in E(G)} \sqrt{d_i^2+d_j^2}\sqrt{d_j} \\
&= \sqrt{d_i^2+d_k^2}\sqrt{d_k} \\
&= \sqrt{1+d_k^2}\sqrt{d_k} \\
&\le \sqrt{(n-3)(n^2-6n+10)} \\
&\le \sqrt{n+1}\sqrt{n^2-6n+15}, \quad k=1,2.
\end{aligned}$$

In summary, we have $SX \le \sqrt{(n+1)(n^2-6n+15)}X$, and so $\mu_1(G) \le \sqrt{n+1}\sqrt{n^2-6n+15}$. ■

Lemma 8. *If $G \in \mathcal{U}_2 \setminus \{G_2\}$, then $\mu_1(G) \le \sqrt{n+1}\sqrt{n^2-6n+15}$.*

Proof. Since $G \in \mathcal{U}_2 \setminus \{G_2\}$, we have $d_1+d_2=n, d_3=3, d_4=\cdots=d_n=1$, and $3 \le d_1, d_2 \le n-3$. Then

$$(SX)_1 = \sum_{v_1v_j\in E(G)} \sqrt{d_1^2+d_j^2}\sqrt{d_j}$$

$$
\begin{aligned}
&= \sqrt{d_1^2+d_2^2}\sqrt{d_2}+\sqrt{d_1^2+d_3^2}\sqrt{d_3}+(d_1-2)\sqrt{d_1^2+1}\\
&\leq \sqrt{d_1^2+d_2^2+d_1^2+d_3^2+(d_1-2)(d_1^2+1)}\sqrt{d_2+d_3+d_1-2}\\
&= \sqrt{n+1}\sqrt{d_1^3+d_1^2+(1-2n)d_1+n^2+7}\\
&= \sqrt{n+1}\sqrt{d_1^2+d_1+1-2n+\frac{n^2+7}{d_1}}\sqrt{d_1}\\
&\leq \sqrt{d_1^2+d_1-2n-1+\frac{n^2+2n+3}{d_1}}\sqrt{d_1}\\
&\leq \sqrt{n+1}\sqrt{n^2-6n+15}\sqrt{d_1}.
\end{aligned}
$$

Similarly,

$$(SX)_2 \leq \sqrt{n+1}\sqrt{n^2-6n+15}\sqrt{d_2}.$$

For $i=3$, we have

$$
\begin{aligned}
(SX)_3 &= \sum_{v_3v_j\in E(G)}\sqrt{d_3^2+d_j^2}\sqrt{d_j}\\
&= \sqrt{d_3^2+d_1^2}\sqrt{d_1}+\sqrt{d_3^2+d_2^2}\sqrt{d_2}+\sqrt{d_3^2+1}\sqrt{1}\\
&\leq \sqrt{3d_3^2+d_1^2+d_2^2+1}\sqrt{n+1}\\
&= \sqrt{2d_1^2-2nd_1+n^2+28}\sqrt{n+1}\\
&= \sqrt{\frac{1}{3}(2d_1^2-2nd_1+n^2+28)}\sqrt{n+1}\sqrt{d_3}\\
&\leq \sqrt{n+1}\sqrt{n^2-6n+15}\sqrt{d_3}.
\end{aligned}
$$

For $4\leq i\leq n$, we have

$$
\begin{aligned}
(SX)_i &= \sqrt{d_i^2+d_k^2}\sqrt{d_k}\\
&= \sqrt{1+d_k^2}\sqrt{d_k}\\
&\leq \sqrt{n+1}\sqrt{n^2-6n+15}, k=1,2,3.
\end{aligned}
$$

In summary, we have $SX\leq\sqrt{(n+1)(n^2-6n+15)}X$, and so $\mu_1(G)\leq\sqrt{n+1}\sqrt{n^2-6n+15}$. ■

Lemma 9. *If $G \in \mathcal{U}_3 \setminus \{G_3\}$, then $\mu_1(G) \le \sqrt{n+1}\sqrt{n^2-6n+14}$.*

