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Maximum Balaban Index and Sum–Balaban Index of Bicyclic Graphs[*]

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Abstract

In [Z. Chen, M. Dehmer, Y. Shi, H. Yang, Sharp upper bounds for the Balaban index of bicyclic graphs, MATCH Communications in Mathematical and in Computer Chemistry, 75 (2016) 105–128.], the authors gave sharp upper bounds on Balaban index and sum–Balaban index for bicyclic graphs. We find that there are some flaws in this paper, and that there exists bicyclic graphs which having greater Balaban index and sum–Balaban index than what are claimed by Chen at al. In this paper, we amend the upper bounds of Balaban index and sum–Balaban index for bicyclic graphs, and characterize the bicyclic graphs which attain the new bounds.

1 Introduction

Let G be a simple and connected graph with $|V(G)| = n$ and $|E(G)| = m$. Let $N_G(u)$ be the neighbor vertex set of vertex u. Then $d_G(u) = |N_G(u)|$ is called the

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degree of u. The distance between vertices u and v in G is denoted by $d_G(u,v)$, and $D_G(u) = \sum_{v \in V(G)} d_G(u,v)$ is the distance sum of vertex u in G.

Let G be a graph and $\emptyset \neq U \subseteq V(G)$. The subgraph with vertex set U and edge set consisting of those pairs of vertices that are edges in G is called the induced subgraph of G, denoted by $G[U]$. For any vertex $v \in V(G)$, we define $D_G(v,U) = \sum_{u \in U} d_G(v,u)$.

The cyclomatic number μ of G is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph. It is known that $\mu = \mid E(G) \mid - \mid V(G) \mid + 1 = m - n + 1$.

The Balaban index of a simple connected graph G is defined as

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

It was proposed by Balaban in [1, 2], which is also called the average distance–sum connectivity or J index. It appears to be a very useful molecular descriptor with attractive properties. In 2010, Balaban et al. [3] also proposed the sum–Balaban index $SJ(G)$ of a connected graph G, which is defined as

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

Balaban index and sum–Balaban index were used in various quantitative structure-property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies. It has been shown that Balaban index has a strong correlation with the chemical properties of the chemical compound and other topological indices octanes. Mathematical properties of Balaban index and sum–Balaban index can be found in [3–13].

A bicyclic graph G is a connected simple graph which satisfies $|E(G)| = |V(G)|+1$. There are two basic bicyclic graphs: ∞-graph and θ-graph. More concisely, an ∞-graph, denoted by $\infty(p,q,l)$, is obtained from two vertex-disjoint cycles C_p and C_q by connecting one vertex of C_p and one vertex of C_q with a path P_l of length $l-1$ (in the case of $l=1$, identifying the above two vertices); and a θ-graph, denoted by $\theta(p,q,l)$, is a union of three internally disjoint paths $P_{p+1}, P_{q+1}, P_{l+1}$ of length p, q, l respectively with common end vertices, where $p, q, l \geq 1$ and at most one of them is

1. Observe that any bicyclic graph G is obtained from an ∞-graph or a θ-graph G_0 (possibly) by attaching trees to some of its vertices. We call G_0 the kernel of G.

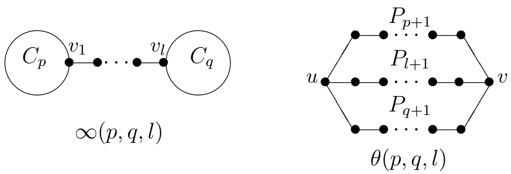

Figure 1.1 ∞-graph and θ-graph

In the recent paper [3], sharp upper bounds for Balaban and sum–Balaban indices were given for bicyclic graphs. We find that there are some flaws in this paper, and that there exists the bicyclic graph which has the bigger Balaban index and sum–Balaban index than earlier claimed.

In this paper, we amend the upper bounds for the Balaban and sum–Balaban indices for bicyclic graphs, and characterize the bicyclic graphs which attain the new bounds. In Section 2, we introduce some useful graph transformations, and research the changes of Balaban index and sum–Balaban index of a bicyclic graph after these transformations. In Section 3, we obtain upper bounds for Balaban index and sum–Balaban index for bicyclic graphs, which are better than the upper bounds of [3], and characterize the bicyclic graphs which attain the bounds. In Section 4, we give some examples to show that there are flaws in the paper [3].

2 Some useful graph transformations

In this section, we introduce some useful graph transformations.

2.1 Edge–lifting transformation ([4, 5])

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).

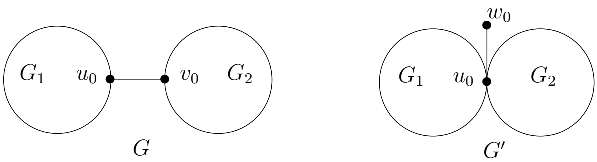

Figure 2.1 The edge–lifting transformation

Lemma 2.1 ([4,5]). *Let G' be the edge–lifting transformation of G. Then $J(G) < J(G')$, and $SJ(G) < SJ(G')$.*

Denote $\mathcal{B}_n$ by the set of all bicyclic graphs of order n. By Lemma 2.1, we can verify that if $B \in \mathcal{B}_n$ attains the maximum Balaban index and sum–Balaban index of all graphs in $\mathcal{B}_n$, then the following two conditions hold.

(C1) The kernel B_0 of B is $\infty(p, q, 1)$ or $\theta(p, q, l)$;

(C2) The graph B is obtained from B_0 by attaching some pendant edges.

Let n, p, q, t be positive integers with $1 \le t < p$, $1 \le t < q$ and $p + q - t \le n$. Let $B(p, q, t)$ be a digraph of order $p + q - t$ as in Figure 2.2, and $\hat{B}(p, q, t)$ be a digraph of order n obtained from $B(p, q, t)$ by attaching $n - p - q + t$ pendant edges to its vertices. It is clear that $\hat{B}(p, q, t) \in \mathcal{B}_n$.

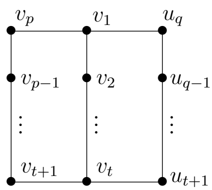

Figure 2.2 Graph $B(p, q, t)$

Let n, p, q, t be positive integers. Denote $\hat{\mathcal{B}}_n = \{\hat{B}(p, q, t) \mid p + q - t \le n, 1 \le t \le \frac{p}{2} + 1, 1 \le t \le \frac{q}{2} + 1\}$. In order to determine the bicyclic graph which attains the maximum Balaban index and maximum sum–Balaban index of all graphs in $\mathcal{B}_n$, we just need to discuss the graphs $\hat{B}(p, q, t)$ in $\hat{\mathcal{B}}_n$.

In the following, we define three new graph transformations.

2.2 Cycle transformation

Let $\hat{B}(p,q,t) \in \hat{\mathcal{B}}_n$, where $W_{v_i} = \{w \mid wv_i \in E(\hat{B}(p,q,t)) \text{ and } d_{\hat{B}(p,q,t)}(w) = 1\}$ and $|W_{v_i}| = k_i$ for $1 \le i \le p$, and $W_{u_j} = \{w \mid wu_j \in E(\hat{B}(p,q,t)) \text{ and } d_{\hat{B}(p,q,t)}(w) = 1\}$ and $|W_{u_j}| = l_j$ for $t+1 \le j \le q$. If p is even and $p \ge 4$, then $\hat{B}'(p,q,t)$ is the graph obtained from $\hat{B}(p,q,t)$ by deleting the edge v_pv_{p-1} and all pendent vertices of v_p, meanwhile, adding the edge v_1v_{p-1} and k_{p-1} pendent edges to v_1. If p is odd and $p \ge 5$, then $\hat{B}'(p,q,t)$ is the graph obtained from $\hat{B}(p,q,t)$ by deleting the edge $v_pv_{p-1}, v_{p-1}v_{p-2}$ and all pendent edges of v_p, v_{p-1}, meanwhile, adding the edge v_1v_{p-1} and $k_p + k_{p-1}$ pendent edges to v_1.

We say that $\hat{B}'(p,q,t)$ is obtained from $\hat{B}(p,q,t)$ by the cycle transformation (see Figure 2.3).

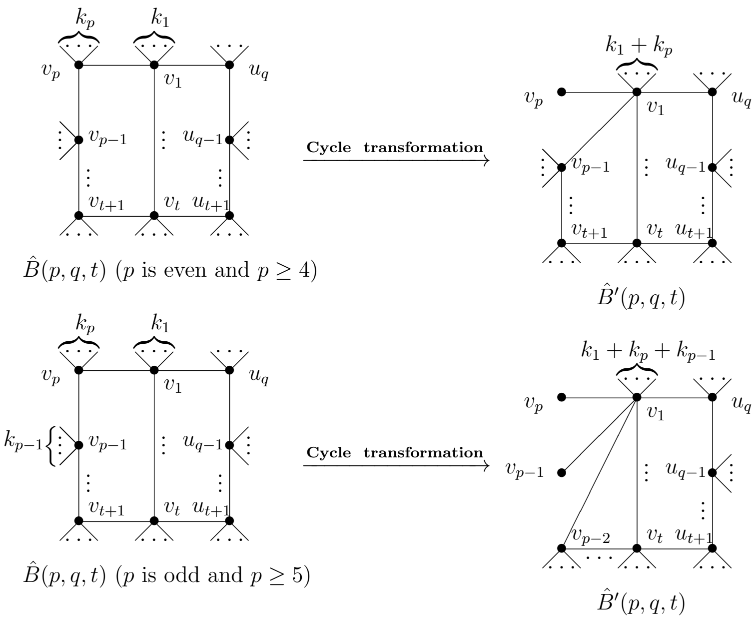

Figure 2.3 The cycle transformation

Lemma 2.2 ([7]). *Let $x, y, a \in R^+$ such that $x \geq y + a$. Then $\frac{1}{\sqrt{xy}} \geq \frac{1}{\sqrt{(x-a)(y+a)}}$, and the equality holds if and only if $x = y + a$.*

Lemma 2.3 ([11]). *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 2.4. *Let $\hat{B} = \hat{B}(p, q, t) \in \hat{\mathcal{B}}_n$ with $p \geq q$ and $p \geq 4$, and $\hat{B}' = \hat{B}'(p, q, t)$ is obtained from $\hat{B}(p, q, t)$ by the cycle transformation (see Figure 2.3). Then $J(\hat{B}) < J(\hat{B}')$.*

Proof Let $V = \{v_1, v_2, \cdots, v_p\}$, $U = \{u_{t+1}, u_{t+2}, \cdots, u_q\}$, $W_{v_i} = \{w \mid wv_i \in E(\hat{B})$ and $d_{\hat{B}}(w) = 1\}$ and $|W_{v_i}| = k_i$ for $1 \leq i \leq p$, $W_{u_j} = \{w \mid wu_j \in E(\hat{B})$ and $d_{\hat{B}}(w) = 1\}$ and $|W_{u_j}| = l_j$ for $t + 1 \leq j \leq q$.

