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The Second Largest Balaban Index (Sum-Balaban Index) of Unicyclic Graphs

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Abstract Balaban index and Sum-Balaban index were used in various quantitative structure-property relationship and quantitative structure activity relationship studies. In this paper, the unicyclic graphs with the second largest Balaban index and the second largest Sum-Balaban index among all unicyclic graphs on n vertices are characterized, respectively.

Keywords Balaban index; Sum-Balaban index; unicyclic graph

MR(2010) Subject Classification 05C35; 05C50

1. Introduction

Let G be a simple and connected graph with $|V(G)| = n$ and $|E(G)| = m$. Then $\mu = |E(G)| - |V(G)| + 1 = m - n + 1$ is the cyclomatic number. As usual, let $N_G(u)$ be the neighbor vertex set of vertex u, and $d_G(u, v)$ be the distance between vertices u and v in G. Then $d_G(u) = |N_G(u)|$ is called the degree of u, and $D_G(u) = \sum_{v\in V(G)} d_G(u, v)$ (or $D(u)$ for short) is the distance sum of vertex u in G.

Balaban index was proposed by Balaban [1,2] which is also called the average distance-sum connectivity or J index. The Balaban index of a simple connected graph G is defined as

$$J(G) = \frac{m}{\mu + 1} \sum_{uv\in E(G)} \frac{1}{\sqrt{D_G(u)D_G(v)}}.$$

Balaban et al. [3] also proposed the Sum-Balaban index $SJ(G)$ of a connected graph G, which is defined as

$$SJ(G) = \frac{m}{\mu + 1} \sum_{uv\in E(G)} \frac{1}{\sqrt{D_G(u) + D_G(v)}}.$$

For chemical applications, it may be interesting to identify the graph with the maximum and minimum topological indices in given class of graphs. Deng [4] proved that among all trees

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with n vertices, the star S_n and the path P_n have the maximal and the minimal Balaban index. Fang and Gao et al. [5] gave the sharp upper bounds of Balaban index and Sum-Balaban index for bicyclic graphs, and characterize the bicyclic graphs which attain the upper bounds. You and Dong [6] gave the unicyclic graphs with the maximum Balaban index and the maximum Sum-Balaban index among all unicyclic graphs on n vertices. More mathematical propertices of Balaban index can be found in [7–10]. More mathematical propertices of Sum-Balaban index can be found in [8,9,11,12].

Although in [6], Lihua YOU has characterized unicyclic graphs with the maximum Balaban index (Sum-Balaban index) and calculated the corresponding value of the maximum index, in order to find unicyclic graphs with the second largest Balaban index (Sum-Balaban index) we shall first use a new method to find unicyclic graphs with the maximum Balaban index (Sum-Balaban index).

2. The maximum Balaban index (Sum-Balaban index) of unicyclic graphs

We first introduce some useful graph transformations.

2.1. The edge-lifting transformation

The edge-lifting transformation ([4,12]) Let G_1 and G_2 be two graphs with $n_1 \geq 2$ and $n_2 \geq 2$ vertices, respectively. If G is the graph obtained from G_1 and G_2 by adding an edge between a vertex u_0 of G_1 and a vertex v_0 of G_2, G' is the graph obtained by identifying u_0 of G_1 to v_0 of G_2 and adding a pendent edge to $u_0(v_0)$, then G' is called the edge-lifting transformation of G (see Figure 2.1).

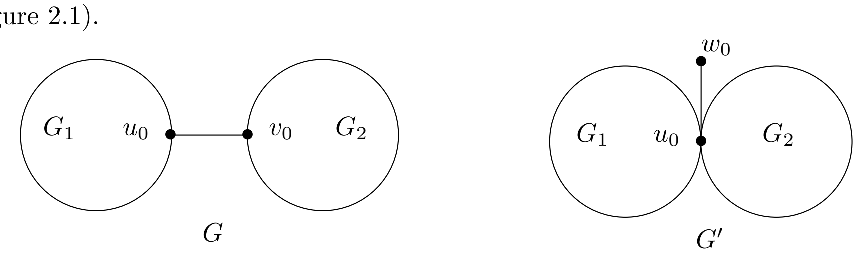


Figure 2.1 The edge-lifting transformation

Lemma 2.1 ([4,12]) *Let G' be the edge-lifting transformation of G. Then $J(G) < J(G')$, and $SJ(G) < SJ(G')$.*

A rooted graph has one of its vertices, called the root, distinguished from the others. If T is a rooted star, then the root is its center.

Let $T_1, T_2, \ldots, T_k$ be k rooted trees with $|V(T_i)| \geq 2$ $(1 \leq i \leq k)$ and roots $u_1, u_2, \ldots, u_k$, respectively. Let C_r be a cycle with length r $(r \geq 3)$.

Let $\mathbb{U}_n$ be the set of all unicyclic graphs on n vertices, $G(n, r, k)$ be a unicyclic graph on n vertices obtained from $C_r, T_1, T_2, \ldots, T_k$ by attaching k rooted trees $T_1, T_2, \ldots, T_k$ to k distinct vertices of the cycle C_r. Let $\mathbb{G}^*(n, r, k)$ be the set of all unicyclic graphs on n vertices obtained from C_r by attaching k rooted stars to k distinct vertices of C_r (see Figure 2.2).

For any $G(n,r,k) \in \mathbb{U}_n$, by repeating edge-lifting transformations on $G(n,r,k)$, we will get a unicyclic graph $G^*(n,r,k) \in \mathbb{G}^*(n,r,k)$ from $G(n,r,k)$. By Lemma 2.1, we have $J(G(n,r,k)) < J(G^*(n,r,k))$ and $SJ(G(n,r,k)) < SJ(G^*(n,r,k))$.

