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Maximal Balaban Index of Graphs *

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Abstract

The Balaban index (also called J index) of a connected graph G is denoted as

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

where $\sigma_G(u) = \sum_{w \in V(G)} d_G(u, w)$ and μ is the cyclomatic number. It has been used in various QSAR and QSPR studies. Let U_n^3 be an unicyclic graph obtained from a triangle C_3 by attaching $n-3$ pendent edges at one vertex of C_3. Let B_n $(n \geq 4)$ be a bicyclic graph obtained from U_n^3 by adding an edge between one pendent vertex and a vertex of degree 2 of U_n^3. In this paper, we show that U_n^3 and B_n have the largest Balaban index among all n-vertex unicyclic graphs and n-vertex bicyclic graphs, respectively.

1 Introduction

For a simple graph G, denote the edge set and vertex set of G by $E(G)$ and $V(G)$, respectively. Let $m = |E(G)|$ and $n = |V(G)|$, i.e., the edge number and vertex number of G. $N_G(v)$ denotes the set of neighbors of vertex v in G. If H is subgraph of G, its edge set and vertex set are denoted by $E_G(H)$ and $V_G(H)$, respectively. If Y is a vertex subset of $V(G)$, the vertex-induced subgraph of G induced by Y is denoted by $G[Y]$. The distance between vertices u and v in G is denoted by $d_G(u, v)$, and the sum of the distance between vertex u and each vertex of G is denoted by $\sigma_G(u)$. That is $\sigma_G(u) = \sum_{w \in V(G)} d_G(u, w)$.

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In 1982, A.T.Balaban in [1] introduced a new topological index for a connected graph G, which is called the Balaban index nowadays or J index for short. It is defined as

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

where μ is the cyclomatic number.

The Balaban index has been widely used in various QSAR and QSPR studies. The Balaban index and Wiener index [2] are two kinds of important topological indices based on the distance. Balaban et al. [3] compare the sequence of the isomers of alkane with k carbon atoms, where $6 \leq k \leq 9$. The result shows that the sequence of the isomers of alkane based on the Balaban index is parallel with that based on the Wiener index. Moreover, the former has smaller degeneracy than latter, which means that using the Balaban index to characterize molecular structure is better than the Wiener index. Until now, there are many results on the maximal and minimal Wiener index [4–8]. However, there are few similar results on the Balaban index [9–11].

We denoted by C_n a n-vertex cycle. Let U_n^3 be an unicyclic graph obtained from C_3 by attaching $n-3$ pendent edges at one vertex of C_3. Let B_n be a bicyclic graph obtained from U_n^3 by adding an edge between one pendent vertex and a vertex of degree 2 of U_n^3. Two graphs U_n^3 and B_n are shown in Fig 1. In this paper, we show that U_n^3 and B_n have the largest Balaban index among all n-vertex unicyclic graphs and n-vertex bicyclic graphs, respectively.

Fig. 1. Graphs U_n^3 and B_n

2 Preliminaries

Let G be a graph, and $G - xy$ denotes the graph that arises from G by deleting the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from G by adding an edge $xy \notin E(G)$, where $x, y \in V(G)$. We will use $\mathcal{U}_n$ and $\mathcal{B}_n$ to denote the sets of all unicyclic and bicyclic graphs with n vertices, respectively.

For each i, $i = 1, 2, \cdots, g$, let T_i be a rooted tree attached at the root vertex w_i of the cycle C_g. Of course, some of T_is may be just the root w_i. Then we may denote the n- vertex unicyclic graph by $U_n(T_{w_1}, T_{w_2}, \cdots, T_{w_g})$. The center of a star means its vertex with maximum degree. If each T_{w_i}, $i = 1, 2, \cdots, g$, is a star S_{w_i} whose root is w_i the center of S_{w_i}, the n- vertex unicyclic graph $U_n(T_{w_1}, T_{w_2}, \cdots, T_{w_g})$ is denoted by $U_n(S_{w_1}, S_{w_2}, \cdots, S_{w_g})$. The set of all this kind of unicyclic graphs is denoted by $\mathcal{U}^*_{n,g}$.

3 Main results

The main result in this section is as follows.

Theorem 1. The graph U_n^3 has the largest Balaban index among all n-vertex unicyclic graphs.

Before given the proof of Theorem 1, we need some more preparations.

Let G_1 and G_2 be two graphs, and $v_i \in V(G_i)$, $i = 1, 2$. Suppose $n_1 = |V(G_1)|$ and $n_2 = |V(G_2)|$, where $n_1 \geq 1, n_2 \geq 1$. The graph H_1 is obtained from G_1 and G_2 by joining two vertices v_1 and v_2 by an edge v_1v_2. The graph H_2 is obtained from H_1 by identifying two vertices v_1 and v_2 and changing the edge v_1v_2 into a pendent edge attached at vertex v_1, that is,

$$H_2 = H_1 - \{v_2x | x \in N_{H_1}(v_2) \setminus \{v_1\}\} + \{v_1x | x \in N_{H_1}(v_2) \setminus \{v_1\}\}$$

Two graphs H_1 and H_2 are shown in Fig 2.

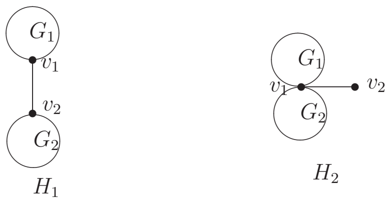


Fig. 2. Graphs H_1 and H_2

Lemma 1. $J(H_1) \leq J(H_2)$.

Proof. By the definition of the Balaban index, we have

$$\begin{aligned} \frac{\mu+1}{m} J(H_1) &= \sum_{uv \in E_{H_1}(G_1)} \frac{1}{\sqrt{\sigma_{H_1}(u)\sigma_{H_1}(v)}} \\ &+ \sum_{ab \in E_{H_1}(G_2)} \frac{1}{\sqrt{\sigma_{H_1}(a)\sigma_{H_1}(b)}} + \frac{1}{\sqrt{\sigma_{H_1}(v_1)\sigma_{H_1}(v_2)}} \end{aligned} \quad (1)$$

$$\begin{aligned}\frac{\mu+1}{m}J(H_2) &= \sum_{uv\in E_{H_2}(G_1)}\frac{1}{\sqrt{\sigma_{H_2}(u)\sigma_{H_2}(v)}}\\ &+ \sum_{ab\in E_{H_2}(G_2)}\frac{1}{\sqrt{\sigma_{H_2}(a)\sigma_{H_2}(b)}}+\frac{1}{\sqrt{\sigma_{H_2}(v_1)\sigma_{H_2}(v_2)}} \qquad (2)\end{aligned}$$

For any vertex $u \in V_{H_1}(G_1)$ (i.e., $u \in V_{H_2}(G_1)$), it's obvious that $\sigma_{H_1}(u) \geq \sigma_{H_2}(u)$. Thus,

$$\sum_{uv\in E_{H_1}(G_1)}\frac{1}{\sqrt{\sigma_{H_1}(u)\sigma_{H_1}(v)}} \leq \sum_{uv\in E_{H_2}(G_1)}\frac{1}{\sqrt{\sigma_{H_2}(u)\sigma_{H_2}(v)}} \qquad (3)$$

Claim 1.1.

$$\sum_{ab\in E_{H_1}(G_2)}\frac{1}{\sqrt{\sigma_{H_1}(a)\sigma_{H_1}(b)}} \leq \sum_{ab\in E_{H_2}(G_2)}\frac{1}{\sqrt{\sigma_{H_2}(a)\sigma_{H_2}(b)}}$$

In fact, it is easy to see that

$$V_{H_2}(G_1) = V_{H_1}(G_1), \quad V_{H_2}(G_2) = V_{H_1}(G_2) - \{v_2\} + \{v_1\}$$

Let N_2 be the set of all neighbors of v_2 in the subgraph G_2 of H_1, i.e., $N_2 = \{y|v_2y \in E_{H_1}(G_2)\}$. Obviously, $N_2 = \{y|v_1y \in E_{H_2}(G_2)\}$. For any vertex $v \in V_{H_1}(G_2) - \{v_2\}$ (i.e., $v \in V_{H_2}(G_2) - \{v_1\}$), we have

$$\sigma_{H_1}(v) = \sum_{x\in V_{H_1}(G_2)-\{v_2\}} d_{H_1}(v,x) + d_{H_1}(v,v_2) + \sum_{y\in V_{H_1}(G_1)} d_{H_1}(v,y) \qquad (4)$$

$$\sigma_{H_2}(v) = \sum_{x\in V_{H_2}(G_2)-\{v_1\}} d_{H_2}(v,x) + d_{H_2}(v,v_2) + \sum_{y\in V_{H_2}(G_1)} d_{H_2}(v,y) \qquad (5)$$

By the structures of H_1 and H_2, one can find that

$$\sum_{x\in V_{H_1}(G_2)-\{v_2\}} d_{H_1}(v,x) = \sum_{x\in V_{H_2}(G_2)-\{v_1\}} d_{H_2}(v,x)$$

and

$$d_{H_2}(v,v_2) = d_{H_1}(v,v_2)+1$$

Since

$$\sum_{y\in V_{H_1}(G_1)} d_{H_1}(v,y) - \sum_{y\in V_{H_2}(G_1)} d_{H_2}(v,y) \geq 1,$$

by (4) and (5), we have

$$\sigma_{H_1}(v) \geq \sigma_{H_2}(v) \qquad (6)$$

Thus,

$$\sum_{ab\in E_{H_1}(G_2)-\{v_2y|y\in N_2\}}\frac{1}{\sqrt{\sigma_{H_1}(a)\sigma_{H_1}(b)}} \leq \sum_{ab\in E_{H_2}(G_2)-\{v_1y|y\in N_2\}}\frac{1}{\sqrt{\sigma_{H_2}(a)\sigma_{H_2}(b)}} \qquad (7)$$

By direct calculation, we have

$$\begin{aligned}\sigma_{H_2}(v_1) &= \sigma_{H_1}(v_1) - n_2 + 1\\ \sigma_{H_1}(v_2) &= \sigma_{H_1}(v_1) - n_2 + n_1\\ \sigma_{H_2}(v_2) &= \sigma_{H_2}(v_1) + n - 2\\ &= \sigma_{H_1}(v_1) + n_1 - 1\end{aligned}$$

Since $n_1 \geq 1$, we have

$$\sigma_{H_1}(v_2) \geq \sigma_{H_2}(v_1) \tag{8}$$

By (6) and (8), we have

$$\sum_{ab\in\{v_2y|y\in N_2\}} \frac{1}{\sqrt{\sigma_{H_1}(a)\sigma_{H_1}(b)}} \leq \sum_{ab\in\{v_1y|y\in N_2\}} \frac{1}{\sqrt{\sigma_{H_2}(a)\sigma_{H_2}(b)}} \tag{9}$$

So Claim 1.1 holds by (7) and (9).