Case 1. p is even.

We first consider the vertex $v_x \in V(\hat{B}) \setminus \{v_p\}$. It easy to see that

$$D_{\hat{B}}(v_x) = D_{\hat{B}}(v_x, V) + \sum_{i=1}^{p} D_{\hat{B}}(v_x, W_{v_i}) + D_{\hat{B}}(v_x, U) + \sum_{j=t+1}^{q} D_{\hat{B}}(v_x, W_{u_j})$$

and

$$D_{\hat{B}'}(v_x) = D_{\hat{B}'}(v_x, V) + \sum_{i=1}^{p} D_{\hat{B}'}(v_x, W_{v_i}) + D_{\hat{B}'}(v_x, U) + \sum_{j=t+1}^{q} D_{\hat{B}'}(v_x, W_{u_j}).$$

From the operation of cycle transformation, note that $\hat{B}[U \cup W_{u_j}] \cong \hat{B}'[U \cup W_{u_j}]$ and $d_{\hat{B}}(v_x, u_j) \geq d_{\hat{B}'}(v_x, u_j)$. Thus, $D_{\hat{B}}(v_x, W_{u_j}) \geq D_{\hat{B}'}(v_x, W_{u_j})$, where $v_x \in V(\hat{B}) \setminus \{v_p\}, t + 1 \leq j \leq q$. Then for any vertex $v_x \in V(\hat{B}) \setminus \{v_p\}$,

$$D_{\hat{B}}(v_x, U) \geq D_{\hat{B}'}(v_x, U), \quad \sum_{j=t+1}^{q} D_{\hat{B}}(v_x, W_{u_j}) \geq \sum_{j=t+1}^{q} D_{\hat{B}'}(v_x, W_{u_j}).$$

Meanwhile, for any vertex $v_x \in V(\hat{B}) \setminus \{v_p\}, 1 \leq i \leq p$,

$$D_{\hat{B}}(v_x, V) \geq D_{\hat{B}'}(v_x, V), \quad \sum_{i=1}^{p} D_{\hat{B}}(v_x, W_{v_i}) \geq \sum_{i=1}^{p} D_{\hat{B}'}(v_x, W_{v_i}).$$

For the vertex $v_x \in V(\hat{B}) \setminus \{v_p\}$, we have

$$D_{\hat{B}}(v_x) - D_{\hat{B}'}(v_x) = [D_{\hat{B}}(v_x, V) - D_{\hat{B}'}(v_x, V)]$$

$$+ \quad \left[\sum_{i=1}^{p} D_{\hat{B}}(v_x, W_{v_i}) - \sum_{i=1}^{p} D_{\hat{B}'}(v_x, W_{v_i})\right] + [D_{\hat{B}}(v_x, U) - D_{\hat{B}'}(v_x, U)]$$

$$+ \quad \left[\sum_{j=t+1}^{q} D_{\hat{B}}(v_x, W_{u_j}) - \sum_{j=t+1}^{q} D_{\hat{B}'}(v_x, W_{u_j})\right] \geq 0\,. \tag{1}$$

It can be checked directly that

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x)D_{\hat{B}'}(v_y)}} \geq \frac{1}{\sqrt{D_{\hat{B}}(v_x)D_{\hat{B}}(v_y)}}, \text{ where } v_x \in V(\hat{B}) \setminus \{v_p\}. \tag{2}$$

In what follows, we consider the edges on vertex v_p of $\hat{B}$: v_pv_1, $v_{p-1}v_p$, the edges on v_p to W_{v_p}.

Case 1.1. $v_pv_1 \in E(\hat{B})$.

It can be checked directly that

$$\begin{aligned} D_{\hat{B}'}(v_p, V) - D_{\hat{B}}(v_p, V) &= \left[2\left(1 + \cdots + \frac{p-2}{2}\right) + p - 1\right] \\ &- \left[2\left(1 + \cdots + \frac{p-2}{2}\right) + \frac{p}{2}\right] = \frac{p}{2} - 1 \end{aligned}$$

$$\begin{aligned} \sum_{i=1}^{p} D_{\hat{B}'}(v_p, W_{v_i}) - \sum_{i=1}^{p} D_{\hat{B}}(v_p, W_{v_i}) &= \sum_{i=1}^{p}[D_{\hat{B}'}(v_p, W_{v_i}) - D_{\hat{B}}(v_p, W_{v_i})] = \sum_{i=\frac{p+2}{2}}^{p} k_i \\ D_{\hat{B}'}(v_p, U) &= D_{\hat{B}}(v_p, U) \\ \sum_{j=t+1}^{q} D_{\hat{B}'}(v_p, W_{u_j}) &= \sum_{j=t+1}^{q} D_{\hat{B}}(v_p, W_{u_j})\,. \end{aligned}$$

Then we have

$$\begin{aligned} &D_{\hat{B}'}(v_p) - D_{\hat{B}}(v_p) \\ &= [D_{\hat{B}'}(v_p, V) - D_{\hat{B}}(v_p, V)] + [\sum_{i=1}^{p} D_{\hat{B}'}(v_p, W_{v_i}) - \sum_{i=1}^{p} D_{\hat{B}}(v_p, W_{v_i})] \\ &\quad + [D_{\hat{B}'}(v_p, U) - D_{\hat{B}}(v_p, U)] + [\sum_{j=t+1}^{q} D_{\hat{B}'}(v_p, W_{u_j}) - \sum_{j=t+1}^{q} D_{\hat{B}}(v_p, W_{u_j})] \\ &= \sum_{i=\frac{p+2}{2}}^{p} k_i + \frac{p}{2} - 1. \end{aligned}$$

Similarly, we have

$$D_{\hat{B}}(v_1) - D_{\hat{B}'}(v_1) = \sum_{i=\frac{p+2}{2}}^{p} k_i + \frac{p}{2} - 1.$$

Then we have

$$D_{\hat{B}'}(v_p) - D_{\hat{B}}(v_p) = D_{\hat{B}}(v_1) - D_{\hat{B}'}(v_1) = \sum_{i=\frac{p+2}{2}}^{p} k_i + \frac{p}{2} - 1. \tag{3}$$

Since $d_{\hat{B}'}(v_p, v_1) = 1$, we have

$$D_{\hat{B}'}(v_p) - D_{\hat{B}'}(v_1) = n - 2 > \sum_{i=\frac{p+2}{2}}^{p} k_i + \frac{p}{2} - 1 = D_{\hat{B}'}(v_p) - D_{\hat{B}}(v_p). \tag{4}$$

Let $x = D_{\hat{B}'}(v_p), y = D_{\hat{B}'}(v_1), a = \sum_{i=\frac{p+2}{2}}^{p} k_i + \frac{p}{2} - 1$. Then $x - y = n - 2 > a$. By Lemma 2.2, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_p)D_{\hat{B}'}(v_1)}} > \frac{1}{\sqrt{(D_{\hat{B}'}(v_p) - a)(D_{\hat{B}'}(v_1) + a)}} = \frac{1}{\sqrt{D_{\hat{B}}(v_p)D_{\hat{B}}(v_1)}}. \tag{5}$$

Case 1.2. $v_{p-1}v_p \in E(\hat{B})$.

By (1) and (4), we have $D_{\hat{B}'}(v_{p-1}) \leq D_{\hat{B}}(v_{p-1})$, $D_{\hat{B}'}(v_1) < D_{\hat{B}}(v_p)$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_{p-1})D_{\hat{B}'}(v_1)}} < \frac{1}{\sqrt{D_{\hat{B}}(v_{p-1})D_{\hat{B}}(v_p)}} . \tag{6}$$

Case 1.3. The edges on v_p to W_{v_p}.

By (1) and (4), we have $D_{\hat{B}}(v_p) > D_{\hat{B}'}(v_1)$, $D_{\hat{B}}(v_x) \geq D_{\hat{B}'}(v_x)$, where $v_x \in W_{v_p}$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)D_{\hat{B}'}(v_x)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_p)D_{\hat{B}}(v_x)}}, \text{ where } v_x \in W_{v_p} . \tag{7}$$

By (2), (5), (6), and (7), it can be checked directly that

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x)D_{\hat{B}'}(v_y)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_x)D_{\hat{B}}(v_y)}}, \text{ where } v_x, v_y \in V(\hat{B}) .$$

From the definition of Balaban index, if p is even, we have $J(\hat{B}') > J(\hat{B})$.

Case 2. p is odd.