Proof. Since $G \in \mathcal{U}_3 \setminus \{G_3\}$, we have $d_1 + d_2 = n, d_3 = d_4 = 2, d_5 = \cdots = d_n = 1$, and $3 \le d_1, d_2 \le n-3$. Then

$$\begin{aligned}
(SX)_1 &= \sum_{v_1 v_j \in E(G)} \sqrt{d_1^2 + d_j^2}\sqrt{d_j} \\
&= \sqrt{d_1^2 + d_2^2}\sqrt{d_2} + \sqrt{d_1^2 + d_3^2}\sqrt{d_3} + \sqrt{d_1^2 + d_4^2}\sqrt{d_4} \\
&\quad + (d_1 - 3)\sqrt{d_1^2 + 1} \\
&\le \sqrt{3d_1^2 + d_2^2 + d_3^2 + d_4^2 + (d_1 - 3)(d_1^2 + 1)}\sqrt{d_2 + d_3 + d_4 + d_1 - 3} \\
&= \sqrt{d_1^3 + d_1^2 + (1 - 2n)d_1 + n^2 + 5}\sqrt{n+1} \\
&= \sqrt{d_1^2 + d_1 + 1 - 2n + \frac{n^2 + 5}{d_1}}\sqrt{n+1}\sqrt{d_1} \\
&\le \sqrt{n+1}\sqrt{n^2 - 6n + 14}\sqrt{d_1}.
\end{aligned}$$

Similarly,

$$(SX)_2 \le \sqrt{n+1}\sqrt{n^2 - 6n + 14}\sqrt{d_2}.$$

For $i = 3, 4, 5$, we have

$$\begin{aligned}
(SX)_3 &= \sum_{v_3 v_j \in E(G)} \sqrt{d_3^2 + d_j^2}\sqrt{d_j} \\
&= \sqrt{d_3^2 + d_1^2}\sqrt{d_1} + \sqrt{d_3^2 + d_2^2}\sqrt{d_2} \\
&\le \sqrt{2d_3^2 + d_1^2 + d_2^2}\sqrt{d_1 + d_2} \\
&= \sqrt{8 + d_1^2 + (n - d_1)^2}\sqrt{n} \\
&= \sqrt{d_1^2 - nd_1 + \frac{n^2}{2} + 4}\sqrt{n}\sqrt{2} \\
&\le \sqrt{\frac{n^2}{2} - 3n + 13}\sqrt{n}\sqrt{2} \\
&\le \sqrt{n^2 - 6n + 14}\sqrt{n+1}\sqrt{d_3},
\end{aligned}$$

$$
\begin{aligned}
(SX)_4 &= \sum_{v_4v_j\in E(G)} \sqrt{d_4^2+d_j^2}\sqrt{d_j}\\
&= \sqrt{d_4^2+d_1^2}\sqrt{d_1}+\sqrt{d_4^2+d_5^2}\sqrt{d_5}\\
&= \sqrt{4+d_1^2}\sqrt{d_1}\sqrt{5}\\
&\le \sqrt{n^2-6n+14}\sqrt{n+1}\sqrt{2}\\
&\le \sqrt{n^2-6n+14}\sqrt{n+1}\sqrt{d_4},
\end{aligned}
$$

and

$$
(SX)_5 = \sqrt{d_5^2+d_4^2}\sqrt{d_4} = 2\sqrt{1+4} \le \sqrt{n+1}\sqrt{n^2-6n+14}.
$$

For $6 \le i \le n$, we have

$$
\begin{aligned}
(SX)_i &= \sqrt{d_i^2+d_k^2}\sqrt{d_k}\\
&= \sqrt{1+d_k^2}\sqrt{d_k}\\
&\le \sqrt{(n_3)^2+1}\sqrt{n-3}\\
&\le \sqrt{n+1}\sqrt{n^2-6n+14}.
\end{aligned}
$$

In summary, we have $SX \le \sqrt{(n+1)(n^2-6n+14)}X$, and so $\mu_1(G) \le \sqrt{n+1}\sqrt{n^2-6n+14}$. ∎

Lemma 10. *If $G \in \mathcal{U}_4 \setminus \{G_1, G_3\}$, then $\mu_1(G) \le \sqrt{n+1}\sqrt{n^2-6n+14}$.*