Moreover, since

$$\begin{aligned}&\sigma_{H_2}(v_1)\sigma_{H_2}(v_2) - \sigma_{H_1}(v_1)\sigma_{H_1}(v_2)\\ &= (\sigma_{H_1}(v_1) - n_2 + 1)(\sigma_{H_1}(v_1) + n_1 - 1) - \sigma_{H_1}(v_1)(\sigma_{H_1}(v_1) + n_1 - n_2)\\ &= (n_2 - 1)(1 - n_1) \leq 0,\end{aligned}$$

then

$$\frac{1}{\sqrt{\sigma_{H_1}(v_1)\sigma_{H_1}(v_2)}} \leq \frac{1}{\sqrt{\sigma_{H_2}(v_1)\sigma_{H_2}(v_2)}} \tag{10}$$

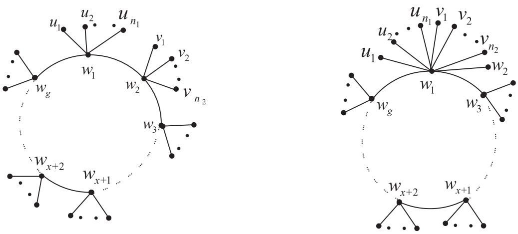
So the result follows immediately from (1), (2), (3), (10) and Claim 1.1. □

Thus, by Lemma 1, we focus on seeking the unicyclic graph with the largest Balaban index in $\mathcal{U}^*_{n,g}$.

Let $U_0 = U_n(S_{w_1}, S_{w_2}, \cdots, S_{w_g})$ be an unicyclic graph in $\mathcal{U}^*_{n,g}$, where $g > 3$, and w_1 and w_2 be the centers of two adjacent stars S_{w_1}, S_{w_2} to which there are some pendent vertices, say $\{u_1, u_2, \cdots, u_{n_1}\}$ and $\{v_1, v_2, \cdots, v_{n_2}\}$ attached, respectively. Let U_1 be the graph obtained from U_0 by identifying two vertices w_1 and w_2 and changing the edge w_1w_2 into a pendent edge attached at w_1, that is,

$$U_1 = U_0 - \{w_2x|x \in N_{U_0}(w_2) \setminus \{w_1\}\} + \{w_1x|x \in N_{U_0}(w_2) \setminus \{w_1\}\}$$

Two graphs U_0 and U_1 are shown in Fig 3.



U_0 U_1

Fig. 3. Graphs U_0 and U_1, where $x = \lfloor \frac{g}{2} \rfloor$

Lemma 2. $J(U_0) < J(U_1)$.

Proof. Let $Y_1(U_0)$ and $Y_2(U_0)$ be two subsets of the vertex set $V(U_0)$ such that

$$Y_1(U_0) = V(S_{w_1}) \cup \{w_2\} \cup V(S_{w_{\lfloor \frac{g}{2} \rfloor+2}}) \cup V(S_{w_{\lfloor \frac{g}{2} \rfloor+3}}) \cdots \cup V(S_{w_g})$$

$$Y_2(U_0) = V(U_0) - Y_1(U_0)$$

Let $E_1(U_0)$ and $E_2(U_0)$ be two subsets of edge set $E(U_0)$ such that

$$E_1(U_0) = E(U_0[Y_1(U_0)]) - \{w_1 w_2\}$$

$$E_2(U_0) = E(U_0) - E_1(U_0) - \{w_1 w_2\}$$

In a similar way, we define the corresponding items for U_1 as follows.

$$Y_1(U_1) = Y_1(U_0), \quad Y_2(U_1) = Y_2(U_0)$$

$$E_1(U_1) = E(U_1[Y_1(U_1)]) - \{w_1 w_2\}$$

$$E_2(U_1) = E(U_1) - E_1(U_1) - \{w_1 w_2\}$$

It is easy to see that

$$E(U_0) = E_1(U_0) \cup E_2(U_0) \cup \{w_1 w_2\}$$

$$E(U_1) = E_1(U_1) \cup E_2(U_1) \cup \{w_1 w_2\}$$

By the definition of the Balaban index, we have

$$\begin{aligned}\frac{2}{m}J(U_0) &= \sum_{uv\in E_1(U_0)} \frac{1}{\sqrt{\sigma_{U_0}(u)\sigma_{U_0}(v)}} \\ &\quad + \sum_{ab\in E_2(U_0)} \frac{1}{\sqrt{\sigma_{U_0}(a)\sigma_{U_0}(b)}} + \frac{1}{\sqrt{\sigma_{U_0}(w_1)\sigma_{U_0}(w_2)}} \qquad (11)\\ \frac{2}{m}J(U_1) &= \sum_{uv\in E_1(U_1)} \frac{1}{\sqrt{\sigma_{U_1}(u)\sigma_{U_1}(v)}} \\ &\quad + \sum_{ab\in E_2(U_1)} \frac{1}{\sqrt{\sigma_{U_1}(a)\sigma_{U_1}(b)}} + \frac{1}{\sqrt{\sigma_{U_1}(w_1)\sigma_{U_1}(w_2)}} \qquad (12)\end{aligned}$$

When $x \in Y_1(U_0)$(i.e., $x \in Y_1(U_1)$) and $x \neq w_2$, since the length of the cycle in U_1 is less exactly one than that in U_0, thus,

$$\sigma_{U_0}(x) > \sigma_{U_1}(x) \qquad (13)$$

So it is easy to see that

$$\sum_{uv\in E_1(U_0)} \frac{1}{\sqrt{\sigma_{U_0}(u)\sigma_{U_0}(v)}} < \sum_{uv\in E_1(U_1)} \frac{1}{\sqrt{\sigma_{U_1}(u)\sigma_{U_1}(v)}} \qquad (14)$$

Claim 2.1.

$$\sum_{ab\in E_2(U_0)} \frac{1}{\sqrt{\sigma_{U_0}(a)\sigma_{U_0}(b)}} < \sum_{ab\in E_2(U_1)} \frac{1}{\sqrt{\sigma_{U_1}(a)\sigma_{U_1}(b)}}$$

By the structures of U_0 and U_1, one can find that

$$\begin{aligned} E_2(U_0) &= \bigcup_{1\le i\le n_2} \{w_2v_i\} \cup \{w_2w_3\} \cup \{w_{\lfloor \frac{g}{2}\rfloor+1}w_{\lfloor \frac{g}{2}\rfloor+2}\} \cup \overline{E_2}(U_0) \qquad (15)\\ E_2(U_1) &= \bigcup_{1\le i\le n_2} \{w_1v_i\} \cup \{w_1w_3\} \cup \{w_{\lfloor \frac{g}{2}\rfloor+1}w_{\lfloor \frac{g}{2}\rfloor+2}\} \cup \overline{E_2}(U_1) \qquad (16)\end{aligned}$$

where

$$\begin{aligned} \overline{E_2}(U_0) &= E_2(U_0) - \bigcup_{1\le i\le n_2} \{w_2v_i\} \cup \{w_2w_3\} \cup \{w_{\lfloor \frac{g}{2}\rfloor+1}w_{\lfloor \frac{g}{2}\rfloor+2}\} \\ \overline{E_2}(U_1) &= E_2(U_1) - \bigcup_{1\le i\le n_2} \{w_1v_i\} \cup \{w_1w_3\} \cup \{w_{\lfloor \frac{g}{2}\rfloor+1}w_{\lfloor \frac{g}{2}\rfloor+2}\}\end{aligned}$$

By direct computation, we have

$$\begin{aligned} \sigma_{U_1}(w_1) &= \sigma_{U_0}(w_1) - |Y_2(U_0)| \\ \sigma_{U_0}(u_i) &= \sigma_{U_0}(w_1) + n - 2 \\ \sigma_{U_1}(u_i) &= \sigma_{U_0}(u_i) - |Y_2(U_0)| \\ &= \sigma_{U_0}(w_1) + |Y_1(U_0)| - 2\end{aligned}$$

$$\begin{aligned}
\sigma_{U_1}(w_1) &= \sigma_{U_0}(w_1) - |Y_2(U_0)| \\
\sigma_{U_0}(w_2) &= \sigma_{U_0}(w_1) + |Y_1(U_0)| - |Y_2(U_0)| - 2 \\
\sigma_{U_0}(v_j) &= 2(n_2 - 1) + \sigma_{U_0}(w_2) - 2n_2 + n \\
&= \sigma_{U_0}(w_1) + 2|Y_1(U_0)| - 4
\end{aligned}$$

where $1 \le i \le n_1$ and $1 \le j \le n_2$.

Since w_2, v_j and u_i are the pendent vertices of w_1 on U_1, then $\sigma_{U_1}(w_2) = \sigma_{U_1}(v_j) = \sigma_{U_1}(u_i)$. By $\sigma_{U_0}(w_2) > \sigma_{U_1}(w_1)$ and $\sigma_{U_0}(v_j) > \sigma_{U_1}(w_2) = \sigma_{U_1}(v_j) = \sigma_{U_1}(u_i)$, we have

$$\sum_{1\le j\le n_2} \frac{1}{\sqrt{\sigma_{U_0}(w_2)\sigma_{U_0}(v_j)}} < \sum_{1\le j\le n_2} \frac{1}{\sqrt{\sigma_{U_1}(w_1)\sigma_{U_1}(v_j)}} \tag{17}$$

We choose a vertex $x \in Y_2(U_0) - \{v_1, v_2, \cdots, v_{n_2}\}$(i.e., $x \in Y_2(U_1) - \{v_1, v_2, \cdots, v_{n_2}\}$).

Since $d_{U_1}(x, w_2) = d_{U_0}(x, w_2) + 1$ and

$$\sum_{y\in V(U_0)-\{w_2\}} d_{U_0}(x, y) - \sum_{y\in V(U_1)-\{w_2\}} d_{U_1}(x, y) > 1,$$

then

$$\begin{aligned}
\sigma_{U_1}(x) &= d_{U_1}(x, w_2) + \sum_{y\in V(U_1)-\{w_2\}} d_{U_1}(x, y) \\
&< d_{U_0}(x, w_2) + 1 + \sum_{y\in V(U_0)-\{w_2\}} d_{U_0}(x, y) - 1 \\
&= \sigma_{U_0}(x)
\end{aligned} \tag{18}$$

Therefore,

$$\sum_{ab\in \overline{E_2}(U_0)} \frac{1}{\sqrt{\sigma_{U_0}(a)\sigma_{U_0}(b)}} < \sum_{ab\in \overline{E_2}(U_1)} \frac{1}{\sqrt{\sigma_{U_1}(a)\sigma_{U_1}(b)}} \tag{19}$$

By (13) and (18), we have

$$\frac{1}{\sqrt{\sigma_{U_0}(w_{\lfloor \frac{g}{2}\rfloor+1})\sigma_{U_0}(w_{\lfloor \frac{g}{2}\rfloor+2})}} < \frac{1}{\sqrt{\sigma_{U_1}(w_{\lfloor \frac{g}{2}\rfloor+1})\sigma_{U_1}(w_{\lfloor \frac{g}{2}\rfloor+2})}} \tag{20}$$

From (18) and $\sigma_{U_0}(w_2) > \sigma_{U_1}(w_1)$, it is easy to see that

$$\frac{1}{\sqrt{\sigma_{U_0}(w_2)\sigma_{U_0}(w_3)}} < \frac{1}{\sqrt{\sigma_{U_1}(w_1)\sigma_{U_1}(w_3)}} \tag{21}$$

Thus, Claim 2.1 follows by (15)-(17) and (19)-(21).

