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Maximum Balaban index and sum-Balaban index of cacti

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Abstract: The Balaban index and sum-Balaban index were used in various quantitative structure-property relationship and quantitative structure activity relationship studies. Here the upper bounds of Balaban index and sum-Balaban index among all cacti were given and the cacti that attain the bounds were characterized.

Key words: cactus; Balaban index; sum-Balaban index; maximum

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仙人掌图的最大 Balaban 指数和 sum-Balaban 指数

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摘要:Balaban 指数与 sum-Balaban 指数被广泛地应用于定量结构性质和定量活性性质的研究.确定了仙人掌图 Balaban 指数与 sum-Balaban 指数的上界,并刻画了所有取得上界的极图.

关键词:仙人掌图;Balaban 指数;sum-Balaban 指数;极大值

0 Introduction

Molecular topology can be expressed numerically in term of molecular descriptors, and among these descriptors topological indices occupy a special place because they are more complex than counts of atoms, groups or bonds, but less complicated than quantum-chemical parameters.

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Consequently, they can be computed in a very short time from various types of input data on atom connectivities, and be used for quantitative structure-property relationship (QSPR) and quantitative structure activity relationship (QSAR).

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

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

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

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

where the distance between vertices u and v in G is denoted by $d_G(u,v)$ and $D_G(u)=\sum_{v\in V(G)} d_G(u,v)$ (or $D(u)$ for short) is the distance sum of vertex u in G. $\mu=|E(G)|-|V(G)|+1=m-n+1$ is the cyclomatic number.

In 2002, Balaban[4] compared the ordering of constitutional isomers of alkanes with 6～9 carbon atoms. It was shown that the ordering induced by Balaban index parallels the ordering induced by Wiener index, but reduces the degeneracy of the latter index and provides a much higher discriminating ability.

The behavior of Balaban index mimics the behavior of the melting temperatures and glass transition temperatures for linear macromolecules, which possess an asymptotic limit for these physical properties. The asymptotic value of Balaban index for an infinite path is the number $\pi=3.14159$ in Ref. [3] and the asymptotic properties for Fibonacci trees are analyzed in Ref. [5].

For chemical applications, it may be interesting to identify the graphs with the maximum and minimum topological indices in a given class of graphs. Deng[6] proved that among all trees with n vertices, the star S_n and the path P_n have the maximal and the minimal Balaban index, respectively. Fang et al.[7] gave the upper bounds of Balaban index and sum-Balaban index for bicyclic graphs, and characterized the bicyclic graphs which attain the sharp upper bounds. You and Dong[8] gave the unicyclic graphs with the maximum Balaban index and the maximum sum-Balaban index among all unicyclic graphs on n vertices. More mathematical properties of Balaban index can be found in Refs. [9-12]. More mathematical properties of sum-Balaban index can be found in Refs. [10-11,13-14].

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

Let G be a graph and $\emptyset\neq U\subseteq V(G)$. The subgraph of G whose vertex set is U and whose edge set is the set of edges of G that have both ends in U is called the subgraph of G induced by U and is denoted by $G[U]$. We say that $G[U]$ is an induced subgraph of G. The induced subgraph $G[V(G)\backslash U]$ is denoted by $G-U$. If $U=\{v\}$, we write $G-v$ for $G-\{v\}$. For any vertex $v\in V(G)$, we define $D_G(v,U)=\sum_{u\in U} d_G(v,u)$.

A block of a graph G is a maximal 2-connected subgraph of G. A cactus graph is a connected graph in which no edge lies in more than one cycle, such that each block of a cactus graph is either an edge or a cycle. A vertex shared by two or more cycles is called a cut-vertex. We denote C_n^l the set of all cactus graphs of order n and l cycles. Obviously, C_n^0 are trees and C_n^1 are unicyclic graphs. Refs. [6,8] obtained the upper bounds on the Balaban index (sum-Balaban index) of trees and unicyclic graphs, respectively. In this paper, we let $l\geqslant 2$ and then $n\geqslant 2l+1$.

If all blocks of a cactus G are cycles of the same length m, the cactus is m-uniform. A hexagonal cactus is a 6-uniform cactus such that every block of the graph is a hexagon. If each hexagon of a hexagonal cactus G has at most two cut-vertices and each cut-vertex is shared by exactly two hexagons, we say that G is a chain hexagonal cactus (see Fig. 1). More information on cacti can be found in Refs. [15-20].

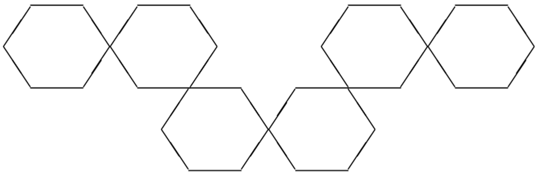

Fig. 1 A chain hexagonal cactus

In this paper, we obtain the upper bounds of Balaban index and sum-Balaban index among cacti, and characterize the cacti which attain the bounds. In Section 1, we introduce some useful lemmas and some useful graph transformations, and study the changes of Balaban index and sum-Balaban index of a cactus graph after these transformations. In Section 2, we will give sharp upper bounds on Balaban index and sum-Balaban index of cacti.