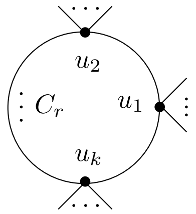
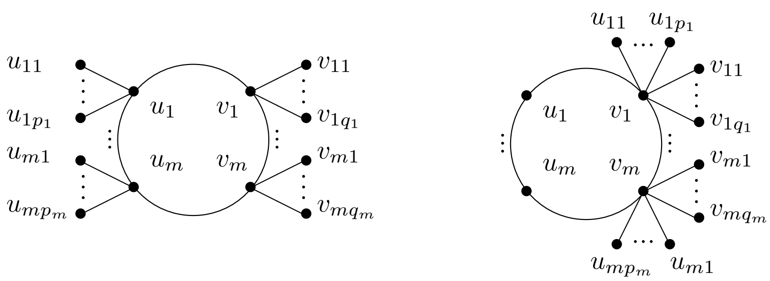


Figure 2.2 $\mathbb{G}^*(n,r,k)$

2.2. Branch transformation

Branch transformation ([6]) Let $G = G^*(n,r,k) \in \mathbb{G}^*(n,r,k)$ and $m = \lfloor \frac{r}{2} \rfloor$. Define $C_r = v_1v_2 \cdots v_m u_m \cdots u_2u_1v_1$ for even r and $C_r = v_1v_2 \cdots v_m v_{m+1} u_m \cdots u_2u_1v_1$ for odd r. Then G' is obtained from G by deleting the pendent edge u_iw and adding the pendent edge v_iw for any $i \in \{1, 2, \ldots, m\}$ (if there exists the pendent edge u_iw), where $w \in V(G)\backslash V(C_r)$. We say G' is obtained from G by branch transformation (see Figure 2.3, where $p_i \geq 0$, $q_i \geq 0$ for any $i \in \{1, 2, \ldots, m\}$).



$G = G^*(n,r,k)$ for r is even $\qquad$ G'

Figure 2.3 The branch transformation

Lemma 2.2 ([6]) *Let n, r, k be positive integers with $2 \leq k \leq r$, $3 \leq r \leq n-k$, $G = G^*(n,r,k) \in \mathbb{G}^*(n,r,k)$, G' be the graph obtained from G by branch transformation. Then $J(G) < J(G')$, $SJ(G) < SJ(G')$.*

Lemma 2.3 ([6]) *Let n, r, k be positive integers with $2 \leq k \leq r$, $3 \leq r \leq n-k$, $G = G^*(n,r,k) \in \mathbb{G}^*(n,r,k)$, G' be the graph obtained from G by repeating the branch transformation, and we cannot get other graph from G' by repeating branch transformation. Then*

(i) $G' \in \mathbb{G}^*(n,r,1)$ (see Figure 2.4).

(ii) $J(G) \leq J(G')$, the equality holds if and only if $G \cong G'$.

(iii) $J(G) \leq SJ(G')$, the equality holds if and only if $G \cong G'$.

2.3. The cycle transformation

The cycle transformation Let $G = G^*(n,r,1) \in \mathbb{G}^*(n,r,1)$ be defined as in Figure 2.4, where $V(C_r) = u_1, u_2, \ldots, u_r$, and n, r be positive integers with $3 \le r \le n$.

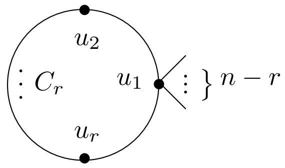


Figure 2.4 Graph $G^*(n,r,1) \in \mathbb{G}^*(n,r,1)$

(i) If $r \ge 4$ is even, then G' is the graph obtained from G by deleting the edge u_2u_3 and adding the edge u_1u_3.

(ii) If $r \ge 5$ is odd, then G' is the graph obtained from G by deleting the edges u_2u_3 and u_3u_4, and adding the edges u_1u_3 and u_1u_4.

We say G' is obtained from G by the cycle transformation (see Figure 2.5).

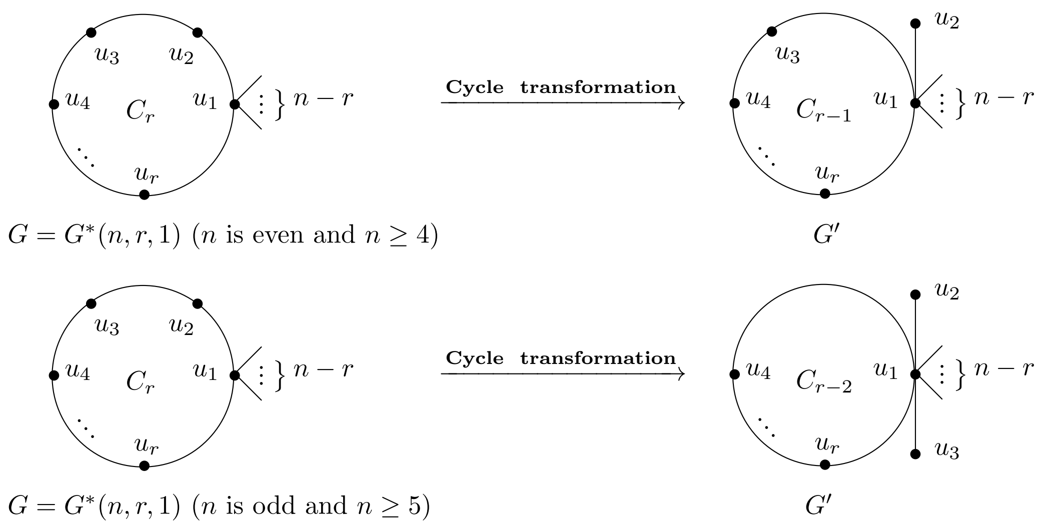


Figure 2.5 The cycle transformation

Lemma 2.4 ([7]) *Let $x, y, a \in R^+$ such that $x \ge y + a$. Then $\frac{1}{\sqrt{xy}} \ge \frac{1}{\sqrt{(x-a)(y+a)}}$, and the equality holds if and only if $x = y + a$.*