We first consider the vertex $v_x \in V(\hat{B}) \setminus \{v_p, v_{p-1}\}$. From the operation of cycle transformation, noting that $\hat{B}'[U \cup W_{u_j}] \cong \hat{B}[U \cup W_{u_j}]$ and $d_{\hat{B}}(v_x, u_j) \geq d_{\hat{B}'}(v_x, u_j)$,

$D_{\hat{B}}(v_x, W_{u_j}) \geq D_{\hat{B}'}(v_x, W_{u_j})$, where $v_x \in V(\hat{B}) \setminus \{v_p, v_{p-1}\},\ t+1 \leq j \leq q$. Then for any vertex $v_x \in V(\hat{B}) \setminus \{v_p, v_{p-1}\}$, we have

$$D_{\hat{B}}(v_x, U) \geq D_{\hat{B}'}(v_x, U) \quad , \quad \sum_{j=t+1}^{q} D_{\hat{B}}(v_x, W_{u_j}) \geq \sum_{j=t+1}^{q} D_{\hat{B}'}(v_x, W_{u_j})\,.$$

Meanwhile, for any $v_x \in V(\hat{B}) \setminus \{v_p, v_{p-1}\},\ 1 \leq i \leq p$, we have

$$D_{\hat{B}}(v_x, V) \geq D_{\hat{B}'}(v_x, V), \quad \sum_{i=1}^{p} D_{\hat{B}}(v_x, W_{v_i}) \geq \sum_{i=1}^{p} D_{\hat{B}'}(v_x, W_{v_i}).$$

Then for the vertices $v_x \in V(\hat{B}) \setminus \{v_p, v_{p-1}\}$, we have

$$D_{\hat{B}}(v_x) \geq D_{\hat{B}'}(v_x)\,. \tag{8}$$

For the vertex $v_x, v_y \in V(\hat{B}) \setminus \{v_p, v_{p-1}\}$, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x) D_{\hat{B}'}(v_y)}} \geq \frac{1}{\sqrt{D_{\hat{B}}(v_x) D_{\hat{B}}(v_y)}}\,. \tag{9}$$

In what follows, we consider the edges on the vertices v_p, v_{p-1} of $\hat{B}$: $v_p v_1$, $v_{p-1} v_p$, $v_{p-2} v_{p-1}$, the edges on v_p to W_{v_p} and v_{p-1} to $W_{v_{p-1}}$.

Case 2.1. $v_p v_1 \in E(\hat{B})$.

It can be checked directly that

$$\begin{aligned}
& D_{\hat{B}'}(v_p, V) - D_{\hat{B}}(v_p, V) = 1 \\
& \sum_{i=1}^{p} D_{\hat{B}'}(v_p, W_{v_i}) - \sum_{i=1}^{p} D_{\hat{B}}(v_p, W_{v_i}) = k_p \\
& D_{\hat{B}'}(v_p, U) = D_{\hat{B}}(v_p, U) \\
& \sum_{j=t+1}^{q} D_{\hat{B}'}(v_p, W_{u_j}) = \sum_{j=t+1}^{q} D_{\hat{B}}(v_p, W_{u_j})\,.
\end{aligned}$$

Then

$$D_{\hat{B}'}(v_p) - D_{\hat{B}}(v_p) = k_p + 1\,. \tag{10}$$

Similarly, we have

$$D_{\hat{B}}(v_1, V) - D_{\hat{B}'}(v_1, V) = p - 3$$

$$D_{\hat{B}}(v_1, U) = D_{\hat{B}'}(v_1, U)$$

$$\sum_{j=t+1}^{q} D_{\hat{B}}(v_1, W_{u_j}) = \sum_{j=t+1}^{q} D_{\hat{B}'}(v_1, W_{u_j})$$

$$\sum_{i=1}^{p} D_{\hat{B}}(v_1, W_{v_i}) - \sum_{i=1}^{p} D_{\hat{B}'}(v_1, W_{v_i}) = \sum_{i=1}^{p} [D_{\hat{B}}(v_1, W_{v_i}) - D_{\hat{B}'}(v_1, W_{v_i})] \geq k_p \,.$$

Then

$$D_{\hat{B}}(v_1) - D_{\hat{B}'}(v_1) \geq k_p + p - 3 > k_p + 1 = D_{\hat{B}'}(v_p) - D_{\hat{B}}(v_p) \,. \tag{11}$$

Since $d_{\hat{B}'}(v_p, v_1) = 1$, we have

$$D_{\hat{B}'}(v_p) - D_{\hat{B}'}(v_1) = n - 2 > k_p + 1 = D_{\hat{B}'}(v_p) - D_{\hat{B}}(v_p) \,. \tag{12}$$

Let $x = D_{\hat{B}'}(v_p)$, $y = D_{\hat{B}'}(v_1)$, $a = k_p + 1$. Then $x - y = n - 2 > a$. By Lemma 2.2, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_p) D_{\hat{B}'}(v_1)}} \geq \frac{1}{\sqrt{(D_{\hat{B}'}(v_p) - a)(D_{\hat{B}'}(v_1) + a)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_p) D_{\hat{B}}(v_1)}} \,. \tag{13}$$

Case 2.2. $v_{p-1}v_p \in E(\hat{B})$.

It can be checked directly that

$$\begin{aligned} D_{\hat{B}}(v_{p-1}) - D_{\hat{B}'}(v_1) &\geq [D_{\hat{B}}(v_{p-1}, V) - D_{\hat{B}'}(v_1, V)] \\ &+ [D_{\hat{B}}(v_{p-1}, W_{v_i}) - D_{\hat{B}'}(v_1, W_{v_i})] \geq p - 3 + k_p > k_p + 1 \\ D_{\hat{B}'}(v_{p-1}) &= D_{\hat{B}'}(v_p) \,. \end{aligned}$$

By (10) and (12), we have $D_{\hat{B}'}(v_{p-1}) - D_{\hat{B}}(v_p) = D_{\hat{B}'}(v_p) - D_{\hat{B}}(v_p) = k_p + 1$ and $D_{\hat{B}}(v_p) > D_{\hat{B}'}(v_1)$. Then $D_{\hat{B}'}(v_{p-1}) > D_{\hat{B}}(v_p) > D_{\hat{B}'}(v_1)$. Let $x = D_{\hat{B}'}(v_{p-1})$, $y = D_{\hat{B}'}(v_1)$, $a = k_p + 1$. Then $x > y + a$. By Lemma 2.2, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_{p-1}) D_{\hat{B}'}(v_1)}} > \frac{1}{\sqrt{(D_{\hat{B}'}(v_{p-1}) - a)(D_{\hat{B}'}(v_1) + a)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_p) D_{\hat{B}}(v_{p-1})}} \,. \tag{14}$$

Case 2.3. $v_{p-2}v_{p-1} \in E(\hat{B})$.

It can be checked directly that $D_{\hat{B}}(v_{p-2}) \geq D_{\hat{B}'}(v_{p-2})$, $D_{\hat{B}}(v_{p-1}) > D_{\hat{B}'}(v_1)$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_{p-2}) D_{\hat{B}'}(v_1)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_{p-2}) D_{\hat{B}}(v_{p-1})}} \,. \tag{15}$$

Case 2.4. The edges on v_p to W_{v_p} and the edges on v_{p-1} to $W_{v_{p-1}}$ of $\hat{B}$.

By (8) and (12), we have $D_{\hat{B}}(v_p) > D_{\hat{B}'}(v_1)$, $D_{\hat{B}}(v_x) \geq D_{\hat{B}'}(v_x)$, where $v_x \in W_{v_p}$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)D_{\hat{B}'}(v_x)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_p)D_{\hat{B}}(v_x)}}, \text{ where } v_x \in W_{v_p}. \tag{16}$$

Since $D_{\hat{B}}(v_{p-1}) > D_{\hat{B}'}(v_1)$ and $D_{\hat{B}}(v_x) \geq D_{\hat{B}'}(v_x)$, where $v_x \in W_{v_{p-1}}$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)D_{\hat{B}'}(v_x)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_{p-1})D_{\hat{B}}(v_x)}}, \text{ where } v_x \in W_{v_{p-1}}. \tag{17}$$

By (9) and (13)–(17), it can be checked directly that

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x)D_{\hat{B}'}(v_y)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_x)D_{\hat{B}}(v_y)}}, \text{ where } v_x, v_y \in V(\hat{B})\,.$$

From the definition of Balaban index, if p is odd, we have $J(\hat{B}') > J(\hat{B})$. $\square$

Lemma 2.5. *Let $\hat{B} = \hat{B}(p,q,t) \in \hat{\mathcal{B}}_n$ with $p \geq q$ and $p \geq 4$, and $\hat{B}' = \hat{B}'(p,q,t)$ is obtained from $\hat{B}(p,q,t)$ by the cycle transformation (see Figure 2.3). Then $SJ(\hat{B}) < SJ(\hat{B}')$.*

Proof Let V, U, W_{v_i}, W_{u_j} be defined as in the proof of Lemma 2.4.

Case 1. p is even.

For the vertices $v_x, v_y \in V(\hat{B}) \setminus \{v_p\}$, by (1), we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x)+D_{\hat{B}'}(v_y)}} \geq \frac{1}{\sqrt{D_{\hat{B}}(v_x)+D_{\hat{B}}(v_y)}}, \text{where } v_x, v_y \in V(\hat{B}) \setminus \{v_p\}. \tag{18}$$

We following consider the edges on vertex v_p of $\hat{B}$: v_pv_1, $v_{p-1}v_p$, the edges on v_p to W_{v_p}.

Case 1.1. $v_pv_1 \in E(\hat{B})$.

By (3), we have $D_{\hat{B}'}(v_1) + D_{\hat{B}'}(v_p) = D_{\hat{B}}(v_1) + D_{\hat{B}}(v_p)$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_p)+D_{\hat{B}'}(v_1)}} = \frac{1}{\sqrt{D_{\hat{B}}(v_p)+D_{\hat{B}}(v_1)}}\,. \tag{19}$$

Case 1.2. $v_{p-1}v_p \in E(\hat{B})$.