1 Some useful graph transformations

In this section, we will introduce some useful lemmas and some useful graph transformations.

Lemma 1.1[9] Let $x, y, a \in \mathbb{R}^+$ such that $x \geqslant y + a$. Then $\frac{1}{\sqrt{xy}} \geqslant \frac{1}{\sqrt{(x-a)(y+a)}}$, and the equality holds if and only if $x = y + a$.

Lemma 1.2[8] Let $x_1, x_2, y_1, y_2 \in \mathbb{R}^+$ such that $x_1 > y_1$ and $x_2 - x_1 = y_2 - y_1 > 0$. Then $\frac{1}{\sqrt{x_1}} + \frac{1}{\sqrt{y_2}} < \frac{1}{\sqrt{x_2}} + \frac{1}{\sqrt{y_1}}$.

1.1 Edge-lifting transformation

Let G_1 and G_2 be two graphs with $n_1 \geqslant 2$ and $n_2 \geqslant 2$ 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 v_0, then G' is called the edge-lifting transformation of G (see Fig. 2).

Lemma 1.3[6,14] Let G' be the edge-lifting transformation of G. Then $J(G) < J(G')$, and $SJ(G) < SJ(G')$.

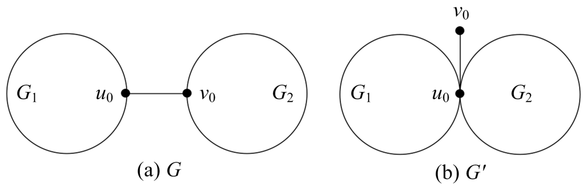

Fig. 2 The edge-lifting transformation

By Lemma 1.3, we can verify that if $C \in C_n^l$ attains the maximum Balaban index and sum-Balaban index of all graphs in C_n^l, then C is a cactus graph as shown in Fig. 3 and the following five conditions hold.

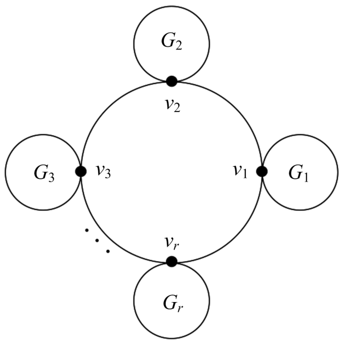

Fig. 3 The cactus graph C

(i) $3 \leqslant r \leqslant n - 2l + 2$;

(ii) each cycle of cactus graph C has at least one cut-vertex;

(iii) G_i is a cactus graph, or pendent edges, or a vertex, where $1 \leqslant i \leqslant r$;

(iv) $G_i \cap G_j = \varnothing$ for any $1 \leqslant i < j \leqslant r$;

(v) there are $l-1$ cycles in $G_1 \cup G_2 \cup G_3 \cup \cdots \cup G_r$.

Fig. 4 shows an example of how to obtain C by repeating edge-lifting transformations from a cactus graph $\mathscr{G}$, where $V(G_1) = \{v_1, v_5, v_6, v_7\}$; $E(G_1) = \{v_1v_5, v_1v_6, v_1v_7, v_6v_7\}$; $V(G_2) = \{v_2, v_8\}$; $E(G_2) = \{v_2v_8\}$; $V(G_3) = \{v_3, v_9, v_{10}\}$; $E(G_3) = \{v_3v_9, v_3v_{10}\}$; $V(G_4) = \{v_4\}$; $E(G_4) = \varnothing$.

Remark 1.1 In order to determine the cacti which attain the maximum Balaban index and maximum sum-Balaban index of all graphs in C_n^l, we just need to discuss the cactus graph $C \in C_n^l$ as shown in Fig. 3.