Lemma 2.5 ([6]) *Let $x_1, x_2, y_1, y_2 \in R^+$ such that $x_1 > y_1$ and $x_2 - x_1 = y_2 - y_1 > 0$. Then $\frac{1}{\sqrt{x_1}} + \frac{1}{\sqrt{y_2}} < \frac{1}{\sqrt{x_2}} + \frac{1}{\sqrt{y_1}}$.*

Lemma 2.6 ([7]) *Let $a, a', b, b', w, x, y, z \in R^+$ such that $\frac{b}{x} \ge \frac{a}{w}, \frac{b'}{y} \ge \frac{a'}{z}, w \ge x$ and $z \ge y$. Then $\frac{1}{\sqrt{(w+a)(z+a')}} + \frac{1}{\sqrt{xy}} \ge \frac{1}{\sqrt{wz}} + \frac{1}{\sqrt{(x+b)(y+b')}}$, and the equality holds if and only if $b = a, b' = a', w = x$ and $z = y$.*

Lemma 2.7 *Let $G = G^*(n,r,1) \in \mathbb{G}^*(n,r,1)$, G' be the graph obtained from G by cycle* *transformation (see Figure 2.5). Then $J(G) < J(G')$ and $SJ(G) < SJ(G')$.*

Proof Let $V(C_r) = \{u_1, u_2, \ldots, u_r\}$ and $W_{u_1} = \{w | wu_1 \in G$ and $d_G(w) = 1\}$.

Case 1 r is even.

We first consider the vertex $u_x \in V(C_r)\backslash\{u_2\}$. It is easy to see that

$$D_G(u_x) = D_G(u_x, C_r) + D_G(u_x, W_{u_1}) = [2(1+2+\cdots+\frac{r-2}{2}) + \frac{r}{2}] + (n-r)(D_G(u_x, u_1)+1),$$

$$D_{G'}(u_x) = D_{G'}(u_x, C_r) + D_{G'}(u_x, W_{u_1}) = 2(1+2+\cdots+\frac{r-2}{2}) + (n-r+1)(D_{G'}(u_x, u_1)+1).$$

Since $D_G(u_x, u_1) \geq D_{G'}(u_x, u_1)$ and $D_{G'}(u_x, u_1) + 1 < \frac{r}{2}$, where $u_x \in V(C_r)\backslash\{u_2\}$, we have

$$D_G(u_x) - D_{G'}(u_x) = \frac{r}{2} + (n-r)[D_G(u_x, u_1) - D_{G'}(u_x, u_1)] - [D_{G'}(u_x, u_1) + 1] > 0. \quad (1)$$

Next we consider u_2 and the vertices in W_{u_1}. Clearly

$$D_G(w) > D_{G'}(w), \text{ where } w \in W_{u_1}, \quad (2)$$

and

$$D_G(u_2) = 2(1+2+\cdots+\frac{r-2}{2}) + \frac{r}{2} + 2(n-r),$$
$$D_{G'}(u_2) = 2(1+2+\cdots+\frac{r-2}{2}) + (r-1) + 2(n-r),$$
$$D_G(u_1) = 2(1+2+\cdots+\frac{r-2}{2}) + \frac{r}{2} + (n-r),$$
$$D_{G'}(u_1) = 2(1+2+\cdots+\frac{r-2}{2}) + 1 + (n-r).$$

As such, we have

$$D_{G'}(u_2) - D_G(u_2) = \frac{r}{2} - 1,$$
$$D_G(u_1) - D_{G'}(u_1) = \frac{r}{2} - 1,$$
$$D_{G'}(u_2) - D_{G'}(u_1) = n - 2.$$

Let $x = D_{G'}(u_2)$, $y = D_{G'}(u_1)$, $a = \frac{r}{2} - 1$. Then $x - y = n - 2 > a$. By Lemma 2.4, we have

$$\frac{1}{\sqrt{D_{G'}(u_2)D_{G'}(u_1)}} > \frac{1}{\sqrt{[D_{G'}(u_2) - a][D_{G'}(u_1) + a]}} = \frac{1}{\sqrt{D_G(u_2)D_G(u_1)}}, \quad (3)$$

$$\frac{1}{\sqrt{D_{G'}(u_2) + D_{G'}(u_1)}} = \frac{1}{\sqrt{D_G(u_2) + D_G(u_1)}}. \quad (4)$$

Since $D_{G'}(u_3) < D_G(u_3)$ and $D_{G'}(u_1) < D_G(u_2)$, we have

$$\frac{1}{\sqrt{D_{G'}(u_3)D_{G'}(u_1)}} > \frac{1}{\sqrt{D_G(u_3)D_G(u_2)}}, \quad (5)$$

$$\frac{1}{\sqrt{D_{G'}(u_3) + D_{G'}(u_1)}} > \frac{1}{\sqrt{D_G(u_3) + D_G(u_2)}}. \quad (6)$$

From (1) and (2), we have

$$\frac{1}{\sqrt{D_{G'}(u_x)D_{G'}(u_y)}} > \frac{1}{\sqrt{D_G(u_x)D_G(u_y)}}, \quad (7)$$

$$\frac{1}{\sqrt{D_{G'}(u_x)+D_{G'}(u_y)}} > \frac{1}{\sqrt{D_G(u_x)+D_G(u_y)}}, \tag{8}$$

$$\frac{1}{\sqrt{D_{G'}(u_1)D_{G'}(w)}} > \frac{1}{\sqrt{D_G(u_1)D_G(w)}}, \tag{9}$$

$$\frac{1}{\sqrt{D_{G'}(u_1)+D_{G'}(w)}} > \frac{1}{\sqrt{D_G(u_1)+D_G(w)}}, \tag{10}$$

where $u_x, u_y \in V(C_r)\backslash\{u_2\}$ and $w \in W_{u_1}$.