By (1) and (4), we have $D_{\hat{B}'}(v_{p-1}) < D_{\hat{B}}(v_{p-1})$, $D_{\hat{B}'}(v_1) \leq D_{\hat{B}}(v_p)$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_{p-1})+D_{\hat{B}'}(v_1)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_{p-1})+D_{\hat{B}}(v_p)}}\,. \tag{20}$$

Case 1.3. The edges on v_p to W_{v_p}.

By (1) and (4), we have $D_{\hat{B}'}(v_1) \leq D_{\hat{B}}(v_p)$, $D_{\hat{B}'}(v_x) \leq D_{\hat{B}}(v_x)$, where $v_x \in W_{v_p}$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1) + D_{\hat{B}'}(v_x)}} \geq \frac{1}{\sqrt{D_{\hat{B}'}(v_p) + D_{\hat{B}'}(v_x)}}, \text{ where } v_x \in W_{v_p}\,. \tag{21}$$

By (18)–(21) and the definition of sum–Balaban index, if p is even, we have $SJ(\hat{B}') > SJ(\hat{B})$.

Case 2. p is odd ($p \geq 5$).

For the vertices $v_x, v_y \in V(\hat{B}) \setminus \{v_p, v_{p-1}\}$, by (8), we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x) + D_{\hat{B}'}(v_y)}} \geq \frac{1}{\sqrt{D_{\hat{B}}(v_x) + D_{\hat{B}}(v_y)}} \tag{22}$$

where $v_x, v_y \in V(\hat{B}) \setminus \{v_p, v_{p-1}\}$.

In what follows, we consider the edges on vertices v_p, v_{p-1} of $\hat{B}$: $v_p v_1$, $v_{p-1}v_p$, $v_{p-2}v_{p-1}$, the edges on v_p to W_{v_p} and v_{p-1} to $W_{v_{p-1}}$.

Case 2.1. $v_p v_1 \in E(\hat{B})$.

By (11), we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_p) + D_{\hat{B}'}(v_1)}} \geq \frac{1}{\sqrt{D_{\hat{B}}(v_p) + D_{\hat{B}}(v_1)}}\,. \tag{23}$$

Case 2.2. $v_{p-1}v_p \in E(\hat{B})$.

It can be checked directly that $D_{\hat{B}}(v_{p-1}) - D_{\hat{B}'}(v_1) > k_p + 1 = D_{\hat{B}'}(v_{p-1}) - D_{\hat{B}}(v_p)$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1) + D_{\hat{B}'}(v_{p-1})}} > \frac{1}{\sqrt{D_{\hat{B}}(v_{p-1}) + D_{\hat{B}}(v_p)}}. \tag{24}$$

Case 2.3. $v_{p-2}v_{p-1} \in E(\hat{B})$.

Since $D_{\hat{B}}(v_{p-2}) \geq D_{\hat{B}'}(v_{p-2})$ and $D_{\hat{B}}(v_{p-1}) > D_{\hat{B}'}(v_1)$, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_{p-2}) + D_{\hat{B}'}(v_1)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_{p-2}) + D_{\hat{B}}(v_{p-1})}}\,. \tag{25}$$

Case 2.4. The edges on v_p to W_{v_p} and the edges on v_{p-1} to $W_{v_{p-1}}$ of $B_{p,q}$.

By (8) and (12), we have $D_{\hat{B}}(v_p) > D_{\hat{B}'}(v_1)$, $D_{\hat{B}}(v_x) \geq D_{\hat{B}'}(v_x)$, where $v_x \in W_{v_p}$. Then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)+D_{\hat{B}'}(v_x)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_p)+D_{\hat{B}}(v_x)}}, \text{ where } v_x \in W_{v_p}. \tag{26}$$

Since $D_{\hat{B}}(v_{p-1}) > D_{\hat{B}'}(v_1)$ and $D_{\hat{B}}(v_x) \geq D_{\hat{B}'}(v_x)$, where $v_x \in W_{v_{p-1}}$, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)+D_{\hat{B}'}(v_x)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_{p-1})+D_{\hat{B}}(v_x)}}, \text{ where } v_x \in W_{v_{p-1}}. \tag{27}$$

By (22)–(27), we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x)+D_{\hat{B}'}(v_y)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_x)+D_{\hat{B}}(v_y)}}, \text{ where } v_x, v_y \in V(\hat{B}).$$

From the definition of sum–Balaban index, if p is odd, we have $SJ(\hat{B}') > SJ(\hat{B})$. $\square$

By repeating cycle transformations, for any graph $\hat{B}(p,q,t) \in \hat{\mathcal{B}}_n$, we will get $\hat{B}(3,3,1)$ (when $t=1$) and $\hat{B}(3,3,2)$ (when $t \geq 2$) from $\hat{B}(p,q,t)$, where graphs $\hat{B}(3,3,1)$ and $\hat{B}(3,3,2)$ are defined in Figure 2.4.

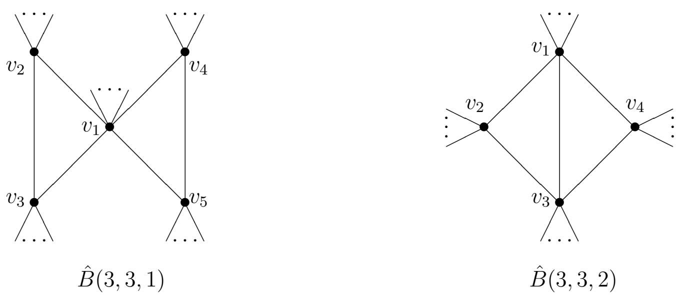

Figure 2.4 Graphs $\hat{B}(3,3,1)$ and $\hat{B}(3,3,2)$

Figure 2.5 shows an example how to obtain $\hat{B}(3,3,2)$ by repeating cycle transformations from graph $\hat{B}(7,6,5)$.

We say that $\hat{B}'(3,3,1)$ is obtained from $\hat{B}(3,3,1)$ by pendent edges transformation (see Figure 2.6).

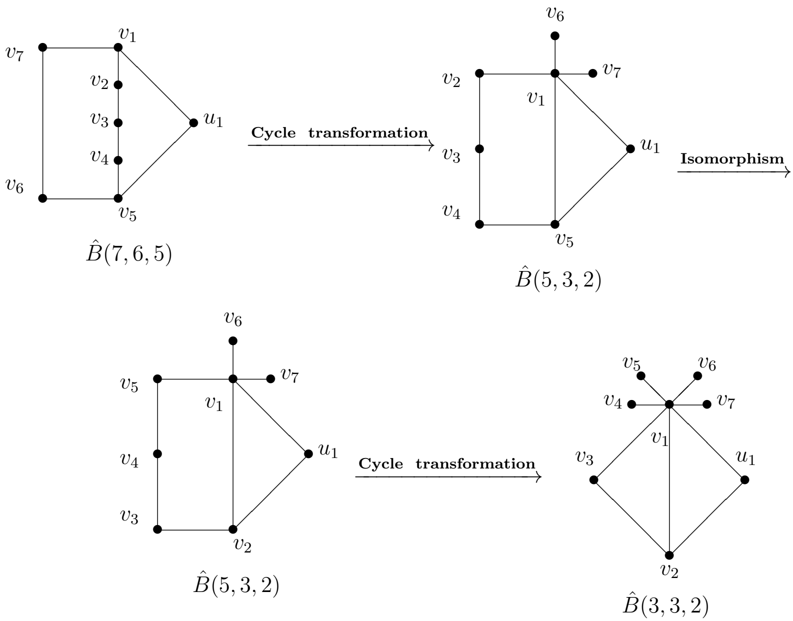

Figure 2.5 An example

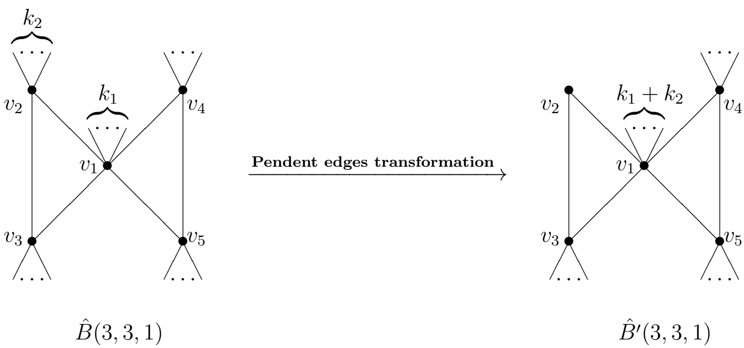

Figure 2.6 The pendent edges transformation (Choose $i = 2$)

By Lemmas 2.4 and 2.5, we now only need to consider the Balaban indices and sum–Balaban indices of the graphs $\hat{B}(3,3,1)$ and $\hat{B}(3,3,2)$.

2.3 Pendent edges transformation on $\hat{B}(3,3,1)$

Let $C_1 = v_1v_2v_3$, $C_2 = v_1v_4v_5$, $W_{v_i} = \{w \mid wv_i \in E(\hat{B}(3,3,1))$ and $d_{\hat{B}(3,3,1)}(w) = 1\}$, and $|W_{v_i}| = k_i$ for $1 \le i \le 5$. Choose any $i \in \{2,3,4,5\}$. The graph $\hat{B}'(3,3,1)$ is obtained from $\hat{B}(3,3,1)$ by deleting the pendent edges of v_i, and adding k_i pendent edges to v_1.