1.2 Cycle-edge transformation

Let $C \in C_n^l$ be a cactus graph as shown in

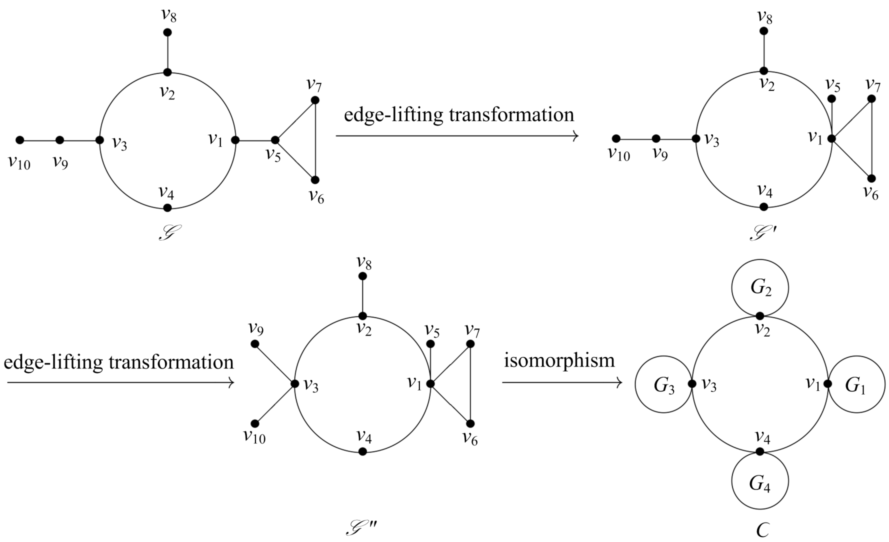

Fig. 4 An example

Fig. 3, where $C_r = v_1 v_2 \cdots v_r$ is the biggest cycle of C, and $|V(G_i)| = t_i + 1$. Denote the vertex set $W_{v_i} = N_C(v_i) \cap V(G_i)$ and $|W_{v_i}| = k_i$ for $1 \leqslant i \leqslant r$. Obviously, $t_i \geqslant k_i$ for $1 \leqslant i \leqslant r$.

(i) If r is even and $r \geqslant 4$, then C' is the graph obtained from C by deleting the edge $v_2 v_3$ and the edges from v_2 to W_{v_2}, meanwhile, adding the edges $v_1 v_3$ and from v_1 to W_{v_2}.

(ii) If r is odd and $r \geqslant 5$, then C' is the graph obtained from C by deleting the edges $v_2 v_3, v_3 v_4$, from v_2 to W_{v_2} and v_3 to W_{v_3}, meanwhile, adding the edges $v_1 v_4, v_1 v_3$, from v_1 to W_{v_2} and v_1 to W_{v_3}.

Then $C' \in \mathcal{C}_n^l$. We say that C' is the cycle-edge transformation of C (see Fig. 5).

Lemma 1.4 Let $C \in \mathcal{C}_n^l$ be a cactus graph as shown in Fig. 3 with $r \geqslant 4$, and C' be the cycle-edge transformation of C (see Fig. 5). Then $J(C) < J(C')$.

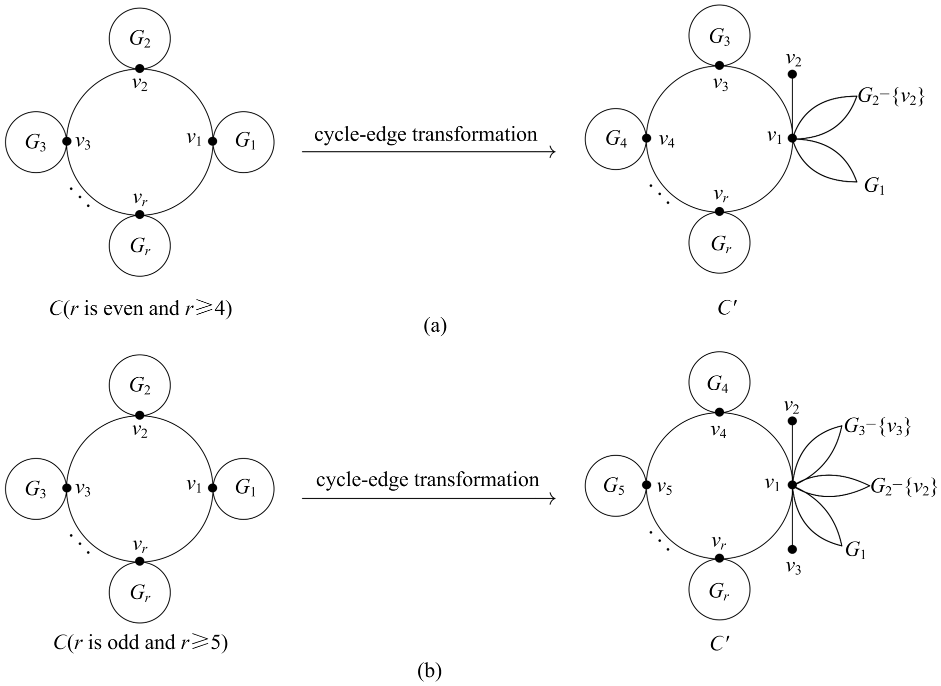

Fig. 5 The cycle-edge transformation

Proof Case 1 r is even and $r\geqslant 4$.

We first consider the vertex $v_x \in V(C)\backslash\{v_2\}$. It is easy to see that

$$D_C(v_x)=\sum_{i=1}^{r} D_C(v_x,G_i)+D_C(v_x,C_r),$$

$$D_{C'}(v_x)=\sum_{i=1}^{r} D_{C'}(v_x,G_i)+D_{C'}(v_x,C_r).$$

From the operation of cycle-edge transformation, noting that $C-\{V(G_2)\}\cong C'-\{V(G_2)\}$ and $D_C(v_x,C_r)\geqslant D_{C'}(v_x,C_r)$, $D_C(v_x,G_2)\geqslant D_{C'}(v_x,G_2)$, where $v_x\in V(C)\backslash\{v_2\}$. Then we have $D_C(v_x,G_i)\geqslant D_{C'}(v_x,G_i)$, where $1\leqslant i\leqslant r$, and

$$D_C(v_x)-D_{C'}(v_x)\geqslant 0 \tag{1}$$

where $v_x\in V(C)\backslash\{v_2\}$.