Proof. Since $G \in \mathcal{U}_4 \setminus \{G_1, G_3\}$, we have $d_1+d_2 = n, d_3 = d_4 = 2, d_5 = \cdots = d_n = 1$, and $3 \le d_1, d_2 \le n-3$. Then

$$
\begin{aligned}
(SX)_1 &= \sum_{v_1v_j\in E(G)} \sqrt{d_1^2+d_j^2}\sqrt{d_j}\\
&= \sqrt{d_1^2+d_2^2}\sqrt{d_2}+\sqrt{d_1^2+d_3^2}\sqrt{d_3}+\sqrt{d_1^2+d_4^2}\sqrt{d_4}\\
&\quad +(d_1-3)\sqrt{d_1^2+1}\\
&\le \sqrt{3d_1^2+d_2^2+d_3^2+d_4^2+(d_1-3)(d_1^2+1)}\sqrt{d_2+d_3+d_4+d_1-3}\\
&= \sqrt{d_1^3+d_1^2+(1-2n)d_1+n^2+5}\sqrt{n+1}
\end{aligned}
$$

$$= \sqrt{d_1^2 + d_1 + 1 - 2n + \frac{n^2+5}{d_1}}\sqrt{n+1}\sqrt{d_1}$$
$$\leq \sqrt{n+1}\sqrt{n^2-6n+14}\sqrt{d_1}.$$

Similarly,

$$(SX)_2 \leq \sqrt{n+1}\sqrt{n^2-6n+14}\sqrt{d_2}.$$

For $i = 3, 4$, we have

$$\begin{aligned}(SX)_3 &= \sqrt{d_3^2+d_1^2}\sqrt{d_1} + \sqrt{d_3^2+d_4^2}\sqrt{d_4}\\ &\leq \sqrt{2d_3^2+d_1^2+d_4^2}\sqrt{d_1+d_4}\\ &= \sqrt{d_1^2+12}\sqrt{d_1+2}\\ &\leq \sqrt{n^2-6n+14}\sqrt{n+1}\sqrt{2},\end{aligned}$$

and

$$(SX)_4 \leq \sqrt{n^2-6n+14}\sqrt{n+1}\sqrt{2}.$$

For $5 \leq i \leq n$, we have

$$\begin{aligned}(SX)_i &= \sqrt{d_i^2+d_k^2}\sqrt{d_k}\\ &= \sqrt{1+d_k^2}\sqrt{d_k}\\ &\leq \sqrt{n+1}\sqrt{n^2-6n+14}, \quad k=1,2.\end{aligned}$$

In summary, we have $SX \leq \sqrt{(n+1)(n^2-6n+14)}X$, and so $\mu_1(G) \leq \sqrt{n+1}\sqrt{n^2-6n+14}$. ■

Lemma 11. *If $G \in \mathcal{U}_5 \setminus \{G_5\}$, then $\mu_1(G) \leq \sqrt{n+1}\sqrt{n^2-6n+13}$.*

Proof. Since $G \in \mathcal{U}_5 \setminus \{G_4\}$, we have $d_1 + d_2 = n, d_3 = d_4 = 2, d_5 = \cdots = d_n = 1$, and $3 \leq d_1, d_2 \leq n-3$. Then

$$\begin{aligned}(SX)_1 &= \sum_{v_1v_j \in E(G)} \sqrt{d_1^2+d_j^2}\sqrt{d_j}\\ &= \sqrt{d_1^2+d_2^2}\sqrt{d_2} + \sqrt{d_1^2+d_4^2}\sqrt{d_4} + (d_1-2)\sqrt{d_1^2+1}\end{aligned}$$

$$
\begin{aligned}
&\leq \sqrt{2d_1^2 + d_2^2 + d_4^2 + (d_1-2)(d_1^2+1)}\sqrt{d_2 + d_4 + d_1 - 2} \\
&= \sqrt{d_1^3 + d_1^2 + (1-2n)d_1 + n^2 + 2}\sqrt{n} \\
&= \sqrt{d_1^2 + d_1 + 1 - 2n + \frac{n^2+2}{d_1}}\sqrt{n}\sqrt{d_1} \\
&\leq \sqrt{n+1}\sqrt{n^2-6n+13}\sqrt{d_1}.
\end{aligned}
$$