When $1 \le i \le n_1$, we know that $\sigma_{U_1}(w_2) = \sigma_{U_1}(u_i)$. Since

$$\sigma_{U_0}(w_1)\sigma_{U_0}(w_2) - \sigma_{U_1}(w_1)\sigma_{U_1}(w_2) = |Y_2(U_0)|(|Y_1(U_0)| - 2) > 0,$$

then

$$\frac{1}{\sqrt{\sigma_{U_0}(w_1)\sigma_{U_0}(w_2)}} < \frac{1}{\sqrt{\sigma_{U_1}(w_1)\sigma_{U_1}(w_2)}} \tag{22}$$

Thus, the result holds from (11), (12), (14), (22) and Claim 2.1. □

Hence, any unicyclic graph in $\mathcal{U}^*_{n,g}$ can be transformed into the unicyclic graph $U_n(S_{w_1}, S_{w_2}, S_{w_3})$ by using Lemma 3 repeatedly and the corresponding Balaban index increases gradually along with the length of cycle decreasing.

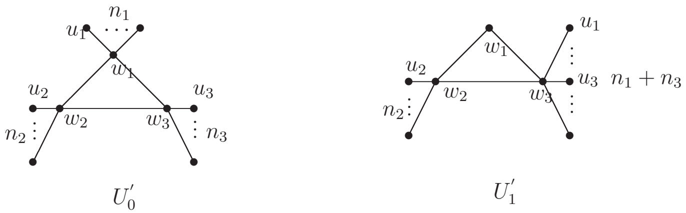


Fig. 4. Graphs U_0' and U_1'

Let $U_0' = U_n(S_{w_1}, S_{w_2}, S_{w_3})$. Let U_1' be the graph obtained from U_0' by changing all the pendent edges attached at the vertex w_1 into the pendent edges attached at the vertex w_3, that is

$$U_1' = U_0' - \{w_1x | x \in N_{U_0'}(w_1) \setminus \{w_2, w_3\}\} + \{w_3x | x \in N_{U_0'}(w_1) \setminus \{w_2, w_3\}\}$$

In U_0', vertex w_i has n_i pendent vertices and u_i is a pendent vertex of w_i, where $i = 1, 2, 3$ and $n_1 \geq 1$, $n_3 \geq 1$. The graphs U_0' and U_1' are shown in Fig 4.

Lemma 3. $J(U_0') < J(U_1')$.

Proof. From the definition of the Balaban index and the structures of the graphs U_0' and U_1', we know that

$$\begin{aligned} \frac{2}{m}J(U_0') &= \frac{n_1}{\sqrt{\sigma_{U_0'}(w_1)\sigma_{U_0'}(u_1)}} + \frac{n_2}{\sqrt{\sigma_{U_0'}(w_2)\sigma_{U_0'}(u_2)}} \\ &+ \frac{n_3}{\sqrt{\sigma_{U_0'}(w_3)\sigma_{U_0'}(u_3)}} + \frac{1}{\sqrt{\sigma_{U_0'}(w_1)\sigma_{U_0'}(w_2)}} \\ &+ \frac{1}{\sqrt{\sigma_{U_0'}(w_3)\sigma_{U_0'}(w_2)}} + \frac{1}{\sqrt{\sigma_{U_0'}(w_1)\sigma_{U_0'}(w_3)}} \end{aligned} \tag{23}$$

$$\frac{2}{m}J(U_1') = \frac{n_2}{\sqrt{\sigma_{U_1'}(w_2)\sigma_{U_1'}(u_2)}} + \frac{n_1+n_3}{\sqrt{\sigma_{U_1'}(w_3)\sigma_{U_1'}(u_3)}} + \frac{1}{\sqrt{\sigma_{U_1'}(w_1)\sigma_{U_1'}(w_2)}} + \frac{1}{\sqrt{\sigma_{U_1'}(w_3)\sigma_{U_1'}(w_2)}} + \frac{1}{\sqrt{\sigma_{U_1'}(w_1)\sigma_{U_1'}(w_3)}} \tag{24}$$

By direct calculation, we have

$$\begin{aligned}
&\sigma_{U_0'}(w_1) = 2n - n_1 - 4, \quad \sigma_{U_0'}(u_1) = 3n - n_1 - 6\\
&\sigma_{U_0'}(w_2) = 2n - n_2 - 4, \quad \sigma_{U_0'}(u_2) = 3n - n_2 - 6\\
&\sigma_{U_0'}(w_3) = 2n - n_3 - 4, \quad \sigma_{U_0'}(u_3) = 3n - n_3 - 6\\
&\sigma_{U_1'}(w_1) = 2n - 4, \quad \sigma_{U_1'}(w_2) = \sigma_{U_0'}(w_2) = 2n - n_2 - 4\\
&\sigma_{U_1'}(u_2) = \sigma_{U_0'}(u_2) = 3n - n_2 - 6, \quad \sigma_{U_1'}(w_3) = n + n_2 - 1\\
&\sigma_{U_1'}(u_3) = \sigma_{U_1'}(u_1) = 2n + n_2 - 3
\end{aligned}$$

Thus, one can see that

$$\begin{aligned}
&\sigma_{U_0'}(w_1)\sigma_{U_0'}(u_1) > \sigma_{U_1'}(w_3)\sigma_{U_1'}(u_3), \quad \sigma_{U_0'}(w_3)\sigma_{U_0'}(u_3) > \sigma_{U_1'}(w_3)\sigma_{U_1'}(u_3)\\
&\sigma_{U_0'}(w_1)\sigma_{U_0'}(w_2) < \sigma_{U_1'}(w_1)\sigma_{U_1'}(w_2), \quad \sigma_{U_0'}(w_3)\sigma_{U_0'}(w_2) > \sigma_{U_1'}(w_3)\sigma_{U_1'}(w_2)\\
&\sigma_{U_0'}(w_1)\sigma_{U_0'}(w_3) > \sigma_{U_1'}(w_1)\sigma_{U_1'}(w_3), \quad \sigma_{U_0'}(w_2)\sigma_{U_0'}(u_2) = \sigma_{U_1'}(w_2)\sigma_{U_1'}(u_2)
\end{aligned}$$

So, we have

$$\begin{aligned}
&\frac{n_2}{\sqrt{\sigma_{U_0'}(w_2)\sigma_{U_0'}(u_2)}} = \frac{n_2}{\sqrt{\sigma_{U_1'}(w_2)\sigma_{U_1'}(u_2)}}\\
&\frac{n_1}{\sqrt{\sigma_{U_0'}(w_1)\sigma_{U_0'}(u_1)}} + \frac{n_3}{\sqrt{\sigma_{U_0'}(w_3)\sigma_{U_0'}(u_3)}} < \frac{n_1+n_3}{\sqrt{\sigma_{U_1'}(w_3)\sigma_{U_1'}(u_3)}}\\
&\frac{1}{\sqrt{\sigma_{U_0'}(w_3)\sigma_{U_0'}(w_2)}} < \frac{1}{\sqrt{\sigma_{U_1'}(w_3)\sigma_{U_1'}(w_2)}}\\
&\frac{1}{\sqrt{\sigma_{U_0'}(w_1)\sigma_{U_0'}(w_3)}} < \frac{1}{\sqrt{\sigma_{U_1'}(w_1)\sigma_{U_1'}(w_3)}}\\
&\frac{1}{\sqrt{\sigma_{U_0'}(w_1)\sigma_{U_0'}(w_2)}} > \frac{1}{\sqrt{\sigma_{U_1'}(w_1)\sigma_{U_1'}(w_2)}}
\end{aligned} \tag{25}$$

Claim 3.1.

$$\frac{1}{\sqrt{\sigma_{U_0'}(w_1)\sigma_{U_0'}(w_2)}}+\frac{1}{\sqrt{\sigma_{U_0'}(w_3)\sigma_{U_0'}(w_2)}}<\frac{1}{\sqrt{\sigma_{U_1'}(w_1)\sigma_{U_1'}(w_2)}}+\frac{1}{\sqrt{\sigma_{U_1'}(w_3)\sigma_{U_1'}(w_2)}}$$

i.e.,

$$\frac{1}{\sqrt{2n-n_2-4}}\left(\frac{1}{\sqrt{2n-n_1-4}}+\frac{1}{\sqrt{2n-n_3-4}}-\frac{1}{\sqrt{2n-4}}-\frac{1}{\sqrt{n+n_2-1}}\right)<0$$

Let $r=2n-n_1-4$ and $t=2n-n_3-4$. Obviously, $r,t>0$. Then

$$\begin{aligned}&\frac{1}{\sqrt{2n-n_1-4}}+\frac{1}{\sqrt{2n-n_3-4}}-\left(\frac{1}{\sqrt{2n-4}}+\frac{1}{\sqrt{n+n_2-1}}\right)\\&=\frac{1}{\sqrt{r}}+\frac{1}{\sqrt{t}}-\left(\frac{1}{\sqrt{r+n_1}}+\frac{1}{\sqrt{t-n_1}}\right)\\&=(-\sqrt{rt(t-n_1)}-\sqrt{rt(r+n_1)}+\sqrt{r(t-n_1)(r+n_1)}+\\&\sqrt{t(t-n_1)(r+n_1)})/\sqrt{rt(t-n_1)(r+n_1)}\end{aligned}\tag{26}$$

We just concern the sign of the numerator of above equation. Thus, from (26), we know

$$\begin{aligned}&(\sqrt{rt(t-n_1)}+\sqrt{rt(r+n_1)})^2-(\sqrt{r(t-n_1)(r+n_1)}+\sqrt{t(t-n_1)(r+n_1)})^2\\&=-2r^{3/2}t^{3/2}+2rt\sqrt{t-n_1}\sqrt{r+n_1}+(\sqrt{r}+\sqrt{t})^2n_1(r-t+n_1)\end{aligned}\tag{27}$$