It can be checked directly that

$$\frac{1}{\sqrt{D_{C'}(v_x)D_{C'}(v_y)}}\geqslant\frac{1}{\sqrt{D_C(v_x)D_C(v_y)}} \tag{2}$$

where $v_x,v_y\in V(C)\backslash\{v_2\}$.

In the following, we consider the edges on vertex v_2 of C: v_1v_2, v_2v_3 and from v_2 to W_{v_2}.

For $v_1v_2\in E(C)$, it can be checked directly that

$$D_{C'}(v_2)-D_C(v_2)=\sum_{i=2}^{\frac{r+2}{2}} t_i+\frac{r}{2}-1,$$

$$D_C(v_1)-D_{C'}(v_1)=\sum_{i=2}^{\frac{r+2}{2}} t_i+\frac{r}{2}-1.$$

Then

$$D_{C'}(v_2)-D_C(v_2)=D_C(v_1)-D_{C'}(v_1)=\sum_{i=2}^{\frac{r+2}{2}} t_i+\frac{r}{2}-1 \tag{3}$$

Since $d_{C'}(v_2,v_1)=1$, we have

$$D_{C'}(v_2)-D_{C'}(v_1)=n-2>\sum_{i=2}^{\frac{r+2}{2}} t_i+\frac{r}{2}-1=D_{C'}(v_2)-D_C(v_2) \tag{4}$$

Let $x=D_{C'}(v_2)$, $y=D_{C'}(v_1)$, $a=\sum_{i=2}^{\frac{r+2}{2}} t_i+\frac{r}{2}-1$. Then $x-y=n-2>a$. By Lemma 1.1, we have

$$\frac{1}{\sqrt{D_{C'}(v_2)D_{C'}(v_1)}}>\frac{1}{\sqrt{(D_{C'}(v_2)-a)(D_{C'}(v_1)+a)}}=\frac{1}{\sqrt{D_C(v_2)D_C(v_1)}} \tag{5}$$

For $v_2v_3\in E(C)$, by (1) and (4), we have $D_{C'}(v_3)\leqslant D_C(v_3)$, $D_{C'}(v_1)<D_C(v_2)$. Then

$$\frac{1}{\sqrt{D_{C'}(v_1)D_{C'}(v_3)}}>\frac{1}{\sqrt{D_C(v_2)D_C(v_3)}} \tag{6}$$

For the edges from v_2 to W_{v_2}, by (1) and (4), we have $D_C(v_2)>D_{C'}(v_1)$, and $D_C(w)\geqslant D_{C'}(w)$ for any $w\in W_{v_2}$. Then

$$\frac{1}{\sqrt{D_{C'}(v_1)D_{C'}(w)}}>\frac{1}{\sqrt{D_C(v_2)D_C(w)}} \tag{7}$$

for any $w\in W_{v_2}$.

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

$$\frac{1}{\sqrt{D_{C'}(v_x)D_{C'}(v_y)}}>\frac{1}{\sqrt{D_C(v_x)D_C(v_y)}}.$$

From the definition of Balaban index, if p is even, we have $J(C')>J(C)$.

Case 2 r is odd and $r\geqslant 5$.

We first consider the vertex $v_x\in V(C)\backslash\{v_2,v_3\}$. From the operation of cycle-edge transformation, noting that $D_C(v_x,C_r)\geqslant D_{C'}(v_x,C_r)$ and $D_C(v_x,G_i)\geqslant D_{C'}(v_x,G_i)$ for $1\leqslant i\leqslant r$. Then for any vertex $v_x\in V(C)\backslash\{v_2,v_3\}$, we have

$$D_C(v_x)\geqslant D_{C'}(v_x) \tag{8}$$

Then

$$\frac{1}{\sqrt{D_{C'}(v_x)D_{C'}(v_y)}}\geqslant\frac{1}{\sqrt{D_C(v_x)D_C(v_y)}} \tag{9}$$

where $v_x,v_y\in V(C)\backslash\{v_2,v_3\}$.

We now consider the edges on vertices v_2,v_3 of C: v_1v_2, v_2v_3, v_3v_4, from v_2 to W_{v_2} and v_3 to W_{v_3}.

For $v_1v_2\in E(C)$, it can be checked directly that

$$D_{C'}(v_2)-D_C(v_2)=t_2+1 \tag{10}$$

$$D_C(v_1)-D_{C'}(v_1)\geqslant t_2+r-3>t_2+1=D_{C'}(v_2)-D_C(v_2) \tag{11}$$

Since $d_{C'}(v_2,v_1)=1$, we have

$$D_{C'}(v_2)-D_{C'}(v_1)=n-2>t_2+1=D_{C'}(v_2)-D_C(v_2) \tag{12}$$

Let $x=D_{C'}(v_2)$, $y=D_{C'}(v_1)$, and $a=t_2+1$. Then $x-y=n-2>a$. By Lemma 1.1, we have

$$\frac{1}{\sqrt{D_{C'}(v_2)D_{C'}(v_1)}} \geqslant \frac{1}{\sqrt{(D_{C'}(v_2)-a)(D_{C'}(v_1)+a)}} > \frac{1}{\sqrt{D_C(v_2)D_C(v_1)}} \quad (13)$$