Similarly,

$$
(SX)_2 \leq \sqrt{n+1}\sqrt{n^2-6n+13}\sqrt{d_2}.
$$

For $i = 3, 4$, we have

$$
\begin{aligned}
(SX)_3 &= \sqrt{d_3^2 + d_2^2}\sqrt{d_2} + \sqrt{d_3^2 + d_4^2}\sqrt{d_4} \\
&\leq \sqrt{2d_3^2 + d_2^2 + d_4^2}\sqrt{d_2 + d_4} \\
&= \sqrt{d_2^2 + 12}\sqrt{d_2 + 2} \\
&\leq \sqrt{n^2-6n+13}\sqrt{n+1}\sqrt{2},
\end{aligned}
$$

and

$$
(SX)_4 \leq \sqrt{n^2-6n+13}\sqrt{n+1}\sqrt{2}.
$$

For $5 \leq i \leq n$, we have

$$
\begin{aligned}
(SX)_i &= \sqrt{d_i^2 + d_k^2}\sqrt{d_k} = \sqrt{1 + d_k^2}\sqrt{d_k} \\
&\leq \sqrt{1 + (n-3)^2}\sqrt{n-3} \\
&\leq \sqrt{n+1}\sqrt{n^2-6n+13}, \qquad k = 1, 2.
\end{aligned}
$$

In summary, we have $SX \leq \sqrt{(n+1)(n^2-6n+13)}X$, and so $\mu_1(G) \leq \sqrt{n+1}\sqrt{n^2-6n+13}$. ■

Lemma 12. *Let $F = \{G_1, G_2, G_3, G_4\}$. Then G_1 has the largest Sombor spectral radius among F.*

Proof. For G_1, we have

$$M(G_1) = \begin{bmatrix} 0 & \beta & \beta & \alpha & \cdots & a \\ \beta & 0 & 2\sqrt{2} & 0 & \cdots & 0 \\ \beta & 2\sqrt{2} & 0 & 0 & \cdots & 0 \\ \alpha & 0 & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \alpha & 0 & 0 & 0 & \cdots & 0 \end{bmatrix},$$

where

$$\alpha = \sqrt{(n-1)^2+1}, \beta = \sqrt{(n-1)^2+4}.$$

Then

$$f_{G_1}(\lambda) = \det(\lambda I - M(G_1)) = (\lambda + 2\sqrt{2})\lambda^{n-4} f_1(\lambda),$$

where

$$f_1(\lambda) = \lambda^3 - 2\sqrt{2}\lambda^2 - (n^3 - 3n^2 + 4n + 4)\lambda + 2\sqrt{2}(n^3 - 5n^2 + 8n - 6).$$

It is easy that

$$f_1(-n\sqrt{n+1}) < 0, \qquad f_1(0) > 0,$$

$$f_1(\sqrt{n+1}\sqrt{n^2-5n+8}) < 0, \qquad f_1(n\sqrt{n+1}) > 0.$$

By zero point theorem, we have

$$\mu_1(G_1) \in (\sqrt{n+1}\sqrt{n^2-5n+8}, n\sqrt{n+1}).$$

For G_2, we have

$$M(G_2) = \begin{bmatrix} 0 & c & b & 0 & a & \cdots & a \\ c & 0 & \sqrt{13} & \sqrt{10} & 0 & \cdots & 0 \\ b & \sqrt{13} & 0 & 0 & 0 & \cdots & 0 \\ 0 & \sqrt{10} & 0 & 0 & 0 & \cdots & 0 \\ a & 0 & 0 & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a & 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix},$$

where

$$a = \sqrt{(n-2)^2+1}, b = \sqrt{(n-2)^2+4}, c = \sqrt{(n-2)^2+9}.$$

Then

$$f_{G_2}(\lambda) = \det(\lambda I - M(G_2)) = \lambda^{n-4} f_2(\lambda),$$

where

$$f_2(\lambda) = \lambda^4 - (n^3 - 6n^2 + 13n + 24)\lambda^2 + 23n^3 - 174n^2 + 443n - 380.$$

It is easy that

$$\begin{aligned}
&f_2(-\sqrt{n+1}\sqrt{n^2-5n+8}) > 0,\\
&f_2\left(-\sqrt{\frac{1}{2}(n+1)(n^2-7n+20)}\right) < 0,\\
&f_2(0) > 0,\\
&f_2\left(\sqrt{\frac{1}{2}(n+1)(n^2-7n+20)}\right) < 0,\\
&f_2(\sqrt{n+1}\sqrt{n^2-5n+8}) > 0.
\end{aligned}$$