Lemma 2.6. *Let $\hat{B} = \hat{B}(3,3,1)$ and $\hat{B}' = \hat{B}'(3,3,1)$ be defined as Figure 2.6 and $k_2 > 0$. Then $J(\hat{B}') > J(\hat{B})$ and $SJ(\hat{B}') > SJ(\hat{B})$.*

Proof Let $V_1 = \{v_1, v_2, v_3, v_4, v_5\}$, $W_{v_i} = \{w \mid wv_i \in E(\hat{B})$ and $d_{\hat{B}}(w) = 1\}$, and $|W_{v_i}| = k_i$ for $1 \le i \le 5$.

Case 1. $v_x \in V(\hat{B})\backslash\{v_2\}$.

It can be checked directly that $D_{\hat{B}}(v_x) \ge D_{\hat{B}'}(v_x)$, then for any vertices $v_x, v_y \in V(\hat{B})\backslash\{v_2\}$, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x)D_{\hat{B}'}(v_y)}} \ge \frac{1}{\sqrt{D_{\hat{B}}(v_x)D_{\hat{B}}(v_y)}}, \text{ where } v_x, v_y \in V(\hat{B})\backslash\{v_2\} \tag{28}$$

and

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x)+D_{\hat{B}'}(v_y)}} \ge \frac{1}{\sqrt{D_{\hat{B}}(v_x)+D_{\hat{B}}(v_y)}}, \text{ where } v_x, v_y \in V(\hat{B})\backslash\{v_2\}\,. \tag{29}$$

Case 2. $v_2 \in V(\hat{B})$.

We following consider the edges on vertices v_2 of $\hat{B}$: v_1v_2, v_2v_3 and $v_2w \in E(\hat{B})$, where $w \in W_{v_2}$.

Case 2.1. $v_1v_2 \in E(\hat{B})$.

It can be checked directly that $D_{\hat{B}}(v_1) - D_{\hat{B}'}(v_1) = D_{\hat{B}'}(v_2) - D_{\hat{B}}(v_2) = k_2$ and $D_{\hat{B}'}(v_2) - D_{\hat{B}'}(v_1) > k_1 + k_2$. Let $x = D_{\hat{B}'}(v_2), y = D_{\hat{B}'}(v_1), a = k_2$. Then $x > y + a$.

By Lemma 2.2, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)D_{\hat{B}'}(v_2)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_1)D_{\hat{B}}(v_2)}} \tag{30}$$

and

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)+D_{\hat{B}'}(v_2)}} = \frac{1}{\sqrt{D_{\hat{B}}(v_1)+D_{\hat{B}}(v_2)}}\,. \tag{31}$$

Case 2.2. $v_2w \in E(\hat{B})$, where $w \in W_{v_2}$.

It can be checked directly that $D_{\hat{B}'}(v_2)-D_{\hat{B}}(v_2) = k_2$, $D_{\hat{B}'}(v_2)-D_{\hat{B}'}(v_1) > k_1+k_2$, then $D_{\hat{B}}(v_2) > D_{\hat{B}'}(v_1)$. Noting that $d_{\hat{B}}(v_2, w) = 1$, $d_{\hat{B}'}(v_1, w) = 1$, where $w \in W_{v_2}$, we have $D_{\hat{B}}(w) = D_{\hat{B}}(v_2)+n-2$, $D_{\hat{B}'}(w) = D_{\hat{B}'}(v_1)+n-2$. Then $D_{\hat{B}}(w) > D_{\hat{B}'}(w)$,

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)D_{\hat{B}'}(w)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_2)D_{\hat{B}}(w)}}, \text{ where } w \in W_{v_2} \tag{32}$$

and

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)+D_{\hat{B}'}(w)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_2)+D_{\hat{B}}(w)}}, \text{ where } w \in W_{v_2}\,. \tag{33}$$

Case 2.3. $v_2v_3 \in E(\hat{B})$ and $v_1v_3 \in E(\hat{B})$.

It can be checked directly that $D_{\hat{B}'}(v_2) - D_{\hat{B}}(v_2) = D_{\hat{B}}(v_1) - D_{\hat{B}'}(v_1) = k_2 > 0$, and $D_{\hat{B}}(v_2) > D_{\hat{B}'}(v_1)$. Let $x_2 = D_{\hat{B}'}(v_2)$, $x_1 = D_{\hat{B}}(v_2)$, $y_2 = D_{\hat{B}}(v_1)$, $y_1 = D_{\hat{B}'}(v_1)$. Then $x_2 - x_1 = y_2 - y_1 = k_2 > 0$ and $x_1 > y_1$. By Lemma 2.3, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_2)}} + \frac{1}{\sqrt{D_{\hat{B}'}(v_1)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_2)}} + \frac{1}{\sqrt{D_{\hat{B}}(v_1)}}\,.$$

Meanwhile, $D_{\hat{B}}(v_3) = D_{\hat{B}'}(v_3)$. Then

$$\begin{aligned} &\frac{1}{\sqrt{D_{\hat{B}'}(v_2)D_{\hat{B}'}(v_3)}} + \frac{1}{\sqrt{D_{\hat{B}'}(v_1)D_{\hat{B}'}(v_3)}} \\ > \quad &\frac{1}{\sqrt{D_{\hat{B}}(v_2)D_{\hat{B}}(v_3)}} + \frac{1}{\sqrt{D_{\hat{B}}(v_1)D_{\hat{B}}(v_3)}}\,. \end{aligned} \tag{34}$$

Let $x_2 = D_{\hat{B}}(v_2)+k_2+D_{\hat{B}'}(v_3)$, $x_1 = D_{\hat{B}}(v_2)+D_{\hat{B}}(v_3)$, $y_2 = D_{\hat{B}'}(v_1)+k_2+D_{\hat{B}}(v_3)$, $y_1 = D_{\hat{B}'}(v_1) + D_{\hat{B}'}(v_3)$. Then $x_2 - x_1 = y_2 - y_1 = k_2 > 0$. By Lemma 2.3, we have

$$\begin{aligned}
&\frac{1}{\sqrt{D_{\hat{B}'}(v_2)+D_{\hat{B}'}(v_3)}}+\frac{1}{\sqrt{D_{\hat{B}'}(v_1)+D_{\hat{B}'}(v_3)}}\\
>\ &\frac{1}{\sqrt{D_{\hat{B}}(v_2)+D_{\hat{B}}(v_3)}}+\frac{1}{\sqrt{D_{\hat{B}}(v_1)+D_{\hat{B}}(v_3)}}. \qquad (35)
\end{aligned}$$

By (28), (30), (32), (34), and the definition of Balaban index, we have $J(\hat{B}') > J(\hat{B})$. By (29), (31), (33), (35), and the definition of sum–Balaban index, we have $SJ(\hat{B}') > SJ(\hat{B})$. □

By repeating pendent edges transformations on $\hat{B}(3,3,1)$, we will get $\hat{B}_1(3,3,1)$ from $\hat{B}(3,3,1)$, where graph $\hat{B}_1(3,3,1)$ is defined in Figure 2.7.

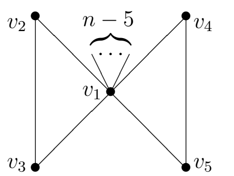

Figure 2.7 Graph $\hat{B}_1(3,3,1)$

2.4 Pendent edges transformation on $\hat{B}(3,3,2)$

Let $W_{v_i} = \{w \mid wv_i \in E(\hat{B}(3,3,2))$ and $d_{\hat{B}(3,3,2)}(w) = 1\}$, and $|W_{v_i}| = k_i$ for $1 \le i \le 4$. Choose any $i \in \{2,3,4\}$. The graph $\hat{B}'(3,3,2)$ is obtained from $\hat{B}(3,3,2)$ by deleting the pendent edges of v_i, and adding k_i pendent edges to v_1.

We say $\hat{B}'(3,3,2)$ is obtained from $\hat{B}(3,3,2)$ by pendent edges transformation (see Figure 2.8).

Lemma 2.7. *Let $\hat{B} = \hat{B}(3,3,2)$ and $\hat{B}' = \hat{B}'(3,3,2)$ be defined as Figure 2.8 and $k_2 > 0$. Then $J(\hat{B}') > J(\hat{B})$ and $SJ(\hat{B}') > SJ(\hat{B})$.*

Proof Let $V_1 = \{v_1, v_2, v_3, v_4\}$, $W_{v_i} = \{w \mid wv_i \in E(\hat{B})$ and $d_{\hat{B}}(w) = 1,\}$, and $|W_{v_i}| = k_i$ for $1 \le i \le 4$.

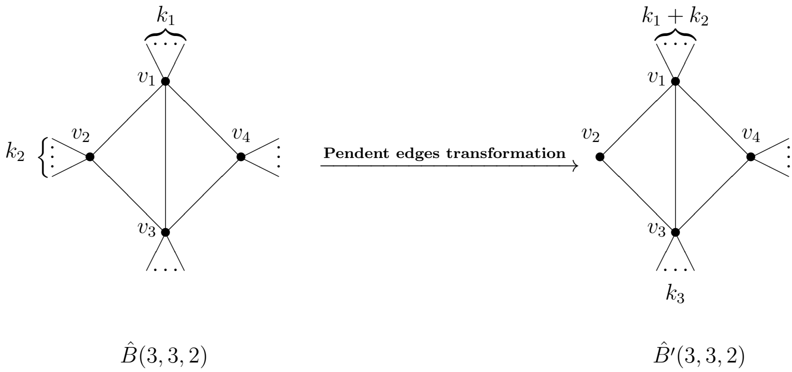

Figure 2.8 The pendent edges transformation (Choose $i = 2$)

Case 1. $v_x \in V(\hat{B})\backslash\{v_2\}$.