Assume $h=t-n_1$. Obviously, $h>0$. By $n_3=r-t+n_1$ and (27), we have

$$\begin{aligned}&[2rt\sqrt{t-n_1}\sqrt{r+n_1}+(\sqrt{r}+\sqrt{t})^2n_1(r-t+n_1)]^2-(2r^{3/2}t^{3/2})^2\\&=[2rt\sqrt{h(r+n_1)}+(\sqrt{r}+\sqrt{t})^2n_1n_3]^2-(2r^{3/2}t^{3/2})^2\\&=[2rt\sqrt{h(r+n_1)}+(\sqrt{r}+\sqrt{t})^2n_1n_3-2r^{3/2}t^{3/2}]\cdot\\&\quad[2rt\sqrt{h(r+n_1)}+(\sqrt{r}+\sqrt{t})^2n_1n_3+2r^{3/2}t^{3/2}]\end{aligned}\tag{28}$$

We choose the first factor from (28), it is easy to see that

$$\begin{aligned}&2rt\sqrt{h(r+n_1)}+(\sqrt{r}+\sqrt{t})^2n_1n_3-2r^{3/2}t^{3/2}\\&=2\sqrt{rt}(-rt+\sqrt{rth(r+n_1)}+n_1n_3)+(r+t)n_1n_3\\&\geq 2\sqrt{rt}(-rt+\sqrt{rth(r+n_1)}+2n_1n_3)\end{aligned}\tag{29}$$

So by (29), it suffices to prove that

$$-rt+\sqrt{rth(r+n_1)}+2n_1n_3>0\tag{30}$$

Let

$$f_1(n) = 12n^2 - 6n(8 + n_1 + n_3) + 12n_1 + 12n_3 - n_1n_3 + 48$$
$$f_2(n) = 20n^2 - 10n(8 + n_1 + n_3) + 20n_1 + 20n_3 + 9n_1n_3 + 80$$

Since $n = n_1 + n_2 + n_3 + 3$, then

$$f_1(n_1 + n_2 + n_3 + 3) > 0, \quad f_2(n_1 + n_2 + n_3 + 3) > 0$$

Thus, we have

$$\begin{aligned} & [2rt\sqrt{rth(r + n_1)}]^2 - [(rt)^2 + rth(r + n_1) - (2n_1n_3)^2]^2 \\ & = n_1^2n_1^3f_1(n)f_2(n) \\ & > 0 \end{aligned} \tag{31}$$

Note that

$$(rt)^2 + rth(r + n_1) - (2n_1n_3)^2 > 0$$

From (31), we can find that

$$\begin{aligned} 2rt\sqrt{rth(r + n_1)} &> (rt)^2 + rth(r + n_1) - (2n_1n_3)^2 \\ &\Longleftrightarrow \\ (2n_1n_3)^2 &> (rt)^2 + rth(r + n_1) - 2rt\sqrt{rth(r + n_1)} \\ &\Longleftrightarrow \\ (2n_1n_3)^2 &> rt(\sqrt{rt} - \sqrt{h(r + n_1)})^2 \end{aligned} \tag{32}$$

Note that $\sqrt{rt} - \sqrt{h(r + n_1)} > 0$. By (32), we know that

$$\begin{aligned} & \sqrt{rt}(\sqrt{h(r + n_1)} - \sqrt{rt}) + 2n_1n_3 \\ & = -rt + \sqrt{r}\sqrt{t}\sqrt{h}\sqrt{r + n_1} + 2n_1n_3 > 0 \end{aligned}$$

Therefore, Claim 3.1 holds by (26)-(30).

Hence, from (23)-(25) and Claim 3.1, the result follows. □

Proof of Theorem 1. Let G and G' be two graphs and denote that graph G is transformed into graph G' by $G \longrightarrow G'$. For any graph U in $\mathcal{U}_n$, we distinguish the following two cases.

Case 1. The length of the cycle in the unicyclic graph U is 3. Then we take transformations as follow:

$$U \longrightarrow U_0^{'} \longrightarrow U_n^3$$

So by Lemma 1 and Lemma 3, we have $J(U) < J(U_0^{'}) < J(U_n^3)$.

Case 2. The length of the cycle in the unicyclic graph U is more than 3. Then we take the following transformations:

$$U \longrightarrow U_0 \longrightarrow U_0^{'} \longrightarrow U_n^3$$

Thus, we have $J(U) < J(U_0) < J(U_0^{'}) < J(U_n^3)$ by lemmas 1-3. This finishes the proof. □

With the similar proof as Theorem 1 but more tedious, we have the following result on bicyclic graphs and the proof is shown in the appendix.

Theorem 2. The graph B_n has the largest Balaban index among all the n-vertex bicyclic graphs.

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Appendix: The proof of Theorem 2.

Before given the proof of Theorem 2, we need some more preparations.

Suppose that v_1 is a vertex of C_p and v_l is a vertex of C_q. Joining v_1 and v_l by a path $v_1, v_2, \cdots, v_l$ of length $l-1$, where $l \geq 1$ and $l = 1$ means identifying v_1 with v_l, the resulting graph (see Fig 5.), denoted by $B(p, l, q)$, is called an ∞-graph. If two cycles C_p and C_q share a common path of length l, where l satisfying $l \leq \lfloor \frac{p}{2} \rfloor, l \leq \lfloor \frac{q}{2} \rfloor$, then the resulting graph (see Fig 5.), denoted by $P(p, l, q)$, is called a θ-graph. Obviously, the set of all bicyclic graphs $\mathcal{B}_n$ consists of two kinds of graphs. one kind, denoted by $\mathcal{B}_n^+$, are those graphs each of them is an ∞-graph with some trees attached; the other kind, denoted by $\mathcal{B}_n^{++}$, are those graphs each of them is a θ-graph with some trees attached. Then we have $\mathcal{B}_n = \mathcal{B}_n^+ \cup \mathcal{B}_n^{++}$.

Fig. 5. Graphs $B(p, l, q)$ and $P(p, l, q)$

If G is a graph obtained by attaching their centers of some stars to some vertices of $B(p, 1, q)$, then $G \in \mathcal{B}_n^+$ obviously. The set of all this kind of bicyclic graphs is denoted by $\mathcal{B}_n^*(p, q)$.

If G is obtained by attaching their centers of some stars to some vertices of $P(p, l, q)$, then $G \in \mathcal{B}_n^{++}$. The set of all this kind of bicyclic graphs is denoted by $\mathcal{B}_n^{**}(p, l, q)$.

Theorem 2. The graph B_n has the largest Balaban index among all the n-vertex bicyclic graphs.

From Lemma 1, we focus on seeking the bicyclic graph with the largest Balaban index in $\mathcal{B}_n^*(p, q)$ or $\mathcal{B}_n^{**}(p, l, q)$.

Let B be a bicyclic graph in $\mathcal{B}_n^*(p, q)$, where $p > 3$ and $q \geq 3$, and w_1 and w_2 be the centers of two adjacent stars S_{w_1}, S_{w_2}, where w_1 is a vertex on the cycle C_p and w_2 is the unique common vertex of two cycles C_p and C_q. Let B' be the graph obtained from B by identifying vertices w_1 and w_2 and changing the edge w_1w_2 into a pendent edge attached at w_1, that is,

$$B' = B - \{w_2x | x \in N_B(w_2) \setminus \{w_1\}\} + \{w_1x | x \in N_B(w_2) \setminus \{w_1\}\}$$

Two graphs B and B' are shown in Fig 6.

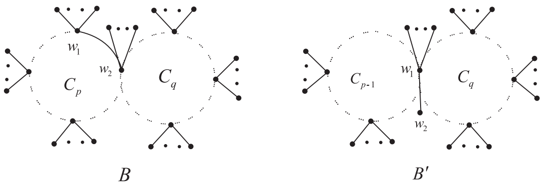

Fig. 6. Graphs B and B'

With the same method as Lemma 2, we have

Lemma 4. $J(B) < J(B^{'})$.

Let B_0 be a bicyclic graph in $\mathcal{B}_n^{**}(p, l, q)$, where $p, q > 3$, with $\{w_1, w_2, \cdots, w_{l+1}, u_{l+2}, \cdots, u_p\}$ and $\{w_1, w_2, \cdots, w_{l+1}, v_{l+2}, \cdots, v_q\}$ as the vertex sets of two cycles C_p and C_q, respectively, and the common vertices w_1 and w_2 of C_p and C_q be the centers of two adjacent stars S_{w_1}, S_{w_2} to which n_1 and n_2 pendent vertices attached, respectively. Let $B_0^{'}$ be the graph obtained from B_0 by identifying vertices w_1 and w_2 and changing the edge w_1w_2 into a pendent edge attached at w_1, that is,

$$B_0^{'} = B_0 - \{w_2x | x \in N_{B_0}(w_2) \setminus \{w_1\}\} + \{w_1x | x \in N_{B_0}(w_2) \setminus \{w_1\}\}$$

The graphs B_0 and $B_0^{'}$ are shown in Fig 7.

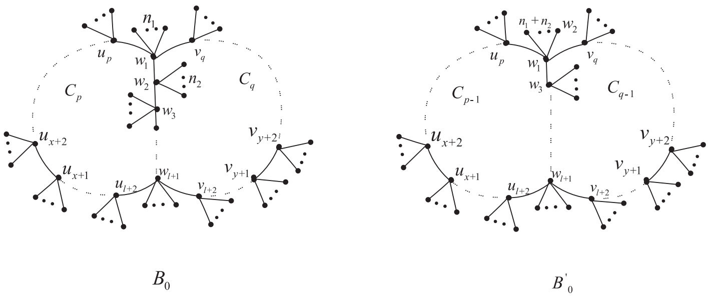

Fig. 7. Graphs B_0 and B'_0, where $x = \left\lfloor \frac{p}{2} \right\rfloor$, $y = \left\lfloor \frac{q}{2} \right\rfloor$

Lemma 5. $J(B_0) < J(B_0^{'})$.