For $v_2v_3 \in E(C)$, it can be checked directly that

$$D_C(v_3)-D_{C'}(v_1) \geqslant r-3+t_2 > t_2+1,$$
$$D_{C'}(v_3)=D_{C'}(v_2).$$

By (10) and (12), we have $D_{C'}(v_3)-D_C(v_2) = D_{C'}(v_2) - D_C(v_2) = t_2 + 1$ and $D_C(v_2) > D_{C'}(v_1)$. Then $D_{C'}(v_3) > D_C(v_2) > D_{C'}(v_1)$. Let $x = D_{C'}(v_3)$, $y = D_{C'}(v_1)$, $a = t_2+1$. Then $x > y+a$. By Lemma 1.1, we have

$$\frac{1}{\sqrt{D_{C'}(v_3)D_{C'}(v_1)}} > \frac{1}{\sqrt{(D_{C'}(v_3)-a)(D_{C'}(v_1)+a)}} > \frac{1}{\sqrt{D_C(v_2)D_C(v_3)}} \quad (14)$$

For $v_3v_4 \in E(C)$, it can be checked directly that $D_C(v_4) \geqslant D_{C'}(v_4)$, and $D_C(v_3) > D_{C'}(v_1)$. Then

$$\frac{1}{\sqrt{D_{C'}(v_1)D_{C'}(v_4)}} > \frac{1}{\sqrt{D_C(v_3)D_C(v_4)}} \quad (15)$$

For the edges from v_2 to W_{v_2} and the edges from v_3 to W_{v_3}, by (8) and (12), we have $D_C(v_2) > D_{C'}(v_1)$, and $D_C(w) \geqslant D_{C'}(w)$ for any $w \in W_{v_2}$. Then

$$\frac{1}{\sqrt{D_{C'}(v_1)D_{C'}(w)}} > \frac{1}{\sqrt{D_C(v_2)D_C(w)}} \quad (16)$$

for $w \in W_{v_2}$.

Since $D_C(v_3) > D_{C'}(v_1)$ and $D_C(w) \geqslant D_{C'}(w)$ for any $w \in W_{v_3}$, we have

$$\frac{1}{\sqrt{D_{C'}(v_1)D_{C'}(w)}} > \frac{1}{\sqrt{D_C(v_3)D_C(w)}} \quad (17)$$

for $w \in W_{v_3}$.

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

$$\frac{1}{\sqrt{D_{C'}(v_x)D_{C'}(v_y)}} > \frac{1}{\sqrt{D_C(v_x)D_C(v_y)}}$$

for $v_x, v_y \in V(C)$.

From the definition of Balaban index, if r is odd, we have $J(C') > J(C)$.

Lemma 1.5 Let $C \in C_n^l$ be a cactus graph as shown in Fig. 3 with $r \geqslant 4$, and C' be the cycle-edge transformation of C (see Fig. 5). Then $SJ(C) < SJ(C')$.

Proof Case 1 r is even and $r \geqslant 4$.

For the vertices $v_x, v_y \in V(C)\backslash\{v_2\}$, by (1), we have

$$\frac{1}{\sqrt{D_{C'}(v_x)+D_{C'}(v_y)}} \geqslant \frac{1}{\sqrt{D_C(v_x)+D_C(v_y)}} \quad (18)$$

for $v_x, v_y \in V(C)\backslash\{v_2\}$.

In the following, we consider the edges on vertex v_2 of C: v_1v_2, v_2v_3, the edges from v_2 to W_{v_2}.

For $v_1v_2 \in E(C)$, by (3), we have $D_{C'}(v_1) + D_{C'}(v_2) = D_C(v_1) + D_C(v_2)$. Then

$$\frac{1}{\sqrt{D_{C'}(v_2)+D_{C'}(v_1)}} = \frac{1}{\sqrt{D_C(v_2)+D_C(v_1)}} \quad (19)$$

For $v_2v_3 \in E(C)$, by (1) and (4), we have $D_{C'}(v_3) < D_C(v_3)$ and $D_{C'}(v_1) \leqslant D_C(v_2)$. Then

$$\frac{1}{\sqrt{D_{C'}(v_1)+D_{C'}(v_3)}} > \frac{1}{\sqrt{D_C(v_2)+D_C(v_3)}} \quad (20)$$

For the edges from v_2 to W_{v_2}, by (1) and (4), we have $D_{C'}(v_1) \leqslant D_C(v_2)$, and $D_{C'}(w) \leqslant D_C(w)$ for any $w \in W_{v_2}$. Then

$$\frac{1}{\sqrt{D_{C'}(v_1)+D_{C'}(w)}} \geqslant \frac{1}{\sqrt{D_C(v_2)+D_C(w)}} \quad (21)$$

for $w \in W_{v_2}$.

By (18) ~ (21) and the definition of sum-Balaban index, we have $SJ(C') > SJ(C)$.

Case 2 r is odd and $r \geqslant 5$.