It can be checked directly that $D_{\hat{B}}(v_x) \geq D_{\hat{B}'}(v_x)$, then for any vertices $v_x, v_y \in V(\hat{B})\backslash\{v_2\}$, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x)D_{\hat{B}'}(v_y)}} \geq \frac{1}{\sqrt{D_{\hat{B}}(v_x)D_{\hat{B}}(v_y)}}, \text{ where } v_x, v_y \in V(\hat{B})\backslash\{v_2\}, \tag{36}$$

and

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_x)+D_{\hat{B}'}(v_y)}} \geq \frac{1}{\sqrt{D_{\hat{B}}(v_x)+D_{\hat{B}}(v_y)}}, \text{ where } v_x, v_y \in V(\hat{B})\backslash\{v_2\}\,. \tag{37}$$

Case 2. $v_2 \in V(\hat{B})$.

We following consider the edges on vertices v_2 of $\hat{B}$: v_1v_2, v_2v_3 and $v_2w \in E(\hat{B})$, where $w \in W_{v_2}$.

Case 2.1. $v_1v_2 \in E(\hat{B})$.

It can be checked directly that $D_{\hat{B}}(v_1) - D_{\hat{B}'}(v_1) = D_{\hat{B}'}(v_2) - D_{\hat{B}}(v_2) = k_2$ and $D_{\hat{B}'}(v_2) - D_{\hat{B}'}(v_1) > k_1 + k_2$. Let $x = D_{\hat{B}'}(v_2), y = D_{\hat{B}'}(v_1), a = k_2$. Then $x > y + a$. By Lemma 2.2, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)D_{\hat{B}'}(v_2)}} > \frac{1}{\sqrt{D_{\hat{B}}(v_1)D_{\hat{B}}(v_2)}} \tag{38}$$

and

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)+D_{\hat{B}'}(v_2)}}=\frac{1}{\sqrt{D_{\hat{B}}(v_1)+D_{\hat{B}}(v_2)}}. \tag{39}$$

Case 2.2. $v_2w \in E(\hat{B})$, where $w \in W_{v_2}$.

It can be checked directly that $D_{\hat{B}'}(v_2)-D_{\hat{B}}(v_2)=k_2$, $D_{\hat{B}'}(v_2)-D_{\hat{B}'}(v_1)>k_1+k_2$, then $D_{\hat{B}}(v_2)>D_{\hat{B}'}(v_1)$. Noting that $d_{\hat{B}}(v_2,w)=1$, $d_{\hat{B}'}(v_1,w)=1$, where $w \in W_{v_2}$, we have $D_{\hat{B}}(w)=D_{\hat{B}}(v_2)+n-2$, $D_{\hat{B}'}(w)=D_{\hat{B}'}(v_1)+n-2$. Then $D_{\hat{B}}(w)>D_{\hat{B}'}(w)$ and

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)D_{\hat{B}'}(w)}}>\frac{1}{\sqrt{D_{\hat{B}}(v_2)D_{\hat{B}}(w)}} \tag{40}$$

and

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_1)+D_{\hat{B}'}(w)}}>\frac{1}{\sqrt{D_{\hat{B}}(v_2)+D_{\hat{B}}(w)}}, \text{ where } w \in W_{v_2}\,. \tag{41}$$

Case 2.3. $v_2v_3 \in E(\hat{B})$ and $v_1v_3 \in E(\hat{B})$.

It can be checked directly that $D_{\hat{B}'}(v_2)-D_{\hat{B}}(v_2)=D_{\hat{B}}(v_1)-D_{\hat{B}'}(v_1)=k_2>0$, and $D_{\hat{B}}(v_2)>D_{\hat{B}'}(v_1)$. Let $x_2=D_{\hat{B}'}(v_2)$, $x_1=D_{\hat{B}}(v_2)$, $y_2=D_{\hat{B}}(v_1)$, $y_1=D_{\hat{B}'}(v_1)$. Then $x_2-x_1=y_2-y_1=k_2>0$ and $x_1>y_1$. By Lemma 2.3, we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_2)}}+\frac{1}{\sqrt{D_{\hat{B}'}(v_1)}}>\frac{1}{\sqrt{D_{\hat{B}}(v_2)}}+\frac{1}{\sqrt{D_{\hat{B}}(v_1)}}.$$

Meanwhile, $D_{\hat{B}}(v_3)=D_{\hat{B}'}(v_3)$, then

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_2)D_{\hat{B}'}(v_3)}}+\frac{1}{\sqrt{D_{\hat{B}'}(v_1)D_{\hat{B}'}(v_3)}}>\frac{1}{\sqrt{D_{\hat{B}}(v_2)D_{\hat{B}}(v_3)}}+\frac{1}{\sqrt{D_{\hat{B}}(v_1)D_{\hat{B}}(v_3)}}. \tag{42}$$

Let $x_2=D_{\hat{B}}(v_2)+k_2+D_{\hat{B}'}(v_3)$, $x_1=D_{\hat{B}}(v_2)+D_{\hat{B}}(v_3)$, $y_2=D_{\hat{B}'}(v_1)+k_2+D_{\hat{B}}(v_3)$, $y_1=D_{\hat{B}'}(v_1)+D_{\hat{B}'}(v_3)$. Then $x_2-x_1=y_2-y_1=k_2>0$ and $x_1>y_1$. By Lemma 2.3 we have

$$\frac{1}{\sqrt{D_{\hat{B}'}(v_2)+D_{\hat{B}'}(v_3)}}+\frac{1}{\sqrt{D_{\hat{B}'}(v_1)+D_{\hat{B}'}(v_3)}}$$
$$>\frac{1}{\sqrt{D_{\hat{B}}(v_2)+D_{\hat{B}}(v_3)}}+\frac{1}{\sqrt{D_{\hat{B}}(v_1)+D_{\hat{B}}(v_3)}}. \tag{43}$$

By (36), (38), (40), (41), and the definition of Balaban index, we have $J(\hat{B}')>J(\hat{B})$. By (37), (39), (41), (43), and the definition of sum–Balaban index, we have $SJ(\hat{B}')>SJ(\hat{B})$. $\square$

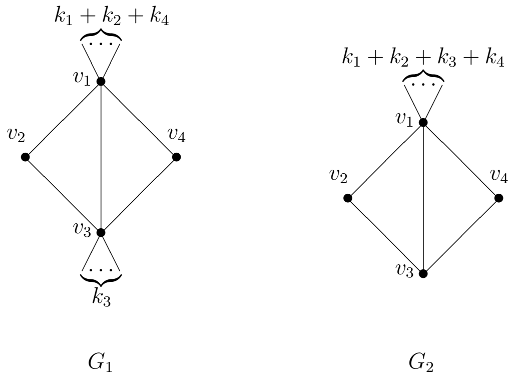

Figure 2.9 Graphs G_1 and G_2

Lemma 2.8. *Let G_1 and G_2 be defined as Figure 2.9, $k_3 > 0$ and $k_1 + k_2 + k_4 > 0$. Then $J(G_2) > J(G_1)$ and $SJ(G_2) > SJ(G_1)$.*

Proof Let $V_1 = \{v_1, v_2, v_3, v_4\}$, $W_{v_i} = \{w \mid wv_i \in E(G_1)$ and $d_{G_1}(w) = 1\}$ for $1 \leq i \leq 4$, $|W_{v_1}| = k_1 + k_2 + k_4$, $|W_{v_2}| = |W_{v_4}| = 0$, and $|W_{v_3}| = k_3$.

We first consider the vertex $v_x \in V(G_1)\backslash\{v_3\}$, secondly, we consider the vertex $v_3 \in V(G_1)$.

Case 1. $v_x \in V(G_1)\backslash\{v_3\}$.

It can be checked directly that $D_{G_2}(v_x) \geq D_{G_1}(v_x)$, then for any vertices $v_x, v_y \in V(G_1)\backslash\{v_3\}$, we have

$$\frac{1}{\sqrt{D_{G_2}(v_x)D_{G_2}(v_y)}} \geq \frac{1}{\sqrt{D_{G_1}(v_x)D_{G_1}(v_y)}}, \text{ where } v_x, v_y \in V(G_1) \tag{44}$$

and

$$\frac{1}{\sqrt{D_{G_2}(v_x) + D_{G_2}(v_y)}} \geq \frac{1}{\sqrt{D_{G_1}(v_x) + D_{G_1}(v_y)}}, \text{ where } v_x, v_y \in V(G_1). \tag{45}$$

Case 2. $v_3 \in V(G_1)$.

We following consider the edges on vertices v_3 of G_1: v_3v_1, v_3v_2, v_3v_4, and $v_3w \in E(G_1)$, where $w \in W_{v_3}$.

Case 2.1. $v_1v_3 \in E(G_1)$.

It can be checked directly that $D_{G_2}(v_3) - D_{G_1}(v_3) = D_{G_1}(v_1) - D_{G_2}(v_1) = k_3$ and $D_{G_2}(v_3) - D_{G_2}(v_1) > k_3$. Let $x = D_{G_2}(v_3), y = D_{G_2}(v_1), a = k_3$. Then $x > y + a$. By Lemma 2.2, we have

$$\frac{1}{\sqrt{D_{G_2}(v_3)D_{G_2}(v_1)}} > \frac{1}{\sqrt{D_{G_1}(v_3)D_{G_1}(v_1)}} \tag{46}$$

and

$$\frac{1}{\sqrt{D_{G_2}(v_1) + D_{G_2}(v_2)}} = \frac{1}{\sqrt{D_{G_1}(v_1) + D_{G_1}(v_2)}}. \tag{47}$$

Case 2.2. $v_2v_3, v_3v_4 \in E(G_1)$.