Proof. Let $Y_1(B_0)$ and $Y_2(B_0)$ be two subsets of the vertex set $V(B_0)$ such that

$$\begin{aligned} Y_2(B_0) &= (V(S_{w_2}) - \{w_2\}) \cup V(S_{w_3}) \cup \cdots \cup V(S_{w_{l+1}}) \\ &\cup V(S_{u_{l+2}}) \cup V(S_{u_{l+3}}) \cup \cdots \cup V(S_{u_{\lfloor \frac{p}{2} \rfloor+1}}) \\ &\cup V(S_{v_{l+2}}) \cup V(S_{v_{l+3}}) \cup \cdots \cup V(S_{v_{\lfloor \frac{q}{2} \rfloor+1}}) \end{aligned}$$

$$Y_1(B_0) \;=\; V(B_0) - Y_2(B_0)$$

Let $E_1(B_0)$ and $E_2(B_0)$ be two subsets of edge set $E(B_0)$ such that

$$\begin{aligned} E_1(B_0) &= E(B_0[Y_1(B_0)]) - \{w_1w_2\} \\ E_2(B_0) &= E(B_0) - E_1(B_0) - \{w_1w_2\} \end{aligned}$$

In a similar way, we define the corresponding items for $B_0^{'}$ as follows.

$$\begin{aligned} &Y_1(B_0^{'}) = Y_1(B_0), \quad Y_2(B_0^{'}) = Y_2(B_0) \\ &E_1(B_0^{'}) = E(B_0^{'}[Y_1(B_0^{'})]) - \{w_1w_2\} \\ &E_2(B_0^{'}) = E(B_0^{'}) - E_1(B_0^{'}) - \{w_1w_2\} \end{aligned}$$

It is easy to see that

$$\begin{aligned} &E(B_0) = E_1(B_0) \cup E_2(B_0) \cup \{w_1w_2\} \\ &E(B_0^{'}) = E_1(B_0^{'}) \cup E_2(B_0^{'}) \cup \{w_1w_2\} \end{aligned}$$

From the definition of the Balaban index, we know that

$$\begin{aligned} \frac{3}{m}J(B_0) &= \sum_{uv\in E_1(B_0)} \frac{1}{\sqrt{\sigma_{B_0}(u)\sigma_{B_0}(v)}} \\ &\quad + \sum_{xy\in E_2(B_0)} \frac{1}{\sqrt{\sigma_{B_0}(x)\sigma_{B_0}(y)}} + \frac{1}{\sqrt{\sigma_{B_0}(w_1)\sigma_{B_0}(w_2)}} \qquad (33) \\ \frac{3}{m}J(B_0^{'}) &= \sum_{uv\in E_1(B_0^{'})} \frac{1}{\sqrt{\sigma_{B_0^{'}}(u)\sigma_{B_0^{'}}(v)}} \\ &\quad + \sum_{xy\in E_2(B_0^{'})} \frac{1}{\sqrt{\sigma_{B_0^{'}}(x)\sigma_{B_0^{'}}(y)}} + \frac{1}{\sqrt{\sigma_{B_0^{'}}(w_1)\sigma_{B_0^{'}}(w_2)}} \qquad (34) \end{aligned}$$

By direct computation, we have

$$\begin{aligned} \sigma_{B_0^{'}}(w_1) &= \sigma_{B_0}(w_1) - |Y_2(B_0)| \\ \sigma_{B_0}(w_2) &= \sigma_{B_0}(w_1) + |Y_1(B_0)| - |Y_2(B_0)| - 2 \end{aligned}$$

Let V and V' be two vertex sets such that

$$\begin{aligned} V &= \{u_i | w_1u_i \in E_{B_0}(S_{w_1}), 1 \le i \le n_1\} \\ V' &= \{u_j | w_1u_j \in E_{B_0^{'}}(S_{w_1}), 1 \le j \le n_1 + n_2 + 1\} \end{aligned}$$

When $u_i \in V$, we can find that

$$\sigma_{B_0}(u_i) \;=\; \sigma_{B_0}(w_1) + n - 2$$

When $1 \le j \le n_1$, $u_j \in V$(i.e., $u_j \in V'$). So we have

$$\begin{aligned}\sigma_{B_0'}(u_j) &= \sigma_{B_0'}(w_2)\\ &= \sigma_{B_0}(u_j) - |Y_2(B_0)|\\ &= \sigma_{B_0}(u_i) - |Y_2(B_0)|\\ &= \sigma_{B_0}(w_1) + |Y_1(B_0)| - 2\end{aligned}$$

When $n_1 + 1 \le j \le n_1 + n_2 + 1$, $u_j \in V'$ and we obtain

$$\sigma_{B_0'}(u_j) = \sigma_{B_0'}(w_2) = \sigma_{B_0}(w_1) + |Y_1(B_0)| - 2$$

Let U be a vertex set such that

$$U = \{u_i | w_2 u_i \in E_{B_0}(S_{w_2}), 1 \le i \le n_2\}$$

When $v \in U$, one can find that

$$\sigma_{B_0}(v) = \sigma_{B_0}(w_2) + n - 2 = \sigma_{B_0}(w_1) + 2|Y_1(B_0)| - 4$$

From the structures of two graphs B_0 and B_0', it is easy to see that

$$E_2(B_0) = \bigcup_{u_i \in U,\ 1 \le i \le n_2} \{w_2 u_i\} \cup \{w_2 w_3\} \cup \overline{E_2}(B_0) \tag{35}$$

$$E_2(B_0') = \bigcup_{u_i \in V',\ 1 \le i \le n_2} \{w_1 u_i\} \cup \{w_1 w_3\} \cup \overline{E_2}(B_0') \tag{36}$$

where

$$\begin{aligned}\overline{E_2}(B_0) &= E_2(B_0) - \bigcup_{u_i \in U,\ 1 \le i \le n_2} \{w_2 u_i\} \cup \{w_2 w_3\}\\ \overline{E_2}(B_0') &= E_2(B_0') - \bigcup_{u_i \in V',\ 1 \le i \le n_2} \{w_1 u_i\} \cup \{w_1 w_3\}\end{aligned}$$

When $u \in Y_2(B_0)$ (i.e., $u \in Y_2(B_0')$), we have

$$\begin{aligned}\sigma_{B_0}(u) &= d_{B_0}(u, w_2) + \sum_{x \in V(B_0) - \{w_2\}} d_{B_0}(u, x)\\ \sigma_{B_0'}(u) &= d_{B_0'}(u, w_2) + \sum_{x \in V(B_0') - \{w_2\}} d_{B_0'}(u, x)\end{aligned}$$

Since $d_{B_0'}(u, w_2) = d_{B_0}(u, w_2) + 1$ and

$$\sum_{x \in V(B_0) - \{w_2\}} d_{B_0}(u, x) - \sum_{x \in V(B_0') - \{w_2\}} d_{B_0'}(u, x) > 1,$$

then

$$\sigma_{B_0}(u) > \sigma_{B_0'}(u) \tag{37}$$

Thus, by (37), we can see that $\sigma_{B_0}(w_3) > \sigma_{B_0'}(w_3)$ and

$$\sum_{xy\in\overline{E_2}(B_0)} \frac{1}{\sqrt{\sigma_{B_0}(x)\sigma_{B_0}(y)}} < \sum_{xy\in\overline{E_2}(B_0')} \frac{1}{\sqrt{\sigma_{B_0'}(x)\sigma_{B_0'}(y)}} \tag{38}$$

Since $\sigma_{B_0}(w_2) > \sigma_{B_0'}(w_1)$, $\sigma_{B_0}(w_3) > \sigma_{B_0'}(w_3)$ and $\sigma_{B_0}(u_i) > \sigma_{B_0'}(u_i)$, where $u_i \in U$ (i.e., $u_i \in V^{'}$), $0 \le i \le n_2$, then

$$\begin{aligned} \sum_{xy\in\{w_2u_i|u_i\in U,1\le i\le n_2\}} \frac{1}{\sqrt{\sigma_{B_0}(x)\sigma_{B_0}(y)}} &< \sum_{xy\in\{w_1u_i|u_i\in V',1\le i\le n_2\}} \frac{1}{\sqrt{\sigma_{B_0'}(x)\sigma_{B_0'}(y)}} \\ \frac{1}{\sqrt{\sigma_{B_0}(w_2)\sigma_{B_0}(w_3)}} &< \frac{1}{\sqrt{\sigma_{B_0'}(w_1)\sigma_{B_0'}(w_3)}} \end{aligned} \tag{39}$$

By (35), (36), (38) and (39), we have

$$\sum_{xy\in E_2(B_0)} \frac{1}{\sqrt{\sigma_{B_0}(x)\sigma_{B_0}(y)}} < \sum_{xy\in E_2(B_0')} \frac{1}{\sqrt{\sigma_{B_0'}(x)\sigma_{B_0'}(y)}} \tag{40}$$

Since $\sigma_{B_0}(w_1)\sigma_{B_0}(w_2) - \sigma_{B_0'}(w_1)\sigma_{B_0'}(w_2) = |Y_2(B_0)|(|Y_1(B_0)| - 2) > 0$, then

$$\frac{1}{\sqrt{\sigma_{B_0}(w_1)\sigma_{B_0}(w_2)}} < \frac{1}{\sqrt{\sigma_{B_0'}(w_1)\sigma_{B_0'}(w_2)}} \tag{41}$$

By the structures of two graphs B_0 and $B_0^{'}$, it is easy to see that

$$E_1(B_0) = \{u_{\lfloor \frac{p}{2}\rfloor+1}u_{\lfloor \frac{p}{2}\rfloor+2}\} \cup \{v_{\lfloor \frac{q}{2}\rfloor+1}v_{\lfloor \frac{q}{2}\rfloor+2}\} \cup \overline{E_1}(B_0) \tag{42}$$

$$E_1(B_0^{'}) = \{u_{\lfloor \frac{p}{2}\rfloor+1}u_{\lfloor \frac{p}{2}\rfloor+2}\} \cup \{v_{\lfloor \frac{q}{2}\rfloor+1}v_{\lfloor \frac{q}{2}\rfloor+2}\} \cup \overline{E_1}(B_0^{'}) \tag{43}$$

where

$$\begin{aligned} \overline{E_1}(B_0) &= E_1(B_0) - \{u_{\lfloor \frac{p}{2}\rfloor+1}u_{\lfloor \frac{p}{2}\rfloor+2}\} \cup \{v_{\lfloor \frac{q}{2}\rfloor+1}v_{\lfloor \frac{q}{2}\rfloor+2}\} \\ \overline{E_1}(B_0^{'}) &= E_1(B_0^{'}) - \{u_{\lfloor \frac{p}{2}\rfloor+1}u_{\lfloor \frac{p}{2}\rfloor+2}\} \cup \{v_{\lfloor \frac{q}{2}\rfloor+1}v_{\lfloor \frac{q}{2}\rfloor+2}\} \end{aligned}$$

When $v \in Y_1(B_0)$ (i.e., $v \in Y_1(B_0^{'})$), since the length of each cycle of $\{C_p, C_q\}$ in $B_0^{'}$ is less exactly one that that in B_0, thus,

$$\sigma_{B_0}(v) > \sigma_{B_0'}(v) \tag{44}$$

Thus, we have

$$\sum_{xy\in\overline{E_1}(B_0)} \frac{1}{\sqrt{\sigma_{B_0}(x)\sigma_{B_0}(y)}} < \sum_{xy\in\overline{E_1}(B_0')} \frac{1}{\sqrt{\sigma_{B_0'}(x)\sigma_{B_0'}(y)}}$$

By (37) and (44), we can see that

$$\frac{1}{\sqrt{\sigma_{B_0}(u_{\lfloor \frac{p}{2}\rfloor+1})\sigma_{B_0}(u_{\lfloor \frac{p}{2}\rfloor+2})}} < \frac{1}{\sqrt{\sigma_{B_0'}(u_{\lfloor \frac{p}{2}\rfloor+1})\sigma_{B_0'}(u_{\lfloor \frac{p}{2}\rfloor+2})}}$$

$$\frac{1}{\sqrt{\sigma_{B_0}(u_{\lfloor \frac{g}{2} \rfloor+1})\sigma_{B_0}(u_{\lfloor \frac{g}{2} \rfloor+2})}} < \frac{1}{\sqrt{\sigma_{B_0'}(u_{\lfloor \frac{g}{2} \rfloor+1})\sigma_{B_0'}(u_{\lfloor \frac{g}{2} \rfloor+2})}}$$

So we obtain

$$\sum_{uv\in E_1(B_0)} \frac{1}{\sqrt{\sigma_{B_0}(u)\sigma_{B_0}(v)}} < \sum_{uv\in E_1(B_0')} \frac{1}{\sqrt{\sigma_{B_0'}(u)\sigma_{B_0'}(v)}} \tag{45}$$

Hence, the result holds from (33), (34), (40), (41) and (45). □

By using Lemma 4 or Lemma 5 repeatedly, the bicyclic graphs B or B_0 may be transformed into the graph B_1 (see Fig 8.), and the corresponding Balaban index increases gradually along with the length of the cycles decreasing.