By (3),(5), (7), (9) and the definition of Balaban index, if r is even we have $J(G) < J(G')$. By (4), (6), (8), (10) and the definition of Sum-Balaban index, if r is even we have $SJ(G) < SJ(G')$.

Case 2 r is odd.

We first consider the vertex $u_x \in V(C_r)\backslash\{u_2, u_3\}$. It is easy to see that

$$D_G(u_x) = D_G(u_x, C_r) + D_G(u_x, W_{u_1}) = 2(1+2+\cdots+\frac{r-1}{2}) + (n-r)(D_G(u_x, u_1)+1)$$

$$D_{G'}(u_x) = D_{G'}(u_x, C_r) + D_{G'}(u_x, W_{u_1}) = 2(1+2+\cdots+\frac{r-3}{2}) + (n-r+2)(D_{G'}(u_x, u_1)+1).$$

Since $D_G(u_x, u_1) \geq D_{G'}(u_x, u_1)$ and $D_{G'}(u_x, u_1) + 1 \leq \frac{r-1}{2}$, we have

$$D_G(u_x) - D_{G'}(u_x) = (r-1) + (n-r)[D_G(u_x, u_1) - D_{G'}(u_x, u_1)] - 2[D_{G'}(u_x, u_1)+1] \geq 0, \tag{11}$$

where $u_x \in V(C_r)\backslash\{u_2, u_3\}$.

Next we consider u_2, u_3 and the vertices in W_{u_1}. Clearly

$$D_G(w) > D_{G'}(w), \text{ where } w \in W_{u_1}, \tag{12}$$

and

$$\begin{aligned}
D_G(u_1) &= 2(1+2+\cdots+\frac{r-1}{2}) + (n-r),\\
D_{G'}(u_1) &= 2(1+2+\cdots+\frac{r-3}{2}) + 2 + (n-r),\\
D_G(u_2) &= 2(1+2+\cdots+\frac{r-1}{2}) + 2(n-r),\\
D_{G'}(u_2) &= D_{G'}(u_1) + (n-2) = 2(1+2+\cdots+\frac{r-3}{2}) + 2n - r,\\
D_G(u_3) &= 2(1+2+\cdots+\frac{r-1}{2}) + 3(n-r),\\
D_{G'}(u_3) &= D_{G'}(u_2) = 2(1+2+\cdots+\frac{r-3}{2}) + 2n - r.
\end{aligned}$$

Thus we have

$$D_{G'}(u_2) - D_G(u_2) = 1, \quad D_G(u_1) - D_{G'}(u_1) = r-3 \geq 2.$$

Let $x = D_{G'}(u_2), y = D_{G'}(u_1), a = 1$. Then $x - y = n-2 > a$. By Lemma 2.4, we have

$$\frac{1}{\sqrt{D_{G'}(u_2)D_{G'}(u_1)}} \geq \frac{1}{\sqrt{[D_{G'}(u_2)-1][D_{G'}(u_1)+1]}} > \frac{1}{\sqrt{D_G(u_2)D_G(u_1)}}, \tag{13}$$

$$\frac{1}{\sqrt{D_{G'}(u_2)+D_{G'}(u_1)}} > \frac{1}{\sqrt{D_G(u_2)+D_G(u_1)}}. \tag{14}$$

Note that $D_G(u_3) - D_{G'}(u_3) = (r-1) + (3n-3r) - (2n-r) = n-r-1$. If $n > r$, then $D_G(u_3) - D_{G'}(u_3) \geq 0$ and we have

$$\frac{1}{\sqrt{D_{G'}(u_3)D_{G'}(u_1)}} > \frac{1}{\sqrt{D_G(u_3)D_G(u_2)}}, \tag{15}$$

$$\frac{1}{\sqrt{D_{G'}(u_3)+D_{G'}(u_1)}} > \frac{1}{\sqrt{D_G(u_3)+D_G(u_2)}}. \tag{16}$$

If $n = r$, then $D_{G'}(u_3) - D_G(u_3) = 1$ and $D_G(u_2) - D_{G'}(u_1) = n-3 \geq 2$. Let $x = D_{G'}(u_3), y = D_{G'}(u_1), a = 1$. Then $x - y > n-2 > a$. By Lemma 2.4, we have

$$\frac{1}{\sqrt{D_{G'}(u_3)D_{G'}(u_1)}} \geq \frac{1}{\sqrt{[D_{G'}(u_2)-1][D_{G'}(u_1)+1]}} > \frac{1}{\sqrt{D_G(u_3)D_G(u_2)}}, \tag{17}$$

$$\frac{1}{\sqrt{D_{G'}(u_3)+D_{G'}(u_1)}} > \frac{1}{\sqrt{D_G(u_3)+D_G(u_2)}}. \tag{18}$$