It can be checked directly that $D_{G_2}(v_3) - D_{G_1}(v_3) = D_{G_1}(v_1) - D_{G_2}(v_1) = k_3$. Let $x_2 = D_{G_2}(v_3)$, $x_1 = D_{G_1}(v_3)$, $y_2 = D_{G_1}(v_1)$, $y_1 = D_{G_2}(v_1)$. Then $x_2 - x_1 = y_2 - y_1 = k_3$ and $x_1 > y_1$. By Lemma 2.3, we have

$$\frac{1}{\sqrt{D_{G_2}(v_3)}} + \frac{1}{\sqrt{D_{G_2}(v_1)}} > \frac{1}{\sqrt{D_{G_1}(v_3)}} + \frac{1}{\sqrt{D_{G_1}(v_1)}}.$$

Since $D_{G_1}(v_2) = D_{G_2}(v_2)$ and $D_{G_1}(v_4) = D_{G_2}(v_4)$, we have

$$\begin{aligned} & \frac{1}{\sqrt{D_{G_2}(v_2)D_{G_2}(v_3)}} + \frac{1}{\sqrt{D_{G_2}(v_1)D_{G_2}(v_2)}} \\ > \; & \frac{1}{\sqrt{D_{G_1}(v_2)D_{G_1}(v_3)}} + \frac{1}{\sqrt{D_{G_1}(v_1)D_{G_1}(v_2)}} \end{aligned} \tag{48}$$

and

$$\begin{aligned} & \frac{1}{\sqrt{D_{G_2}(v_3)D_{G_2}(v_4)}} + \frac{1}{\sqrt{D_{G_2}(v_1)D_{G_2}(v_4)}} \\ > \; & \frac{1}{\sqrt{D_{G_1}(v_3)D_{G_1}(v_4)}} + \frac{1}{\sqrt{D_{G_1}(v_1)D_{G_1}(v_4)}}. \end{aligned} \tag{49}$$

Let $x_2 = D_{G_2}(v_3) + D_{G_2}(v_2)$, $x_1 = D_{G_1}(v_3) + D_{G_1}(v_2)$, $y_2 = D_{G_1}(v_1) + D_{G_1}(v_2)$, $y_1 = D_{G_2}(v_1) + D_{G_2}(v_2)$. Then $x_2 - x_1 = y_2 - y_1 = k_3$ and $x_1 > y_1$. By Lemma 2.3, we have

$$\begin{aligned} & \frac{1}{\sqrt{D_{G_2}(v_3) + D_{G_2}(v_2)}} + \frac{1}{\sqrt{D_{G_2}(v_1) + D_{G_2}(v_2)}} > \\ & \frac{1}{\sqrt{D_{G_1}(v_3) + D_{G_1}(v_2)}} + \frac{1}{\sqrt{D_{G_1}(v_1) + D_{G_1}(v_2)}}. \end{aligned} \tag{50}$$

Similarly, we have

$$\frac{1}{\sqrt{D_{G_2}(v_3)+D_{G_2}(v_4)}}+\frac{1}{\sqrt{D_{G_2}(v_1)+D_{G_2}(v_4)}}>$$
$$\frac{1}{\sqrt{D_{G_1}(v_3)+D_{G_1}(v_4)}}+\frac{1}{\sqrt{D_{G_1}(v_1)+D_{G_1}(v_4)}}. \tag{51}$$

Case 2.3. $v_3w \in E(G_1)$, where $w \in W_{v_3}$.

It can be checked directly that $D_{G_1}(v_3) > D_{G_2}(v_1)$ and $D_{G_1}(w) > D_{G_2}(w)$, where $w \in W_{v_3}$. Then

$$\frac{1}{\sqrt{D_{G_2}(v_1)D_{G_2}(w)}}>\frac{1}{\sqrt{D_{G_1}(v_3)D_{G_1}(w)}} \tag{52}$$

and

$$\frac{1}{\sqrt{D_{G_2}(v_1)+D_{G_2}(w)}}>\frac{1}{\sqrt{D_{G_1}(v_3)+D_{G_1}(w)}}. \tag{53}$$

By (44), (46), (48), (50), (52), and the definition of Balaban index, we have $J(G_2) > J(G_1)$. By (45), (47), (49), (51), (53), and the definition of sum–Balaban index, we have $SJ(G_2) > SJ(G_1)$. $\square$

By repeating pendent edges transformations on $\hat{B}(3,3,2)$, we will get $\hat{B}_2(3,3,2)$ from $\hat{B}(3,3,2)$, where graph $\hat{B}_2(3,3,2)$ is defined in Figure 2.10.

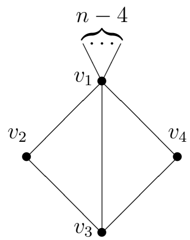

Figure 2.10 Graph $\hat{B}_2(3,3,2)$

3 Maximum Balaban index and sum–Balaban index of bicyclic graphs

From the discussions of Section 2, for any bicyclic graph $\hat{B}(p,q,t) \in \hat{\mathcal{B}}_n$, we finally get the graph $\hat{B}_1(3,3,1)$ (if $t=1$) or $\hat{B}_2(3,3,2)$ (if $t \geq 2$) from $\hat{B}(p,q,t)$ by cycle transformation, pendent edges transformation, or any combination of these, where graphs $\hat{B}_1(3,3,1)$ and $\hat{B}_2(3,3,2)$ are defined in Figures 2.7 and 2.10, respectively. By Lemmas 2.4, 2.5, 2.6, 2.7, and 2.8, we have

$$J(\hat{B}(p,q,t)) \leq \begin{cases} J(\hat{B}_1(3,3,1)), & \text{if } t=1 \\ J(\hat{B}_2(3,3,2)), & \text{if } t \geq 2 \end{cases}$$

and

$$SJ(\hat{B}(p,q,t)) \leq \begin{cases} SJ(\hat{B}_1(3,3,1)), & \text{if } t=1 \\ SJ(\hat{B}_2(3,3,2)), & \text{if } t \geq 2. \end{cases}$$

We now prove $J(\hat{B}_1(3,3,1)) < J(\hat{B}_2(3,3,2))$ and $SJ(\hat{B}_1(3,3,1)) < SJ(\hat{B}_2(3,3,2))$, that is to say, $\hat{B}_2(3,3,2)$ attains the maximum Balaban index and sum–Balaban index of all graphs in $\mathcal{B}_n$.

Lemma 3.1. *Let $\hat{B}_1 = \hat{B}_1(3,3,1)$ and $\hat{B}_2 = \hat{B}_2(3,3,2)$ be defined in Figures 2.7 and 2.10, respectively. Then $J(\hat{B}_1) < J(\hat{B}_2)$ and $SJ(\hat{B}_1) < SJ(\hat{B}_2)$.*

Proof It can be checked directly that

$$\begin{aligned}
D_{\hat{B}_2}(v_1) &= D_{\hat{B}_1}(v_1) = n-1, \\
D_{\hat{B}_2}(v_2) &= D_{\hat{B}_1}(v_2) = 6+2(n-5) = 2n-4, \\
D_{\hat{B}_2}(v_4) &= D_{\hat{B}_1}(v_4) = 6+2(n-5) = 2n-4, \\
D_{\hat{B}_2}(v_3) &= D_{\hat{B}_1}(v_3) - 1 = 2n-5, \\
D_{\hat{B}_2}(v_5) &= D_{\hat{B}_1}(v_5) + 1 = 2n-3, \\
D_{\hat{B}_2}(w) &= D_{\hat{B}_1}(w) = 2n-3, \ \text{where } w \in W_{v_1}.
\end{aligned}$$

We first consider the vertex $v_5 \in V(\hat{B}_1)$, secondly, we consider the vertex $v_x \in V(\hat{B}_1)\backslash\{v_5\}$.

Case 1. $v_5 \in V(\hat{B}_1)$.

we following consider the edges on vertex $v_5 \in V(\hat{B}_1)$: v_1v_5 and v_4v_5.

Case 1.1. $v_1v_5 \in E(\hat{B}_1)$.

For the edges v_1v_5 and v_1v_3, let $x_2 = D_{\hat{B}_2}(v_5) = 2n-3$, $x_1 = D_{\hat{B}_1}(v_3) = 2n-4$, $y_2 = D_{\hat{B}_1}(v_5) = 2n-4$, $y_1 = D_{\hat{B}_2}(v_3) = 2n-5$. Then $x_2 - x_1 = y_2 - y_1 = 1 > 0$ and $x_1 > y_1$. By Lemma 2.3, we have

$$\frac{1}{\sqrt{D_{\hat{B}_2}(v_3)}} + \frac{1}{\sqrt{D_{\hat{B}_2}(v_5)}} > \frac{1}{\sqrt{D_{\hat{B}_1}(v_3)}} + \frac{1}{\sqrt{D_{\hat{B}_1}(v_5)}}.$$

Since $D_{\hat{B}_2}(v_1) = D_{\hat{B}_1}(v_1)$, we have

$$\begin{aligned} & \frac{1}{\sqrt{D_{\hat{B}_2}(v_1)D_{\hat{B}_2}(v_3)}} + \frac{1}{\sqrt{D_{\hat{B}_2}(v_1)D_{\hat{B}_2}(v_5)}} \\ > \; & \frac{1}{\sqrt{D_{\hat{B}_1}(v_1)D_{\hat{B}_1}(v_3)}} + \frac{1}{\sqrt{D_{\hat{B}_1}(v_1)D_{\hat{B}_1}(v_5)}}. \end{aligned} \tag{54}$$

Let $x_2 = D_{\hat{B}_2}(v_5) + D_{\hat{B}_2}(v_1) = 3n-4$, $x_1 = D_{\hat{B}_1}(v_5) + D_{\hat{B}_1}(v_1) = 3n-5$, $y_2 = D_{\hat{B}_1}(v_3) + D_{\hat{B}_1}(v_1) = 3n-5$, $y_1 = D_{\hat{B}_2}(v_3) + D_{\hat{B}_2}(v_1) = 3n-6$. Then $x_2 - x_1 = y_2 - y_1 = 1 > 0$ and $x_1 > y_1$. By Lemma 2.3, we have

$$\begin{aligned} & \frac{1}{\sqrt{D_{\hat{B}_2}(v_5) + D_{\hat{B}_2}(v_1)}} + \frac{1}{\sqrt{D_{\hat{B}_2}(v_3) + D_{\hat{B}_2}(v_1)}} \\ > & \frac{1}{\sqrt{D_{\hat{B}_1}(v_5) + D_{\hat{B}_1}(v_1)}} + \frac{1}{\sqrt{D_{\hat{B}_1}(v_3) + D_{\hat{B}_1}(v_1)}}. \end{aligned} \tag{55}$$

Case 1.2. $v_4v_5 \in E(\hat{B}_1)$.