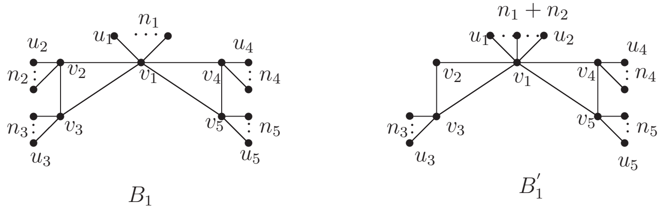

Fig. 8. Graphs B_1 and B_1'

Let B_1 be a bicyclic graph in $\mathcal{B}_n^*(3,3)$ with $\{v_1, v_2, v_3, v_4, v_5\}$ as the vertex set of its two triangles such that each vertex v_i has n_i pendent vertices and u_i is a pendent vertex of v_i, where $1 \le i \le 5$, and v_1 be the unique common vertex of the triangles. Let B_1' be the graph obtained from B_1 by changing all the pendent edges attached at v_2 into the ones attached at v_1 such that there are $n_1 + n_2$ pendent edges attached at v_1, that is,

$$B_1' = B_1 - \{v_2x | x \in N_{B_1}(v_2) \setminus \{v_1, v_3\}\} + \{v_1x | x \in N_{B_1}(v_2) \setminus \{v_1, v_3\}\}$$

Lemma 6. $J(B_1) < J(B_1')$.

Proof. By the definition of the Balaban index and the structures of the graphs B_1 and B_1', we know that

$$\begin{aligned}\frac{3}{m}J(B_1) \;=\; & \frac{n_1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(u_1)}} + \frac{n_2}{\sqrt{\sigma_{B_1}(v_2)\sigma_{B_1}(u_2)}} + \frac{n_3}{\sqrt{\sigma_{B_1}(v_3)\sigma_{B_1}(u_3)}} + \\ & \frac{n_4}{\sqrt{\sigma_{B_1}(v_4)\sigma_{B_1}(u_4)}} + \frac{n_5}{\sqrt{\sigma_{B_1}(v_5)\sigma_{B_1}(u_5)}} + \frac{1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(v_2)}} + \\ & \frac{1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(v_3)}} + \frac{1}{\sqrt{\sigma_{B_1}(v_2)\sigma_{B_1}(v_3)}} + \frac{1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(v_4)}} + \\ & \frac{1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(v_5)}} + \frac{1}{\sqrt{\sigma_{B_1}(v_4)\sigma_{B_1}(v_5)}}\end{aligned} \tag{46}$$

$$\begin{aligned}\frac{3}{m}J(B_1^{'}) &= \frac{n_1+n_2}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(u_1)}}+\frac{n_3}{\sqrt{\sigma_{B_1'}(v_3)\sigma_{B_1'}(u_3)}}+\frac{n_4}{\sqrt{\sigma_{B_1'}(v_4)\sigma_{B_1'}(u_4)}}+\\ &\frac{n_5}{\sqrt{\sigma_{B_1'}(v_5)\sigma_{B_1'}(u_5)}}+\frac{1}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_2)}}+\frac{1}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_3)}}+\\ &\frac{1}{\sqrt{\sigma_{B_1'}(v_2)\sigma_{B_1'}(v_3)}}+\frac{1}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_4)}}+\frac{1}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_5)}}+\\ &\frac{1}{\sqrt{\sigma_{B_1'}(v_4)\sigma_{B_1'}(v_5)}} \qquad (47)\end{aligned}$$

By direct calculation, we have

$$\begin{aligned}&\sigma_{B_1}(v_1)=2n-n_1-6, && \sigma_{B_1}(u_1)=3n-n_1-8\\ &\sigma_{B_1}(v_2)=2n-n_2+n_4+n_5-4, && \sigma_{B_1}(u_2)=3n-n_2+n_4+n_5-6\\ &\sigma_{B_1}(v_3)=2n-n_3+n_4+n_5-4, && \sigma_{B_1}(u_3)=3n-n_3+n_4+n_5-6\\ &\sigma_{B_1}(v_4)=2n-n_4+n_2+n_3-4, && \sigma_{B_1}(u_4)=3n-n_4+n_2+n_3-6\\ &\sigma_{B_1}(v_5)=2n-n_5+n_2+n_3-4, && \sigma_{B_1}(u_5)=3n-n_5+n_2+n_3-6\end{aligned}$$

and

$$\begin{aligned}&\sigma_{B_1'}(v_1)=2n-n_1-n_2-6\\ &\sigma_{B_1'}(u_1)=\sigma_{B_1'}(u_2)=3n-n_1-n_2-8\\ &\sigma_{B_1'}(v_2)=2n+n_4+n_5-4\\ &\sigma_{B_1'}(v_3)=\sigma_{B_1}(v_3), && \sigma_{B_1'}(u_3)=\sigma_{B_1}(u_3)\\ &\sigma_{B_1'}(v_4)=2n+n_3-n_4-4, && \sigma_{B_1'}(v_5)=2n-n_5+n_3-4\\ &\sigma_{B_1'}(u_4)=3n+n_3-n_4-6, && \sigma_{B_1'}(u_5)=3n-n_5+n_3-6\end{aligned}$$

Thus, we easily find that

$$\begin{aligned}&\sigma_{B_1}(v_1)\sigma_{B_1}(u_1)>\sigma_{B_1'}(v_1)\sigma_{B_1'}(u_1), && \sigma_{B_1}(v_2)\sigma_{B_1}(u_2)>\sigma_{B_1'}(v_1)\sigma_{B_1'}(u_1)\\ &\sigma_{B_1}(v_3)\sigma_{B_1}(u_3)=\sigma_{B_1'}(v_3)\sigma_{B_1'}(u_3), && \sigma_{B_1}(v_5)\sigma_{B_1}(u_5)>\sigma_{B_1'}(v_5)\sigma_{B_1'}(u_5)\\ &\sigma_{B_1}(v_4)\sigma_{B_1}(u_4)>\sigma_{B_1'}(v_4)\sigma_{B_1'}(u_4), && \sigma_{B_1}(v_1)\sigma_{B_1}(v_2)>\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_2)\\ &\sigma_{B_1}(v_1)\sigma_{B_1}(v_3)>\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_3), && \sigma_{B_1}(v_1)\sigma_{B_1}(v_4)>\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_4)\\ &\sigma_{B_1}(v_1)\sigma_{B_1}(v_5)>\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_5), && \sigma_{B_1}(v_4)\sigma_{B_1}(v_5)>\sigma_{B_1'}(v_4)\sigma_{B_1'}(v_5)\\ &\sigma_{B_1}(v_2)\sigma_{B_1}(v_3)<\sigma_{B_1'}(v_2)\sigma_{B_1'}(v_3)\end{aligned}$$

So we have

$$\frac{n_1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(u_1)}}+\frac{n_2}{\sqrt{\sigma_{B_1}(v_2)\sigma_{B_1}(u_2)}}<\frac{n_1+n_2}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(u_1)}}$$

$$\frac{n_3}{\sqrt{\sigma_{B_1}(v_3)\sigma_{B_1}(u_3)}} = \frac{n_3}{\sqrt{\sigma_{B_1'}(v_3)\sigma_{B_1'}(u_3)}}, \quad \frac{n_5}{\sqrt{\sigma_{B_1}(v_5)\sigma_{B_1}(u_5)}} < \frac{n_5}{\sqrt{\sigma_{B_1'}(v_5)\sigma_{B_1'}(u_5)}}$$
$$\frac{n_4}{\sqrt{\sigma_{B_1}(v_4)\sigma_{B_1}(u_4)}} < \frac{n_4}{\sqrt{\sigma_{B_1'}(v_4)\sigma_{B_1'}(u_4)}}, \quad \frac{1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(v_2)}} < \frac{1}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_2)}}$$
$$\frac{1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(v_3)}} < \frac{1}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_3)}}, \quad \frac{1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(v_4)}} < \frac{1}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_4)}}$$
$$\frac{1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(v_5)}} < \frac{1}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_5)}}, \quad \frac{1}{\sqrt{\sigma_{B_1}(v_4)\sigma_{B_1}(v_5)}} < \frac{1}{\sqrt{\sigma_{B_1'}(v_4)\sigma_{B_1'}(v_5)}}$$
$$\frac{1}{\sqrt{\sigma_{B_1}(v_2)\sigma_{B_1}(v_3)}} > \frac{1}{\sqrt{\sigma_{B_1'}(v_2)\sigma_{B_1'}(v_3)}} \tag{48}$$

Claim 6.1.

$$\frac{1}{\sqrt{\sigma_{B_1}(v_1)\sigma_{B_1}(v_3)}} + \frac{1}{\sqrt{\sigma_{B_1}(v_2)\sigma_{B_1}(v_3)}} < \frac{1}{\sqrt{\sigma_{B_1'}(v_1)\sigma_{B_1'}(v_3)}} + \frac{1}{\sqrt{\sigma_{B_1'}(v_2)\sigma_{B_1'}(v_3)}}$$

i.e.

$$\frac{1}{\sqrt{2n-n_3+n_4+n_5-4}}\Big(\frac{1}{\sqrt{2n-n_1-6}} + \frac{1}{\sqrt{2n-n_2+n_4+n_5-4}} - \frac{1}{\sqrt{2n-n_1-n_2-6}} - \frac{1}{\sqrt{2n+n_4+n_5-4}}\Big) < 0$$

With the same method as Claim 3.1, Claim 6.1 follows. So the result holds by (46)-(48) and Claim 6.1. □

Hence, by Lemma 6, the bicyclic graph B_1 is transformed into the bicyclic graph B'' (see Fig 11.) and the corresponding Balaban index increases.