Since $D_G(u_3) - D_{G'}(u_1) > 0$, by (11) we have

$$\frac{1}{\sqrt{D_{G'}(u_4)D_{G'}(u_1)}} > \frac{1}{\sqrt{D_G(u_4)D_G(u_3)}}, \tag{19}$$

$$\frac{1}{\sqrt{D_{G'}(u_4)+D_{G'}(u_1)}} > \frac{1}{\sqrt{D_G(u_4)+D_G(u_3)}}, \tag{20}$$

$$\frac{1}{\sqrt{D_{G'}(u_x)D_{G'}(u_y)}} \geq \frac{1}{\sqrt{D_G(u_x)D_G(u_y)}}, \tag{21}$$

$$\frac{1}{\sqrt{D_{G'}(u_x)+D_{G'}(u_y)}} \geq \frac{1}{\sqrt{D_G(u_x)+D_G(u_y)}}, \tag{22}$$

where $u_x, u_y \in V(C_r)\backslash\{u_2, u_3\}$. By (11) and (12) we have

$$\frac{1}{\sqrt{D_{G'}(u_1)D_{G'}(w)}} > \frac{1}{\sqrt{D_G(u_1)D_G(w)}}, \tag{23}$$

$$\frac{1}{\sqrt{D_{G'}(u_1)+D_{G'}(w)}} > \frac{1}{\sqrt{D_G(u_1)+D_G(w)}}, \text{ where } w \in W_{u_1}. \tag{24}$$

By (13), (15), (17), (19), (21), (23) and the definition of Balaban index, if r is odd, we have $J(G) < J(G')$.

By (14), (16), (18), (20), (22), (24) and the definition of Sam-Balaban index, if r is odd, we have $SJ(G) < SJ(G')$. □

From the above discussions, for any unicyclic graph $G \in \mathbb{U}_n$, we finally get the graph G_1 from G by the edge-lifting transformation, branch transformation, cycle transformation, or any combination of these, where G_1 is defined in Figure 2.6. By Lemmas 2.1, 2.2 and Theorem 2.7, we have

$$J(G) \leq J(G_1) \text{ and } SJ(G) \leq SJ(G_1).$$

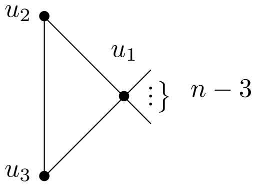


Figure 2.6 Graph G_1

Theorem 2.8 *Let G_1 be defined in Figure 2.6. Then G_1 is the unique unicyclic graph in $\mathbb{U}_n$, which attains the maximum Balaban index and Sum-Balaban index, and*

$$J(G_1)=\frac{n}{\sqrt{2n^2-6n+4}}+\frac{n}{4n-8}+\frac{n^2-3n}{2\sqrt{2n^2-5n+3}},$$
$$SJ(G_1)=\frac{n}{\sqrt{3n-5}}+\frac{n}{4\sqrt{n-2}}+\frac{n^2-3n}{2\sqrt{3n-4}}.$$

Proof It can be checked directly that

$$D_{G_1}(u_1)=n-1,\quad D_{G_1}(u_2)=D_{G_1}(u_3)=2n-4,$$
$$D_{G_1}(w)=2n-3,\ \text{where } w\in W_{u_1}.$$

Thus

$$J(G_1)=\frac{n}{2}\Big[\frac{1}{\sqrt{D_{G_1}(u_1)D_{G_1}(u_2)}}+\frac{1}{\sqrt{D_{G_1}(u_1)D_{G_1}(u_3)}}+\frac{1}{\sqrt{D_{G_1}(u_2)D_{G_1}(u_3)}}+\frac{n-3}{\sqrt{D_{G_1}(u_1)D_{G_1}(w)}}\Big]$$
$$=\frac{n}{\sqrt{2n^2-6n+4}}+\frac{n}{4n-8}+\frac{n^2-3n}{2\sqrt{2n^2-5n+3}},$$

and

$$SJ(G_1)=\frac{n}{2}\Big[\frac{1}{\sqrt{D_{G_1}(u_1)+D_{G_1}(u_2)}}+\frac{1}{\sqrt{D_{G_1}(u_1)+D_{G_1}(u_3)}}+\frac{1}{\sqrt{D_{G_1}(u_2)+D_{G_1}(u_3)}}+$$
$$\frac{n-3}{\sqrt{D_{G_1}(u_1)+D_{G_1}(w)}}\Big]=\frac{n}{\sqrt{3n-5}}+\frac{n}{4\sqrt{n-2}}+\frac{n^2-3n}{2\sqrt{3n-4}}.\ \square$$

3. The second largest Balaban index (Sum-Balaban index) of unicyclic graphs

Let $\tilde{G}$ be the set of graphs which attains the second largest Balaban index (Sum-Balaban index) of unicyclic graphs, obviously, we can obtain G_1 from G_i $(2\le i\le 6)$ by one single transformation (that is, no combination is allowed), then

$$J(\tilde{G})=\max_{2\le i\le 6}J(G_i),\quad SJ(\tilde{G})=\max_{2\le i\le 6}SJ(G_i),$$

where G_i $(2\le i\le 6)$ is defined as in Figure 3.1.