By zero point theorem, we have

$$\mu_1(G_2) \leq \sqrt{n+1}\sqrt{n^2-5n+8}.$$

For G_3, we have

$$M(G_3) = \begin{bmatrix}
0 & b & b & b & 0 & a & \cdots & a\\
b & 0 & 2\sqrt{2} & 0 & 0 & 0 & \cdots & 0\\
b & 2\sqrt{2} & 0 & 0 & 0 & 0 & \cdots & 0\\
b & 0 & 0 & 0 & \sqrt{5} & 0 & \cdots & 0\\
0 & 0 & 0 & \sqrt{5} & 0 & 0 & \cdots & 0\\
a & 0 & 0 & 0 & 0 & 0 & \cdots & 0\\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\
a & 0 & 0 & 0 & 0 & 0 & \cdots & 0
\end{bmatrix},$$

where

$$a = \sqrt{(n-2)^2+1}, b = \sqrt{(n-2)^2+4},$$

Then

$$f_{G_3}(\lambda) = \det(\lambda I - M(G_3)) = (\lambda + 2\sqrt{2})\lambda^{n-6} f_3(\lambda),$$

where

$$\begin{aligned} f_3(\lambda) =& \lambda^5 - 2\sqrt{2}\lambda^4 - (n^3 - 6n^2 + 13n + 4)\lambda^3 + 2\sqrt{2}(n^3 - 8n^2 + 21n \\ & - 12)\lambda^2 + 5(n^3 - 7n^2 + 17n - 9)\lambda - 10\sqrt{2}(n^3 - 9n^2 + 25n - 25). \end{aligned}$$

It is easy that

$$\begin{aligned} & f_3(-\sqrt{n+1})\sqrt{n^2-5n+8}) < 0, \\ & f_3(-\sqrt{(n+1)(n^2-9n)}) > 0, \\ & f_3(0) < 0, \\ & f_3(4\sqrt{2}) > 0, \\ & f_3(\sqrt{(n+1)(n^2-8n)}) < 0, \\ & f_3(\sqrt{n+1}\sqrt{n^2-5n+8}) > 0. \end{aligned}$$

By zero point theorem, we have

$$\mu_1(G_3) \leq \sqrt{n+1}\sqrt{n^2-5n+8}.$$

For G_4, we have

$$M(G_4) = \begin{bmatrix} 0 & b & 0 & b & a & a & \cdots & a \\ b & 0 & 2\sqrt{2} & 0 & 0 & 0 & \cdots & 0 \\ 0 & 2\sqrt{2} & 0 & 2\sqrt{2} & 0 & 0 & \cdots & 0 \\ b & 0 & 2\sqrt{2} & 0 & 0 & 0 & \cdots & 0 \\ b & 0 & 2\sqrt{2} & 0 & 0 & 0 & \cdots & 0 \\ a & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix},$$

where

$$a = \sqrt{(n-2)^2+1}, b = \sqrt{(n-2)^2+4}.$$

Then

$$f_{G_4}(\lambda) = \det(\lambda I - M(G_4)) = \lambda^{n-4} f_4(\lambda),$$

where

$$f_4(\lambda) = \lambda^4 - (n^3 - 6n^2 + 13n + 12)\lambda^2 + 16(n^3 - 8n^2 + 21n - 20).$$

It is easy that

$$f_4(\pm\sqrt{n+1}\sqrt{n^2-5n+8}) > 0,$$

$$f_4(\pm 4) < 0,$$

$$f_4(0) > 0.$$

By zero point theorem, we have

$$\mu_1(G_4) \leq \sqrt{n+1}\sqrt{n^2-5n+8}.$$

In summary, the Sombor spectral radius of G_1 among F is largest. ■

Theorem 2. *If G is the unicyclic graph of order $n \geq 7$, then*

$$\mu_1(G) \leq \mu_1(S_3^+),$$

with equality if and only if $G \cong S_3^+$.