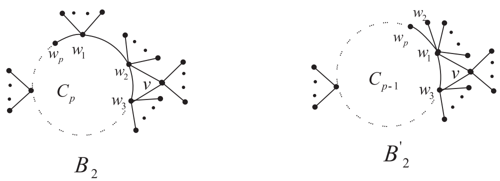

Fig. 9. Graphs B_2 and B'_2

Let B_2 be a bicyclic graph in $\mathcal{B}_n^{**}(p,1,3)$, where $p > 3$, with $\{w_1, w_2, \cdots, w_p\}$ and $\{w_2, w_3, v\}$ as the vertex sets of its cycles C_p and C_3, respectively, where w_2 and w_3 are the common vertices of the cycles, and w_1 and w_2 be the centers of two adjacent stars. Let B_2' be the graph obtained from B_2 by identifying w_1 and w_2 and changing the edge w_1w_2 into a pendent edge attached at w_1, that is,

$$B_2' = B_2 - \{w_2x | x \in N_{B_2}(w_2) \setminus \{w_1\}\} + \{w_1x | x \in N_{B_2}(w_2) \setminus \{w_1\}\}$$

The graphs B_2 and $B_2^{'}$ are shown in Fig 9.

With the same method as Lemma 2, we have

Lemma 7. $J(B_2) < J(B_2^{'})$.

So using Lemma 7 repeatedly, the bicyclic graphs B_2 can be transformed into the graph B_3 (see Fig 10.), and the corresponding Balaban index increases gradually along with the length of the cycle decreasing.

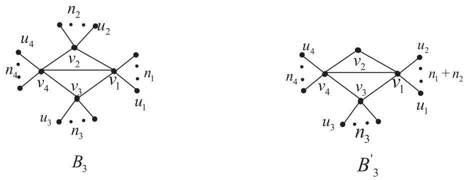

Fig. 10. Graphs B_3 and B'_3

Let B_3 be a bicyclic graph in $\mathcal{B}_n^{**}(3,1,3)$ with $\{v_1, v_2, v_3, v_4\}$ as the vertex set of its two triangles such that each vertex v_i has n_i pendent vertices and u_i is a pendent vertex of vertex v_i, where $1 \leq i \leq 4$, and v_1 and v_3 be the common vertices of the triangles. Let $B_3^{'}$ be the graph obtained from B_3 by changing all the pendent edges attached at v_2 into the ones attached at v_1 such that there are $n_1 + n_2$ pendent edges attached at v_1, that is,

$$B_3^{'} = B_3 - \{v_2x | x \in N_{B_3}(v_2) \setminus \{v_1, v_3\}\} + \{v_1x | x \in N_{B_3}(v_2) \setminus \{v_1, v_3\}\}$$

The graphs B_3 and $B_3^{'}$ are shown in Fig 10.

Lemma 8. $J(B_3) < J(B_3^{'})$.

Proof. By the definition of the Balaban index and the structures of B_3 and $B_3^{'}$, we know that

$$\begin{aligned}\frac{3}{m}J(B_3) &= \frac{n_1}{\sqrt{\sigma_{B_3}(v_1)\sigma_{B_3}(u_1)}} + \frac{n_2}{\sqrt{\sigma_{B_3}(v_2)\sigma_{B_3}(u_2)}} \\ &+ \frac{n_3}{\sqrt{\sigma_{B_3}(v_3)\sigma_{B_3}(u_3)}} + \frac{n_4}{\sqrt{\sigma_{B_3}(v_4)\sigma_{B_3}(u_4)}} \\ &+ \frac{1}{\sqrt{\sigma_{B_3}(v_1)\sigma_{B_3}(v_2)}} + \frac{1}{\sqrt{\sigma_{B_3}(v_2)\sigma_{B_3}(v_3)}} \\ &+ \frac{1}{\sqrt{\sigma_{B_3}(v_1)\sigma_{B_3}(v_3)}} + \frac{1}{\sqrt{\sigma_{B_3}(v_1)\sigma_{B_3}(v_4)}} \\ &+ \frac{1}{\sqrt{\sigma_{B_3}(v_3)\sigma_{B_3}(v_4)}} \end{aligned} \quad (49)$$

$$\begin{aligned}\frac{3}{m}J(B_3') &= \frac{n_1+n_2}{\sqrt{\sigma_{B_3'}(v_1)\sigma_{B_3'}(u_1)}}+\frac{n_3}{\sqrt{\sigma_{B_3'}(v_3)\sigma_{B_3'}(u_3)}}\\ &+\frac{n_4}{\sqrt{\sigma_{B_3'}(v_4)\sigma_{B_3'}(u_4)}}+\frac{1}{\sqrt{\sigma_{B_3'}(v_1)\sigma_{B_3'}(v_2)}}\\ &+\frac{1}{\sqrt{\sigma_{B_3'}(v_2)\sigma_{B_3'}(v_3)}}+\frac{1}{\sqrt{\sigma_{B_3'}(v_1)\sigma_{B_3'}(v_3)}}\\ &+\frac{1}{\sqrt{\sigma_{B_3'}(v_1)\sigma_{B_3'}(v_4)}}+\frac{1}{\sqrt{\sigma_{B_3'}(v_3)\sigma_{B_3'}(v_4)}} \qquad (50)\end{aligned}$$

By direct calculation, we have

$$\begin{aligned}&\sigma_{B_3}(v_1)=2n-n_1-5, \quad \sigma_{B_3}(u_1)=3n-n_1-7\\ &\sigma_{B_3}(v_3)=2n-n_3-5, \quad \sigma_{B_3}(u_3)=3n-n_3-7\\ &\sigma_{B_3}(v_2)=2n+n_4-n_2-4, \quad \sigma_{B_3}(u_2)=3n+n_4-n_2-6\\ &\sigma_{B_3}(v_4)=2n+n_2-n_4-4, \quad \sigma_{B_3}(u_4)=3n+n_2-n_4-6\end{aligned}$$

$$\begin{aligned}&\sigma_{B_3'}(v_1)=n+n_3+n_4-1, \quad \sigma_{B_3'}(u_1)=2n+n_3+n_4-3\\ &\sigma_{B_3'}(v_2)=2n+n_4-4, \quad \sigma_{B_3'}(v_3)=2n-n_3-5\\ &\sigma_{B_3'}(u_3)=3n-n_3-7, \quad \sigma_{B_3'}(v_4)=2n-n_4-4\\ &\sigma_{B_3'}(u_4)=3n-n_4-6\end{aligned}$$

Thus, we easily find that

$$\begin{aligned}\sigma_{B_3}(v_1)\sigma_{B_3}(u_1) &> \sigma_{B_3'}(v_1)\sigma_{B_3'}(u_1)\\ \sigma_{B_3}(v_2)\sigma_{B_3}(u_2) &> \sigma_{B_3'}(v_1)\sigma_{B_3'}(u_1)\\ \sigma_{B_3}(v_1)\sigma_{B_3}(v_2) &> \sigma_{B_3'}(v_1)\sigma_{B_3'}(v_2)\\ \sigma_{B_3}(v_2)\sigma_{B_3}(v_3) &< \sigma_{B_3'}(v_2)\sigma_{B_3'}(v_3)\end{aligned}$$

So by (49) and (50), we have

$$\frac{n_1}{\sqrt{\sigma_{B_3}(v_1)\sigma_{B_3}(u_1)}}+\frac{n_2}{\sqrt{\sigma_{B_3}(v_2)\sigma_{B_3}(u_2)}}<\frac{n_1+n_2}{\sqrt{\sigma_{B_3'}(v_1)\sigma_{B_3'}(u_1)}}$$

$$\frac{n_3}{\sqrt{\sigma_{B_3}(v_3)\sigma_{B_3}(u_3)}}=\frac{n_3}{\sqrt{\sigma_{B_3'}(v_3)\sigma_{B_3'}(u_3)}}, \quad \frac{n_4}{\sqrt{\sigma_{B_3}(v_4)\sigma_{B_3}(u_4)}}<\frac{n_4}{\sqrt{\sigma_{B_3'}(v_4)\sigma_{B_3'}(u_4)}}$$

$$\frac{1}{\sqrt{\sigma_{B_3}(v_1)\sigma_{B_3}(v_2)}}<\frac{1}{\sqrt{\sigma_{B_3'}(v_1)\sigma_{B_3'}(v_2)}}, \quad \frac{1}{\sqrt{\sigma_{B_3}(v_1)\sigma_{B_3}(v_3)}}<\frac{1}{\sqrt{\sigma_{B_3'}(v_1)\sigma_{B_3'}(v_3)}}$$

$$\frac{1}{\sqrt{\sigma_{B_3}(v_1)\sigma_{B_3}(v_4)}}<\frac{1}{\sqrt{\sigma_{B_3'}(v_1)\sigma_{B_3'}(v_4)}}, \quad \frac{1}{\sqrt{\sigma_{B_3}(v_3)\sigma_{B_3}(v_4)}}<\frac{1}{\sqrt{\sigma_{B_3'}(v_3)\sigma_{B_3'}(v_4)}}$$

$$\frac{1}{\sqrt{\sigma_{B_3}(v_2)\sigma_{B_3}(v_3)}} > \frac{1}{\sqrt{\sigma_{B_3'}(v_2)\sigma_{B_3'}(v_3)}} \tag{51}$$

Claim 8.1.

$$\frac{1}{\sqrt{\sigma_{B_3}(v_2)\sigma_{B_3}(v_3)}} + \frac{1}{\sqrt{\sigma_{B_3}(v_1)\sigma_{B_3}(v_3)}} < \frac{1}{\sqrt{\sigma_{B_3'}(v_2)\sigma_{B_3'}(v_3)}} + \frac{1}{\sqrt{\sigma_{B_3'}(v_1)\sigma_{B_3'}(v_3)}}$$

i.e.

$$\frac{1}{\sqrt{2n-n_3-5}}\Big(\frac{1}{\sqrt{2n+n_4-n_2-4}} + \frac{1}{\sqrt{2n-n_1-5}} - \frac{1}{\sqrt{2n+n_4-4}} - \frac{1}{\sqrt{n+n_3+n_4-1}}\Big) < 0$$

With the same method as Claim 3.1, Claim 8.1 follows. Hence, the result follows by (49)-(51) and Claim 8.1. □

From Lemma 8, the bicyclic graphs B_3 can be transformed into the graph B_0'' (see Fig 11.), and the corresponding Balaban index increases.