For the vertices $v_x, v_y \in V(C)\backslash\{v_2, v_3\}$, by (8), we have

$$\frac{1}{\sqrt{D_{C'}(v_x)+D_{C'}(v_y)}} \geqslant \frac{1}{\sqrt{D_C(v_x)+D_C(v_y)}} \quad (22)$$

for $v_x, v_y \in V(C)\backslash\{v_2, v_3\}$.

In the following, we consider the edges on vertices v_2, v_3 of C: v_1v_2, v_2v_3, v_3v_4, the edges from v_2 to W_{v_2} and v_3 to W_{v_3}.

For $v_1v_2 \in E(C)$, by (11), we have

$$\frac{1}{\sqrt{D_{C'}(v_1)+D_{C'}(v_2)}} > \frac{1}{\sqrt{D_C(v_1)+D_C(v_2)}} \tag{23}$$

For $v_2v_3 \in E(C)$, it can be checked directly that $D_C(v_3) - D_{C'}(v_1) > t_2 + 1 = D_{C'}(v_3) - D_C(v_2)$. Then

$$\frac{1}{\sqrt{D_{C'}(v_1)+D_{C'}(v_3)}} > \frac{1}{\sqrt{D_C(v_2)+D_C(v_3)}} \tag{24}$$

For $v_3v_4 \in E(C)$, since $D_C(v_4) \geqslant D_{C'}(v_4)$ and $D_C(v_3) > D_{C'}(v_1)$, we have

$$\frac{1}{\sqrt{D_{C'}(v_4)+D_{C'}(v_1)}} > \frac{1}{\sqrt{D_C(v_4)+D_C(v_3)}} \tag{25}$$

For the edges from v_2 to W_{v_2} and v_3 to W_{v_3} of C, by (8) and (12), we have $D_C(v_2) > D_{C'}(v_1)$, $D_C(w) \geqslant D_{C'}(w)$ for any $w \in W_{v_2}$. Then

$$\frac{1}{\sqrt{D_{C'}(v_1)+D_{C'}(w)}} > \frac{1}{\sqrt{D_C(v_2)+D_C(w)}} \tag{26}$$

for $w \in W_{v_2}$.

Since $D_C(v_3) > D_{C'}(v_1)$ and $D_C(w) \geqslant D_{C'}(w)$ for $w \in W_{v_3}$, we have

$$\frac{1}{\sqrt{D_{C'}(v_1)+D_{C'}(w)}} > \frac{1}{\sqrt{D_C(v_3)+D_C(w)}} \tag{27}$$

for $v_x \in W_{v_3}$.

By (22)～(27), we have

$$\frac{1}{\sqrt{D_{C'}(v_x)+D_{C'}(v_y)}} > \frac{1}{\sqrt{D_C(v_x)+D_C(v_y)}}$$

for $v_x, v_y \in V(C)$.

From the definition of sum-Balaban index, $SJ(C') > SJ(C)$.

Let $C \in C_n^l$ be a cactus graph as shown in Fig. 3. By repeating cycle-edge transformations on C, we will get a cactus graph $C_1 \in C_n^l$ such that $J(C_1) > J(C)$ and $SJ(C_1) > SJ(C)$, where the graph C_1 is defined in Fig. 6 and the following five conditions hold.

(i) G_i is a cactus graph, or pendent edge, or a vertex, where $1 \leqslant i \leqslant 3$;

(ii) there are $l-1$ cycles in $G_1 \cup G_2 \cup G_3$;

(iii) $G_i \cap G_j = \emptyset$ for $1 \leqslant i < j \leqslant 3$;

(iv) each cycle of cactus graph C_1 has at least one cut-vertex;

(v) the length of every cycle of C_1 is 3.

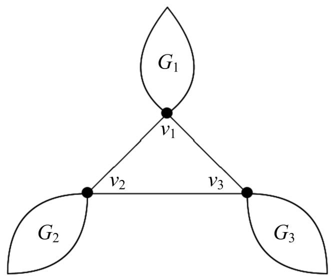

Fig. 6 The cactus graph C_1

Remark 1.2 In order to determine the cacti which attain the maximum Balaban index and maximum sum-Balaban index of all graphs in C_n^l, we just need to discuss the cactus graph $C_1 \in C_n^l$ as shown in Fig. 6.

1.3 Cycle-lifting transformation

Let $C_1 \in C_n^l$ be a cactus graph as shown in Fig. 6. Denote $W_{v_i} = N_{C_1}(v_i) \cap V(G_i)$ and $|W_{v_i}| = k_i$ for $1 \leqslant i \leqslant 3$. Let C'_1 be the graph obtained by deleting the edges v_2v_x for $v_x \in W_{v_2}$, and adding the edges v_1v_x for $v_x \in W_{v_2}$. Then $C'_1 \in C_n^l$. We say that C'_1 is the cycle-lifting transformation of C_1 (see Fig. 7).

Lemma 1.6 Let $C_1 \in C_n^l$ be a cactus graph as shown in Fig. 6, and C'_1 be the cycle-lifting transformation of C_1 (see Fig. 7). Then $J(C_1) < J(C'_1)$, and $SJ(C_1) < SJ(C'_1)$.