Proof. By Lemma 4 and Lemmas 6-11, for all unicyclic graphs of order $n \geq 7$ except $G \in \{G_1, G_2, G_3, G_4\}$, we have

$$\mu_1(G) \leq \sqrt{n+1}\sqrt{n^2-5n+8}.$$

By Lemma 12, we have

$$\mu_1(G_1) \geq \sqrt{n+1}\sqrt{n^2-5n+8} \geq \mu_1(G_i), \quad i = 2, 3, 4.$$

Therefore, G_1 is the unicyclic graph with the largest Sombor spectral radius, which is isomorphic to S_3^+. ■

4 Conclusion

Since, evidently, C_3 be a special form of S_3^+, we obtain our main result as follows.

Theorem 3. *If G is the unicyclic graph of order $n \geq 3$, then*

$$4\sqrt{2} = \mu_1(C_n) \leq \mu_1(G) \leq \mu_1(S_3^+),$$

where the lower bound is achieved by C_n and the upper bound is achieved by S_3^+.

Recently, Li et al. proved the conjecture for the upper and lower bounds of the ABC spectral radius for unicyclic graphs. In this paper, we have researched the spectral radius of the Sombor matrix from an algebraic viewpoint, and characterize the corresponding extremal graphs as Theorem 3. Further, we conjecture that for an unicyclic graph of order $n \geq 3$, the spectral radius ρ of the corresponding matrix based on degree of vertices must satify that $\rho(C_n) \leq \rho(G) \leq \rho(S_3^+)$, with equality if and only if $G \cong C_n$ for the lower bound, and $G \cong S_3^+$ for the upper bound.

***Acknowledgment*:** This work was supported by the National Nature Science Foundation of China (Grant No. 61774137), Shanxi Scholarship Council of China (Grant No.2022-149), and Natural Science Foundation of Shanxi Province(Grant No. 20210302124212).

References

[1] A. E. Brouwer, W. H. Haemers, *Spectra of Graphs*, Springer, New York, 2011.

[2] F. Yang, M. Lu, J. Guo, On the minimum Kirchhoff index of unicyclic graphs with given girth and diameter, *Bull. Malays. Math. Sci. Soc.* **45** (2022) 1287–1299.

[3] Z. Wang, Y. Mao, I. Gutman, J. Wu, Q. Ma, Spectral radius and energy of Sombor matrix of graphs, *Filomat* **35** (2021) 5093–5100.

[4] I. Gutman, Geometric approach to degree–based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.

[5] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.

[6] K. J. Gowtham, N. N. Swamy, On Sombor energy of graphs, *Nanosys. Phys. Chem. Math.* **12** (2021) 411–417.

[7] R. Cruz, I. Gutman, J. Rada, Sombor index of chemical graphs, *Appl. Math. Comput.* **399** (2021)#126018.

[8] H. Deng, Z. Tang, R. Wu, Molecular trees with extremal values of Sombor indices, *Int. J. Quantum Chem.* **121** (2021) #e26622.

[9] H. Ramane, I. Gutman, K. Bhajantri, D. Kitturmath, Sombor index of some graph transformations, *Comm. Comb. Optim.* **8** (2023) 193–205.

[10] K. C. Das, A. S. Çevik, I. N. Cangul, Y. Shang, On Sombor index, *Symmetry* **13** (2021) #140.

[11] M. Ghorbani, X. Li, M. Hakimi–Nezhaad, J. Wang, Bounds on the ABC spectral radius and ABC energy of graphs, *Lin. Algebra Appl.* **598** (2020) 145–164.

[12] R. A. Horn, C. R. Johnson, *Matrix Analysis*, Cambridge Univ. Press, New York, 2012.

[13] B. Horoldagva, C. Xu, On Sombor index of graphs, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 703–713.

[14] V. Kulli, I. Gutman, Computation of Sombor indices of certain networks, *Int. J. Appl. Chem.* **8** (2021) 1–5.

[15] X. Li, J. Wang, On the ABC spectra radius of unicyclic graphs, *Lin. Algebra Appl.* **596** (2020) 71–81.

[16] X. Li, Z. Wang, Trees with extremal spectral radius of weighted adjacency matrices among trees weighted by degree–based indices, *Lin. Algebra Appl.* **620** (2021) 61–75.

[17] I. Redžepović, Chemical applicability of Sombor indices, *J. Serb. Chem. Soc.* **86** (2021) 1–12.

[18] A. Yu, M. Lu, Lower bounds on the (Laplacian) spectral radius of weighted graphs, *Chinese Ann. Math. B* **35** (2014) 669–678.