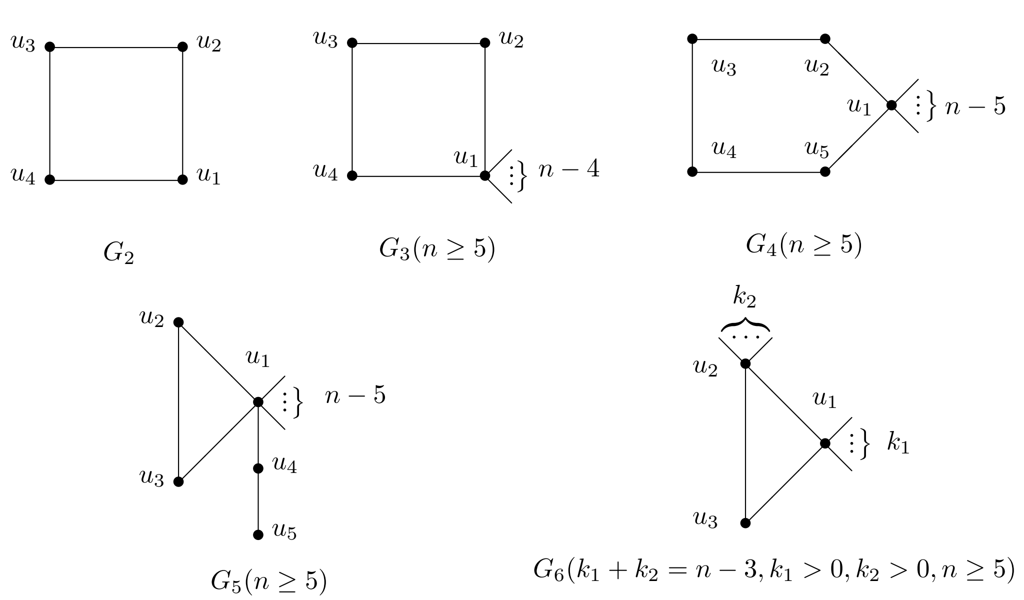


Figure 3.1 Graphs $G_i (2 \leq i \leq 6)$

The pendent edge transformation Let $G = G_6 \in \mathbb{U}_n$, $V(C_3) = \{u_1, u_2, u_3\}$ and $W_{u_1} = \{w | wu_1 \in E(G)$ and $\deg(w) = 1\}$, $|W_{u_1}| = k_1$, $W_{u_2} = \{w | wu_2 \in E(G)$ and $\deg(w) = 1\}$, $|W_{u_2}| = k_2$, where $k_1 > 0, k_2 > 0$ and $k_1 + k_2 + 3 = n$. Without loss of generality, let $k_1 \geq k_2 > 0$. G' is the graph obtained from G by deleting the edge u_2u_4 and adding the edge u_1u_4. We say that G' is obtained from G by the pendent edge transformation (see Figure 3.2).

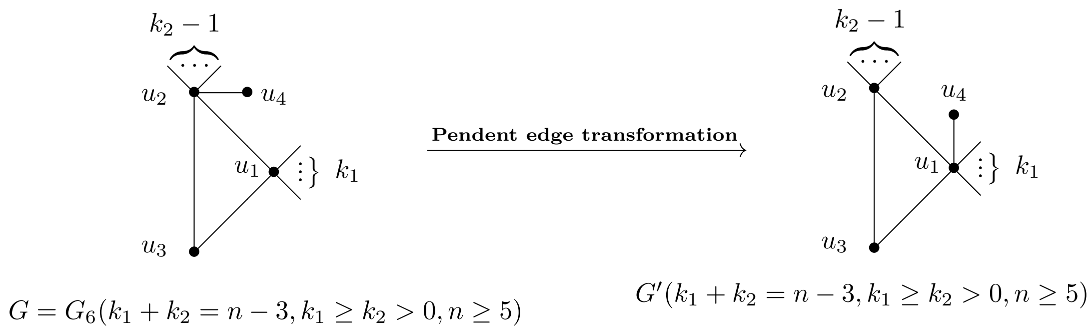


Figure 3.2 The pendent edge transformation on G_6

Theorem 3.1 *Let $G = G_6$ be defined as in Figure 3.2, where $k_1 \geq k_2 > 0$, $k_1 + k_2 = n - 3$ and $n \geq 5$. Let G' be obtained from G by the pendent edge transformation. Then $J(G) < J(G')$ and $SJ(G) < SJ(G')$.*

Proof It is easy to see that

$$D_G(u_1) = D_{G'}(u_1) + 1 = k_1 + 2k_2 + 2,$$
$$D_G(u_2) = D_{G'}(u_2) - 1 = 2k_1 + k_2 + 2 \geq D_G(u_1) \quad (\text{since } k_1 \geq k_2),$$

$$D_G(u_3) = D_{G'}(u_3) = 2k_1 + 2k_2 + 2,$$
$$D_G(u_x) = D_{G'}(u_x) + 1 = 2k_1 + 3k_2 + 3, \quad u_x \in W_{u_1},$$
$$D_G(u_y) = D_{G'}(u_y) - 1 = 3k_1 + 2k_2 + 3, \quad u_y \in W_{u_2}.$$

(i) For the edge $u_1u_2 \in E(G)$.

Let $x = D_{G'}(u_2)$, $y = D_{G'}(u_1)$ and $a = 1$. Then $x - y = k_1 - k_2 + 2 > a$ (since $k_1 \geq k_2$). By Lemma 2.4 we have

$$\frac{1}{\sqrt{D_{G'}(u_2)D_{G'}(u_1)}} \geq \frac{1}{\sqrt{[D_{G'}(u_2)-1][D_{G'}(u_1)+1]}} = \frac{1}{\sqrt{D_G(u_2)D_G(u_1)}} \tag{25}$$

$$\frac{1}{\sqrt{D_{G'}(u_2)+D_{G'}(u_1)}} = \frac{1}{\sqrt{D_G(u_2)+D_G(u_1)}}. \tag{26}$$

(ii) For the edges $u_1u_3, u_2u_3 \in E(G)$.