Proof Let $V(C_1) = \{v_1, v_2, v_3, \cdots, v_n\}$. It can be checked directly that

$$D_{C_1}(v_x) \geqslant D_{C'_1}(v_x) \text{ for } v_x \in V(C_1)\backslash\{v_2\},$$
$$D_{C'_1}(v_2) - D_{C_1}(v_2) = D_{C_1}(v_1) - D_{C'_1}(v_1) > 0,$$
$$D_{C'_1}(v_2) > \max\{D_{C_1}(v_1), D_{C_1}(v_2)\} > D_{C'_1}(v_1).$$

For the vertex $v_x, v_y \in V(C_1)\backslash\{v_2\}$, it is easy to see that

$$\frac{1}{\sqrt{D_{C'_1}(v_x)D_{C'_1}(v_y)}} \geqslant \frac{1}{\sqrt{D_{C_1}(v_x)D_{C_1}(v_y)}} \tag{28}$$

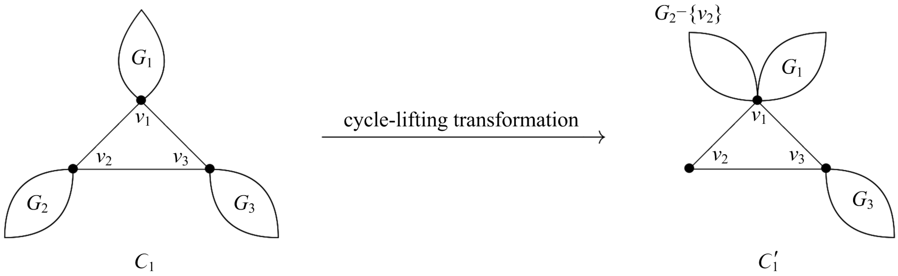

Fig. 7 The cycle-lifting transformation

$$\frac{1}{\sqrt{D_{C_1'}(v_x)+D_{C_1'}(v_y)}} \geqslant \frac{1}{\sqrt{D_{C_1}(v_x)+D_{C_1}(v_y)}} \quad (29)$$

For $v_1v_2 \in E(C_1)$, letting $x = D_{C_1'}(v_2)$, $y = D_{C_1'}(v_1)$, $a = D_{C_1'}(v_2) - D_{C_1}(v_2) = D_{C_1}(v_1) - D_{C_1'}(v_1) > 0$, then $x > y + a$, By Lemma 1.1, we have

$$\frac{1}{\sqrt{D_{C_1'}(v_1)D_{C_1'}(v_2)}} > \frac{1}{\sqrt{D_{C_1}(v_1)D_{C_1}(v_2)}} \quad (30)$$

$$\frac{1}{\sqrt{D_{C_1'}(v_1)+D_{C_1'}(v_2)}} = \frac{1}{\sqrt{D_{C_1}(v_1)+D_{C_1}(v_2)}} \quad (31)$$

For v_2v_3, $v_1v_3 \in E(C_1)$, letting $x_2 = D_{C_1'}(v_2)$, $x_1 = D_{C_1}(v_2)$, $y_2 = D_{C_1}(v_1)$, $y_1 = D_{C_1'}(v_1)$, then $x_1 > y_1$ and $x_2 - x_1 = y_2 - y_1 > 0$. By Lemma 1.2, we have

$$\frac{1}{\sqrt{D_{C_1'}(v_2)}} + \frac{1}{\sqrt{D_{C_1'}(v_1)}} > \frac{1}{\sqrt{D_{C_1}(v_2)}} + \frac{1}{\sqrt{D_{C_1}(v_1)}}.$$

Meanwhile, $D_{C_1}(v_3) = D_{C_1'}(v_3)$, then

$$\frac{1}{\sqrt{D_{C_1'}(v_2)D_{C_1'}(v_3)}} + \frac{1}{\sqrt{D_{C_1'}(v_1)D_{C_1'}(v_3)}} > \frac{1}{\sqrt{D_{C_1}(v_2)D_{C_1}(v_3)}} + \frac{1}{\sqrt{D_{C_1}(v_1)D_{C_1}(v_3)}} \quad (32)$$

Let $x_2 = D_{C_1'}(v_2) + D_{C_1'}(v_3)$, $x_1 = D_{C_1}(v_2) + D_{C_1}(v_3)$, $y_2 = D_{C_1}(v_1) + D_{C_1}(v_3)$, $y_1 = D_{C_1'}(v_1) + D_{C_1'}(v_3)$. Then $x_1 > y_1$ and $x_2 - x_1 = y_2 - y_1 > 0$. By Lemma 1.2, we have

$$\frac{1}{\sqrt{D_{C_1'}(v_2)+D_{C_1'}(v_3)}} + \frac{1}{\sqrt{D_{C_1'}(v_1)+D_{C_1'}(v_3)}} > \frac{1}{\sqrt{D_{C_1}(v_2)+D_{C_1}(v_3)}} + \frac{1}{\sqrt{D_{C_1}(v_1)+D_{C_1}(v_3)}} \quad (33)$$