For the edge $v_4v_5 \in E(\hat{B}_1)$ and $v_3v_4 \in E(\hat{B}_2)$, $D_{\hat{B}_1}(v_4) = D_{\hat{B}_2}(v_4)$ and $D_{\hat{B}_1}(v_5) = 2n-4 < 2n-5 = D_{\hat{B}_2}(v_3)$, then

$$\frac{1}{\sqrt{D_{\hat{B}_2}(v_3)D_{\hat{B}_2}(v_4)}} > \frac{1}{\sqrt{D_{\hat{B}_1}(v_4)D_{\hat{B}_1}(v_5)}} \tag{56}$$

and

$$\frac{1}{\sqrt{D_{\hat{B}_2}(v_3) + D_{\hat{B}_2}(v_4)}} > \frac{1}{\sqrt{D_{\hat{B}_1}(v_4) + D_{\hat{B}_1}(v_5)}}. \tag{57}$$

Case 2. $v_x \in V(\hat{B}_1)\backslash\{v_5\}$.

For the vertex $v_x \in V(\hat{B}_1)\backslash\{v_5\}$, $D_{\hat{B}_2}(v_x) \le D_{\hat{B}_1}(v_x)$. Then

$$\frac{1}{\sqrt{D_{\hat{B}_2}(v_x)D_{\hat{B}_2}(v_y)}} \ge \frac{1}{\sqrt{D_{\hat{B}_1}(v_x)D_{\hat{B}_1}(v_y)}}, \text{ where } v_x, v_y \in V(\hat{B}_1)\backslash\{v_5\}, \tag{58}$$

and

$$\frac{1}{\sqrt{D_{\hat{B}_2}(v_x)+D_{\hat{B}_2}(v_y)}} \ge \frac{1}{\sqrt{D_{\hat{B}_1}(v_x)+D_{\hat{B}_1}(v_y)}}, \text{ where } v_x, v_y \in V(\hat{B}_1)\backslash\{v_5\}. \tag{59}$$

By (54), (56), (58), and the definition of Balaban index, we have $J(\hat{B}_1) < J(\hat{B}_2)$. By (55), (57), (59), and the definition of sum–Balaban index, we have $J(\hat{B}_1) < J(\hat{B}_2)$. $\square$

Theorem 3.2. *Let $\hat{B}_2 = \hat{B}_2(3,3,2)$ be defined in Figure 2.10. Then $\hat{B}_2(3,3,2)$ is the unique unicyclic graph in $\mathcal{B}_n$ which attains the maximum Balaban index and sum–Balaban index of all graphs in $\mathcal{B}_n$, and*

$$\begin{aligned} J(\hat{B}_2(3,3,2)) &= \frac{2n+2}{3\sqrt{2n^2-6n+4}} + \frac{2n+2}{3\sqrt{4n^2-18n+20}} \\ &+ \frac{n+1}{3\sqrt{2n^2-7n+5}} + \frac{n^2-3n-4}{3\sqrt{2n^2-5n+3}} \\ SJ(\hat{B}_2(3,3,2)) &= \frac{2n+2}{3\sqrt{3n-5}} + \frac{2n+2}{3\sqrt{4n-9}} + \frac{n+1}{3\sqrt{3n-6}} + \frac{n^2-3n-4}{3\sqrt{3n-4}}. \end{aligned}$$

Proof From the above discussions, we have that $\hat{B}_2(3,3,2)$ is the unique unicyclic graph of order n which attains the maximum Balaban index and sum–Balaban index of all graphs in $\mathcal{B}_n$. We now calculate the values $J(\hat{B}_2{}'(3,3,2))$ and $SJ(\hat{B}_2{}'(3,3,2))$.

It can be checked directly that

$$\begin{aligned} &D_{\hat{B}_2}(v_1) = n-1, \\ &D_{\hat{B}_2}(v_2) = D_{\hat{B}_2}(v_4) = 2n-4, \\ &D_{\hat{B}_2}(v_3) = 2n-5, \\ &D_{\hat{B}_2}(w) = 2n-3, \text{ where } w \in W_{v_1}. \end{aligned}$$

Thus

$$
\begin{aligned}
J(\hat{B}_2) &= \frac{n+1}{3}\left[\frac{1}{\sqrt{D_{\hat{B}_2}(v_1)D_{\hat{B}_2}(v_2)}}+\frac{1}{\sqrt{D_{\hat{B}_2}(v_2)D_{\hat{B}_2}(v_3)}}+\frac{1}{\sqrt{D_{\hat{B}_2}(v_3)D_{\hat{B}_2}(v_4)}}\right.\\
&+\left.\frac{1}{\sqrt{D_{\hat{B}_2}(v_1)D_{\hat{B}_2}(v_4)}}+\frac{1}{\sqrt{D_{\hat{B}_2}(v_1)D_{\hat{B}_2}(v_3)}}+\sum_{w\in W_{v_1}}\frac{1}{\sqrt{D_{\hat{B}_2}(v_1)D_{\hat{B}_2}(w)}}\right]\\
&= \frac{2n+2}{3\sqrt{2n^2-6n+4}}+\frac{2n+2}{3\sqrt{4n^2-18n+20}}+\frac{n+1}{3\sqrt{2n^2-7n+5}}\\
&+ \frac{n^2-3n-4}{3\sqrt{2n^2-5n+3}}
\end{aligned}
$$

and

$$
\begin{aligned}
SJ(\hat{B}_2) &= \frac{n+1}{3}\left[\frac{1}{\sqrt{D_{\hat{B}_2}(v_1)+D_{\hat{B}_2}(v_2)}}+\frac{1}{\sqrt{D_{\hat{B}_2}(v_2)+D_{\hat{B}_2}(v_3)}}\right.\\
&+ \frac{1}{\sqrt{D_{\hat{B}_2}(v_3)+D_{\hat{B}_2}(v_4)}}+\frac{1}{\sqrt{D_{\hat{B}_2}(v_1)+D_{\hat{B}_2}(v_4)}}+\frac{1}{\sqrt{D_{\hat{B}_2}(v_1)+D_{\hat{B}_2}(v_3)}}\\
&+ \left.\sum_{w\in W_{v_1}}\frac{1}{\sqrt{D_{\hat{B}_2}(v_1)+D_{\hat{B}_2}(w)}}\right]\\
&= \frac{2n+2}{3\sqrt{3n-5}}+\frac{2n+2}{3\sqrt{4n-9}}+\frac{n+1}{3\sqrt{3n-6}}+\frac{n^2-3n-4}{3\sqrt{3n-4}}. \qquad \square
\end{aligned}
$$

It is clear that the upper bounds of Theorem 3.2 is bigger than the upper bounds of Theorems 3.2 and 4.2 in [3].

4 A note on the paper [3]

In this section, we will give three examples to show some flaws in [3].

Example 4.1. *Let G and G' be the bicyclic graphs of order 7 as in Figure 4.1. According to Definition 2.3 in* [3]*, G' is the crossing–edge–lifting transformation of G (see Figure 4.1).*

Take $U_0 = \{u_3, u_4, u_5\}$. By the proof of Case 1 of Lemma 2.9 in [3], for any vertex $u \in U_0$, we have $D_G(u) \geq D_{G'}(u)$. However, $D_G(u_4) = 12$, $D_{G'}(u_4) = 13$, and so $D_G(u_4) < D_{G'}(u_4)$.

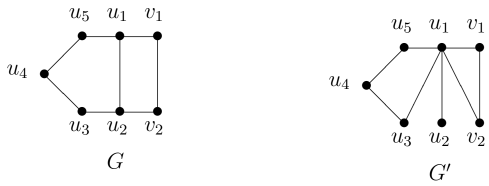

Figure 4.1 Graphs G and G'

Example 4.2. *Let G be the bicyclic graph of order 5 as in Figure 4.2.*

According to Lemma 2.10 in [3], there is the unique graph G' obtained from G by repeating the crossing–edge–lifting transformations until the two cycles of G' have only one crossing point. However, for the graph G as in Figure 4.2, we can not obtained such graph from G.

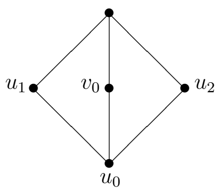

Figure 4.2 Graph G

Example 4.3. *Let G and G' be the bicyclic graphs of order 7 as in Figure 4.3. According to Definition 2.4 in [3], G' is the cycle-edge-transformation of G (see Figure 4.3). Take $U_0 = \{u_0, u_1, u_2, u_3, u_4\}$. By (2.25) in [3], for $u_i, u_j \in U_0$,*

$$\frac{1}{\sqrt{D_G(u_i)\, D_G(u_j)}} < \frac{1}{\sqrt{D_{G'}(u_i)\, D_{G'}(u_j)}}\,.$$

However, since $D_G(u_3) = 12$, $D_{G'}(u_3) = 13$, and $D_G(u_4) = D_{G'}(u_4) = 10$, we have

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

Figure 4.3 Graphs G and G'

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