Let $x_2 = D_{G'}(u_2)$, $x_1 = D_G(u_2)$, $y_2 = D_G(u_1)$, and $y_1 = D_{G'}(u_1)$. Then $x_2 - x_1 = y_2 - y_1 = 1$. By Lemma 2.5 we have

$$\frac{1}{\sqrt{D_G(u_2)}} + \frac{1}{\sqrt{D_G(u_1)}} < \frac{1}{\sqrt{D_{G'}(u_2)}} + \frac{1}{\sqrt{D_{G'}(u_1)}}.$$

From $D_G(u_3) = D_{G'}(u_3)$, it follows

$$\frac{1}{\sqrt{D_G(u_2)D_G(u_3)}} + \frac{1}{\sqrt{D_G(u_1)D_G(u_3)}} < \frac{1}{\sqrt{D_{G'}(u_2)D_{G'}(u_3)}} + \frac{1}{\sqrt{D_{G'}(u_1)D_{G'}(u_3)}}. \tag{27}$$

Let $x_2 = D_{G'}(u_2) + D_{G'}(u_3)$, $x_1 = D_G(u_2) + D_G(u_3)$, $y_2 = D_G(u_1) + D_G(u_3)$, and $y_1 = D_{G'}(u_1) + D_{G'}(u_3)$. Then $x_2 - x_1 = y_2 - y_1 = 1 > 0$. By Lemma 2.5 we have

$$\begin{aligned}&\frac{1}{\sqrt{D_G(u_2)+D_G(u_3)}} + \frac{1}{\sqrt{D_G(u_1)+D_G(u_3)}}\\ &< \frac{1}{\sqrt{D_{G'}(u_2)+D_{G'}(u_3)}} + \frac{1}{\sqrt{D_{G'}(u_1)+D_{G'}(u_3)}}.\end{aligned} \tag{28}$$

(iii) For the edges $u_1u_x, u_2u_y \in E(G)$, where $u_x \in W_{u_1}$ and $u_y \in W_{u_2}$.

Let $w = D_G(u_y)$, $x = D_{G'}(u_x)$, $z = D_G(u_2)$, $y = D_{G'}(u_1)$ and $a = a' = b = b' = 1$. Then $w \geq x$, $z \geq y$. By Lemma 2.6 we have

$$\begin{aligned}&\frac{1}{\sqrt{D_G(u_y)D_G(u_2)}} + \frac{1}{\sqrt{(D_{G'}(u_x)+1)(D_{G'}(u_1)+1)}}\\ &\leq \frac{1}{\sqrt{(D_G(u_y)+1)(D_G(u_2)+1)}} + \frac{1}{\sqrt{D_{G'}(u_x)D_{G'}(u_1)}}\end{aligned}$$

and thus

$$\frac{1}{\sqrt{D_G(u_y)D_G(u_2)}} + \frac{1}{\sqrt{D_G(u_x)D_G(u_1)}} \leq \frac{1}{\sqrt{D_{G'}(u_y)D_{G'}(u_2)}} + \frac{1}{\sqrt{D_{G'}(u_x)D_{G'}(u_1)}}. \tag{29}$$

Let $x_2 = D_{G'}(u_y) + D_{G'}(u_2)$, $x_1 = D_G(u_y) + D_G(u_2)$, $y_2 = D_G(u_1) + D_G(u_x)$, and $y_1 = D_{G'}(u_1) + D_{G'}(u_x)$. Then $x_2 - x_1 = y_2 - y_1 = 2 > 0$. By Lemma 2.5 we have

$$\frac{1}{\sqrt{D_G(u_y)+D_G(u_2)}} + \frac{1}{\sqrt{D_G(u_1)+D_G(u_x)}}$$

$$< \frac{1}{\sqrt{D_{G'}(u_y)+D_{G'}(u_2)}} + \frac{1}{\sqrt{D_{G'}(u_1)+D_{G'}(u_x)}}. \tag{30}$$

(iv) For the edge $u_2u_4 \in E(G)$.

Since $D_G(u_2) - D'_G(u_1) = k_1 - k_2 + 1 > 0$ and $D_G(u_4) - D'_G(u_4) = k_1 + k_2 + 1 > 0$, we have

$$\frac{1}{\sqrt{D_G(u_2)D_G(u_4)}} < \frac{1}{\sqrt{D_{G'}(u_1)D_{G'}(u_4)}}, \tag{31}$$

$$\frac{1}{\sqrt{D_G(u_2)+D_G(u_4)}} < \frac{1}{\sqrt{D_{G'}(u_1)+D_{G'}(u_4)}}. \tag{32}$$

(v) For the edges $u_1u_x \in E(G)$, where $u_x \in W_{u_1}$.

Since $D_G(u_1) > D_{G'}(u_1)$ and $D_G(u_x) > D_{G'}(u_x)$, we have

$$\frac{1}{\sqrt{D_G(u_1)D_G(u_x)}} < \frac{1}{\sqrt{D_{G'}(u_1)D_{G'}(u_x)}}, \tag{33}$$

$$\frac{1}{\sqrt{D_G(u_1)+D_G(u_x)}} < \frac{1}{\sqrt{D_{G'}(u_1)+D_{G'}(u_x)}}. \tag{34}$$

By (25), (27), (29), (31), (33) and the definition of Balaban index, we have $J(G) < J(G')$.

By (26), (28), (30), (32), (34) and the definition of Sum-Balaban index, we have $SJ(G) < SJ(G')$. □

We will get G_7 from G_6 by repeating pendent edge transformations. From Theorem 3.1 we have $J(G_6) \le J(G_7)$ and $SJ(G_6) \le SJ(G_7)$, where G_7 is defined as in Figure 3.3.

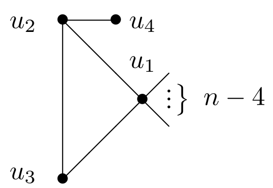


Figure 3.3 Graph G_7

Theorem 3.2 *Let G_i $(2 \le i \le 7)$ be defined as in Figures 3.2 and 3.3.*

(i) If $n = 4$, then G_2 is the unique graph in $\mathbb{U}_n$ which attains the second largest Balaban index and Sum-Balaban index, and $J(G_2) = 2$, $SJ(G_2) = 2\sqrt{2}$.