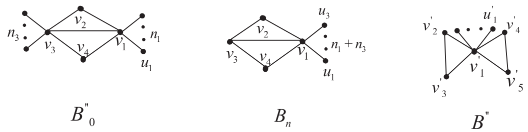

Fig. 11. Graphs B''_0 , B_n and B''

Let B_0'' be a bicyclic graph in $\mathcal{B}_n^{**}(3,1,3)$ with $\{v_1,v_2,v_3,v_4\}$ as the vertex set of its two triangles such that vertex v_i has n_i pendent vertices and u_i is a pendent vertex of v_i, where $1 \le i \le 4$ and $n_2 = n_4 = 0$ when $i = 2,4$, and v_1 and v_3 be the common vertices of the triangles. The bicyclic graph B_n is obtained from B_0'' by changing all the pendent edges attached at v_3 into the ones attached at v_1 such that there are n_1+n_3 pendent edges attached at v_1, that is,

$$B_n = B_0'' - \{v_3x | x \in N_{B_0''}(v_3) \setminus \{v_1,v_2,v_4\}\} + \{v_1x | x \in N_{B_0''}(v_3) \setminus \{v_1,v_2,v_4\}\}$$

Let B'' be a bicyclic graph in $\mathcal{B}_n^{*}(3,3)$ with $\{v_1',v_2',v_3',v_4',v_5'\}$ as the vertex set of its two triangles and u_1' be a pendent vertex of vertex v_1', where v_1' is the unique common vertex of the triangles to which there are $n-5$ pendent edges attached so that there are no ones attached at other vertices on the triangles. Three graphs B_0'', B_n and B'' are shown in Fig 11.

Lemma 9. $J(B_0'') < J(B_n)$.

Proof. From the structures of the graphs B_0'' and B_n, we obtain

$$\sigma_{B_0''}(v_2) = \sigma_{B_0''}(v_4) = \sigma_{B_n}(v_2) = \sigma_{B_n}(v_4)$$

Thus, by the definition of the Balaban index, we know that

$$\begin{aligned}\frac{3}{m}J(B_0'') &= \frac{n_1}{\sqrt{\sigma_{B_0''}(v_1)\sigma_{B_0''}(u_1)}}+\frac{n_3}{\sqrt{\sigma_{B_0''}(v_3)\sigma_{B_0''}(u_3)}}\\&+\frac{1}{\sqrt{\sigma_{B_0''}(v_1)\sigma_{B_0''}(v_3)}}+\frac{2}{\sqrt{\sigma_{B_0''}(v_1)\sigma_{B_0''}(v_2)}}\\&+\frac{2}{\sqrt{\sigma_{B_0''}(v_2)\sigma_{B_0''}(v_3)}}\end{aligned}\tag{52}$$

$$\begin{aligned}\frac{3}{m}J(B_n) &= \frac{n_1+n_3}{\sqrt{\sigma_{B_n}(v_1)\sigma_{B_n}(u_1)}}+\frac{1}{\sqrt{\sigma_{B_n}(v_1)\sigma_{B_n}(v_3)}}+\\&\frac{2}{\sqrt{\sigma_{B_n}(v_1)\sigma_{B_n}(v_2)}}+\frac{2}{\sqrt{\sigma_{B_n}(v_2)\sigma_{B_n}(v_3)}}\end{aligned}\tag{53}$$

By direct computation, we have

$$\begin{aligned}&\sigma_{B_0''}(v_1)=2n-n_1-5, && \sigma_{B_0''}(u_1)=3n-n_1-7\\&\sigma_{B_0''}(v_3)=2n-n_3-5, && \sigma_{B_0''}(u_3)=3n-n_3-7\\&\sigma_{B_0''}(v_2)=\sigma_{B_0''}(v_4)=2n-4, && \sigma_{B_n}(v_1)=n-1\\&\sigma_{B_n}(u_1)=\sigma_{B_n}(u_3)=2n-3, && \sigma_{B_n}(v_2)=\sigma_{B_n}(v_4)=2n-4\\&\sigma_{B_n}(v_3)=2n-5\end{aligned}$$

So we easily find that

$$\begin{aligned}&\sigma_{B_0''}(v_1)\sigma_{B_0''}(u_1)>\sigma_{B_n}(v_1)\sigma_{B_n}(u_1), && \sigma_{B_0''}(v_3)\sigma_{B_0''}(u_3)>\sigma_{B_n}(v_1)\sigma_{B_n}(u_1)\\&\sigma_{B_0''}(v_1)\sigma_{B_0''}(v_3)>\sigma_{B_n}(v_1)\sigma_{B_n}(v_3), && \sigma_{B_0''}(v_1)\sigma_{B_0''}(v_2)>\sigma_{B_n}(v_1)\sigma_{B_n}(v_2)\\&\sigma_{B_0''}(v_2)\sigma_{B_0''}(v_3)<\sigma_{B_n}(v_2)\sigma_{B_n}(v_3)\end{aligned}$$

Thus,

$$\frac{n_1}{\sqrt{\sigma_{B_0''}(v_1)\sigma_{B_0''}(u_1)}}+\frac{n_3}{\sqrt{\sigma_{B_0''}(v_3)\sigma_{B_0''}(u_3)}}<\frac{n_1+n_3}{\sqrt{\sigma_{B_n}(v_1)\sigma_{B_n}(u_1)}}\tag{54}$$

and

$$\begin{aligned}\frac{1}{\sqrt{\sigma_{B_0''}(v_1)\sigma_{B_0''}(v_3)}}&<\frac{1}{\sqrt{\sigma_{B_n}(v_1)\sigma_{B_n}(v_3)}}\\\frac{2}{\sqrt{\sigma_{B_0''}(v_1)\sigma_{B_0''}(v_2)}}&<\frac{2}{\sqrt{\sigma_{B_n}(v_1)\sigma_{B_n}(v_2)}}\\\frac{2}{\sqrt{\sigma_{B_0''}(v_2)\sigma_{B_0''}(v_3)}}&>\frac{2}{\sqrt{\sigma_{B_n}(v_2)\sigma_{B_n}(v_3)}}\end{aligned}\tag{55}$$

Claim 9.1.

$$\frac{2}{\sqrt{\sigma_{B''_0}(v_1)\sigma_{B''_0}(v_2)}}+\frac{2}{\sqrt{\sigma_{B''_0}(v_2)\sigma_{B''_0}(v_3)}}<\frac{2}{\sqrt{\sigma_{B_n}(v_1)\sigma_{B_n}(v_2)}}+\frac{2}{\sqrt{\sigma_{B_n}(v_2)\sigma_{B_n}(v_3)}}$$

i.e.,

$$\frac{2}{\sqrt{2n-4}}\left(\frac{1}{\sqrt{2n-n_1-5}}+\frac{1}{\sqrt{2n-n_3-5}}-\frac{1}{\sqrt{n-1}}-\frac{1}{\sqrt{2n-5}}\right)<0$$

With the same method as Claim 3.1, Claim 9.1 follows. So the result follows by (52)-(55) and Claim 9.1. □

From above lemmas, we focus on seeking the bicyclic graph with the largest Balaban index in the bicyclic graphs B'' and B_n.

Lemma 10. $J(B'') < J(B_n)$.
Proof. By direct calculation, we have

$$\sigma_{B_n}(v_1)=n-1,\quad \sigma_{B_n}(u_1)=2n-3,\quad \sigma_{B_n}(v_2)=2n-4,\quad \sigma_{B_n}(v_3)=2n-5$$
$$\sigma_{B''}(v'_1)=n-1,\quad \sigma_{B''}(u'_1)=2n-3,\quad \sigma_{B''}(v'_2)=2n-4$$

From the structures of two graphs B_n and B'', we obtain

$$\sigma_{B_n}(v_2)=\sigma_{B_n}(v_4)=\sigma_{B''}(v'_2)=\sigma_{B''}(v'_3)=\sigma_{B''}(v'_4)=\sigma_{B''}(v'_5)$$
$$\sigma_{B_n}(v_1)=\sigma_{B''}(v'_1),\quad \sigma_{B_n}(u_1)=\sigma_{B''}(u'_1)$$

Thus,

$$\begin{aligned} J(B_n)-J(B'') &= \frac{1}{\sqrt{(n-1)(2n-5)}}+\frac{2}{\sqrt{(2n-4)(2n-5)}}+\frac{1}{\sqrt{(n-1)(2n-3)}}\\ &\quad -\left(\frac{2}{\sqrt{(n-1)(2n-4)}}+\frac{2}{\sqrt{(2n-4)(2n-4)}}\right)\\ &= \frac{2}{\sqrt{2n-4}}\left(\frac{1}{\sqrt{2n-5}}-\frac{1}{\sqrt{2n-4}}\right)\\ &\quad +\frac{1}{\sqrt{n-1}}\left(\frac{1}{\sqrt{2n-5}}-\frac{2}{\sqrt{2n-4}}+\frac{1}{\sqrt{2n-3}}\right)>0 \end{aligned}$$

This finishes the proof. □

Proof of Theorem 2. Let G and G' be two graphs and denote by $G \longrightarrow G'$ graph G is transformed into graph G' . When $G \in \mathcal{B}_n$, we distinguish the following two cases.
Case 1. $G \in \mathcal{B}_n^+$. Then we take the following transformations:

$$G \longrightarrow B \longrightarrow B_1 \longrightarrow B''$$

So by Lemma 1, Lemma 4 and Lemma 6, we can see that

$$J(G) < J(B) < J(B_1) < J(B^{''})$$

Hence, the result follows from Lemma 10.

Case 2. $G \in \mathcal{B}_n^{++}$. We discuss two subcases as follows.
Subcase 2.1. The graph G has no triangle C_3 as its subgraph. Then we take one of the following two types of transformations (I) and (II):

$$(I)\ G \longrightarrow B_0 \longrightarrow B \longrightarrow B_1 \longrightarrow B^{''}$$

$$(II)\ G \longrightarrow B_0 \longrightarrow B_2 \longrightarrow B_3 \longrightarrow B_0^{''} \longrightarrow B_n$$

When we take transformations (I), by Lemma 1 and lemmas 4-6, we obtain

$$J(G) < J(B_0) < J(B) < J(B_1) < J(B^{''})$$

So the result holds by Lemma 10.
When we take transformations (II), by Lemma 1, Lemma 5 and lemmas 7-9, we have

$$J(G) < J(B_0) < J(B_2) < J(B_3) < J(B_0^{''}) < J(B_n)$$

Thus, the result follows.

Subcase 2.2. The graph G has at least one triangle C_3 as its subgraph. Then we take the following transformations :

$$G \longrightarrow B_2 \longrightarrow B_3 \longrightarrow B_0^{''} \longrightarrow B_n$$

Therefore, by Lemma 1 and lemmas 7-9, we have

$$J(G) < J(B_2) < J(B_3) < J(B_0^{''}) < J(B_n)$$

Hence, this finishes the proof. □