For each edge $v_2v_x \in E(G_2)$, we have $D_{C_1}(v_2) > D_{C_1'}(v_1)$, and $D_{C_1}(v_x) \geqslant D_{C_1'}(v_x)$, where $v_x \in V(G)\backslash\{v_2\}$, then

$$\frac{1}{\sqrt{D_{C_1'}(v_1)D_{C_1'}(v_x)}} > \frac{1}{\sqrt{D_{C_1}(v_2)D_{C_1}(v_x)}} \quad (34)$$

$$\frac{1}{\sqrt{D_{C_1'}(v_1)+D_{C_1'}(v_x)}} > \frac{1}{\sqrt{D_{C_1}(v_2)+D_{C_1}(v_x)}} \quad (35)$$

By (28),(30),(32),(34), and the definition of Balaban index, we have $J(C'_1) > J(C_1)$.

By (29),(31),(33),(35), and the definition of sum-Balaban index, we have

$$SJ(C'_1) > SJ(C_1).$$

By Lemma 1.6 we will get $C_2 \in C_n^l$ from C_1 by repeating cycle-lifting transformations such that $J(C_2) > J(C_1)$ and $SJ(C_2) > SJ(C_1)$, where C_2 is defined in Fig. 8.

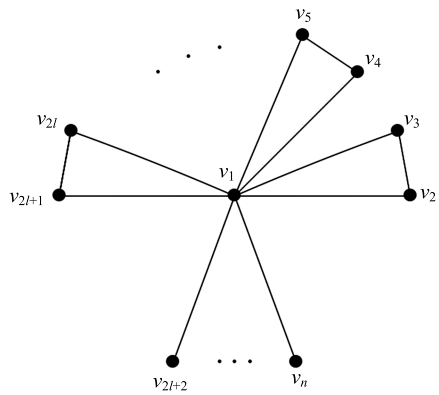

Fig. 8 The cactus graph C_2

Remark 1.3 In order to determine the cacti which attain the maximum Balaban index and maximum sum-Balaban index of all graphs in C_n^l, we just need to discuss the cactus graph $C_2 \in C_n^l$ as shown in Fig. 8.

2 Maximum Balaban index and sum-Balaban index of cacti

From the discussions of Section 1, for any cactus graph $C \in C_n^l$, we finally get the graph C_2 from C by edge-lifting transformation, cycle-edge transformation, cycle-lifting transformation or any combination of these, where graphs $C_2 \in C_n^l$ are defined in Fig. 8. By Lemmas 1.4～1.6, we have

$$J(C) \leqslant J(C_2),\ SJ(C) \leqslant SJ(C_2).$$

That is to say, C_2 attains the maximum Balaban index and maximum sum-Balaban index of all graphs in C_n^l.

Theorem 2.1 Let C_2 be defined in Fig. 8. Then C_2 is the unique cactus graph in C_n^l which attains the maximum Balaban index and sum-Balaban index of all graphs in C_n^l, and

$$\max J(C_n^l) = J(C_2) = \frac{n+l-1}{l+1}\left(\frac{2l}{\sqrt{2n^2-6n+4}} + \frac{n-2l-1}{\sqrt{2n^2-5n+3}} + \frac{l}{2n-4}\right),$$

$$\max SJ(C_n^l) = SJ(C_2) = \frac{n+l-1}{l+1}\left(\frac{2l}{\sqrt{3n-5}} + \frac{n-2l-1}{\sqrt{3n-4}} + \frac{l}{2\sqrt{n-2}}\right).$$

Proof From the above discussions, we have that C_2 is the unique graph of order n and l cycles which attains the maximum Balaban index and sum-Balaban index of all graphs in C_n^l. We now calculate the values $J(C_2)$ and $SJ(C_2)$.

It can be checked directly that

$$D(v_1) = n-1;$$
$$D(v_i) = 2n-4, \text{ where } 2 \leqslant i \leqslant 2l+1;$$
$$D(v_j) = 2n-3, \text{ where } 2l+2 \leqslant j \leqslant n.$$

Thus

$$J(C_2) = \frac{n+l-1}{l+1}\left[\sum_{i=2}^{n} \frac{1}{\sqrt{D(v_1)D(v_i)}} + \frac{l}{\sqrt{D(v_2)D(v_3)}}\right] = \frac{n+l-1}{l+1}\left(\frac{2l}{\sqrt{2n^2-6n+4}} + \frac{n-2l-1}{\sqrt{2n^2-5n+3}} + \frac{l}{2n-4}\right),$$

and

$$SJ(C_2) = \frac{n+l-1}{l+1}\left[\sum_{i=2}^{n} \frac{1}{\sqrt{D(v_1)+D(v_i)}} + \frac{l}{\sqrt{D(v_2)+D(v_3)}}\right] = \frac{n+l-1}{l+1}\left(\frac{2l}{\sqrt{3n-5}} + \frac{n-2l-1}{\sqrt{3n-4}} + \frac{l}{2\sqrt{n-2}}\right).$$

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