(ii) If $n \ge 5$, then G_7 is the unique graph in $\mathbb{U}_n$ which attains the second largest Balaban index and Sum-Balaban index, and

$$J(G_7) = \frac{n}{2}\Big[\frac{1}{\sqrt{n(2n-5)}} + \frac{1}{\sqrt{n(2n-4)}} + \frac{1}{\sqrt{(2n-5)(2n-4)}} + \frac{1}{\sqrt{(2n-5)(3n-7)}} + \frac{n-4}{\sqrt{n(2n-2)}}\Big],$$

$$SJ(G_7) = \frac{n}{2}\Big(\frac{1}{\sqrt{3n-5}} + \frac{1}{\sqrt{3n-4}} + \frac{1}{\sqrt{4n-9}} + \frac{1}{\sqrt{5n-12}} + \frac{n-4}{\sqrt{3n-2}}\Big).$$

Proof It can be directly checked that

$$J(G_2) = \frac{n}{2}\Big(\frac{4}{\sqrt{4\cdot 4}}\Big) = \frac{n}{2},$$

$$SJ(G_2)=\frac{n}{2}(\frac{4}{\sqrt{4+4}})=\frac{\sqrt{2}}{2}n,$$

$$J(G_3)=\frac{n}{2}[\frac{2}{\sqrt{(3n-8)(2n-4)}}+\frac{2}{\sqrt{n(2n-4)}}+\frac{n-4}{\sqrt{n(2n-2)}}],$$

$$SJ(G_3)=\frac{n}{2}(\frac{2}{\sqrt{5n-12}}+\frac{2}{\sqrt{3n-4}}+\frac{n-4}{\sqrt{3n-2}}),$$

$$J(G_4)=\frac{n}{2}[\frac{2}{\sqrt{(2n-4)(n+1)}}+\frac{2}{\sqrt{(2n-4)(3n-9)}}+\frac{1}{3n-9}+\frac{n-5}{\sqrt{(2n-1)(n+1)}}],$$

$$SJ(G_4)=\frac{n}{2}(\frac{2}{\sqrt{3n-3}}+\frac{2}{\sqrt{5n-13}}+\frac{1}{\sqrt{6n-18}}+\frac{n-5}{\sqrt{3n}}),$$

$$J(G_5)=\frac{n}{2}[\frac{2}{\sqrt{n(2n-3)}}+\frac{1}{2n-3}+\frac{1}{\sqrt{n(2n-4)}}+\frac{1}{\sqrt{(2n-4)(3n-6)}}+\frac{n-5}{\sqrt{n(2n-2)}}],$$

$$SJ(G_5)=\frac{n}{2}(\frac{2}{\sqrt{3n-3}}+\frac{1}{\sqrt{4n-6}}+\frac{1}{\sqrt{3n-4}}+\frac{1}{\sqrt{5n-10}}+\frac{n-5}{\sqrt{3n-2}}),$$

$$J(G_7)=\frac{n}{2}[\frac{1}{\sqrt{n(2n-5)}}+\frac{1}{\sqrt{n(2n-4)}}+\frac{1}{\sqrt{(2n-5)(2n-4)}}+\frac{1}{\sqrt{(2n-5)(3n-7)}}+\frac{n-4}{\sqrt{n(2n-2)}}],$$

$$SJ(G_7)=\frac{n}{2}(\frac{1}{\sqrt{3n-5}}+\frac{1}{\sqrt{3n-4}}+\frac{1}{\sqrt{4n-9}}+\frac{1}{\sqrt{5n-12}}+\frac{n-4}{\sqrt{3n-2}}).$$

So the case $n=4$ is clear.

If $n\geq 5$, we have

$$\begin{aligned}J(G_7)-J(G_3)=&\frac{n}{2}[(\frac{1}{\sqrt{n(2n-5)}}-\frac{1}{\sqrt{n(2n-4)}})+(\frac{1}{\sqrt{(2n-5)(2n-4)}}-\frac{1}{\sqrt{(3n-8)(2n-4)}})\\&(\frac{1}{\sqrt{(3n-7)(2n-5)}}-\frac{1}{\sqrt{(3n-8)(2n-4)}})]\\&>\frac{n}{2}(\frac{1}{\sqrt{(3n-7)(2n-5)}}-\frac{1}{\sqrt{(3n-8)(2n-4)}})>0\ \ \text{(by Lemma 2.2)}\end{aligned}$$

and

$$SJ(G_7)-SJ(G_3)=\frac{n}{2}[(\frac{1}{\sqrt{3n-5}}-\frac{1}{\sqrt{3n-4}})+(\frac{1}{\sqrt{4n-9}}-\frac{1}{\sqrt{5n-12}})]>0.$$

Therefore $J(G_7)>J(G_3)$ and $SJ(G_7)>SJ(G_3)$. It can be proved in a similar way that if $n\geq 5$, $J(G_7)>J(G_i)$ and $SJ(G_7)>SJ(G_i)$ for all $3\leq i\leq 6$. Hence

$$\begin{aligned}\max_{3\leq i\leq 7}J(G_i)=J(G_7)=&\frac{n}{2}[\frac{1}{\sqrt{n(2n-5)}}+\frac{1}{\sqrt{n(2n-4)}}+\frac{1}{\sqrt{(2n-5)(2n-4)}}+\\&\frac{1}{\sqrt{(2n-5)(3n-7)}}+\frac{n-4}{\sqrt{n(2n-2)}}],\end{aligned}$$

$$\max_{3\leq i\leq 7}SJ(G_i)=SJ(G_7)=\frac{n}{2}(\frac{1}{\sqrt{3n-5}}+\frac{1}{\sqrt{3n-4}}+\frac{1}{\sqrt{4n-9}}+\frac{1}{\sqrt{5n-12}}+\frac{n-4}{\sqrt{3n-2}}).$$

The theorem now holds. □

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