*Journal of Mathematical Research with Applications*
Jul., 2014, Vol. 34, No. 4, pp. 392–402
DOI:10.3770/j.issn:2095-2651.2014.04.002
Http://jmre.dlut.edu.cn

# The Maximum Balaban Index (Sum-Balaban Index) of Unicyclic Graphs

**Lihua YOU*, Xin DONG**
*School of Mathematical Sciences, South China Normal University, Guangdong* 510631*, P. R. China*

**Abstract** The Balaban index of a connected graph $G$ is defined as

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

and the Sum-Balaban index is defined as

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

where $D_G(u) = \sum_{w\in V(G)} d_G(u,w)$, and $\mu$ is the cyclomatic number of $G$. In this paper, the unicyclic graphs with the maximum Balaban index and the maximum Sum-Balaban index among all unicyclic graphs on $n$ vertices are characterized, respectively.

**Keywords** Balaban index; Sum-Balaban index; unicyclic; maximum.

**MR(2010) Subject Classification** 05C35; 05C50

## 1. Introduction

Let $G$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The distance between vertices $u$ and $v$ in $G$, denoted by $d_G(u,v)$, is the length of the shortest path connecting $u$ and $v$ in $G$. Let $D_G(u) = \sum_{v\in V(G)} d_G(u,v)$, which is the distance sum of vertex $u$ in $G$.

Let $|V(G)| = n$ and $|E(G)| = m$. The cyclomatic number $\mu$ 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 $\mu = m - n + 1$ (see [1]).

The Balaban index of a 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 A. T. Balaban [2, 3], which is also called the average distance-sum connectivity index or $J$ index. It appears to be a very useful molecular descriptor with attractive properties.

Received May 5, 2013; Accepted January 28, 2014
Supported by the Zhujiang Technology New Star Foundation of Guangzhou (Grant No. 2011J2200090), and Program on International Cooperation and Innovation, Department of Education, Guangdong Province (Grant No. 2012gjhz0007).
* Corresponding author
E-mail address: ylhua@scnu.edu.cn (Lihua YOU); 303903094@qq.com (Xin DONG)

Balaban et al. [4] also proposed the study of the Sum-Balaban index 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 subsequently in various QSAR and QSPR studies. It has been shown that Balaban index and Sum-Balaban index have a strong correlation with chemical properties of the chemical compound and other topological indices of octanes and lower benzenoids. Mathematical properties of Balaban index can be found in [5–11]. Mathematical properties of Sum-Balaban index can be found in [10] and [12, 13].

**Theorem 1.1** ([5–9, 12, 13]) *Let $T$ be a tree on $n(\geq 2)$ vertices. Then*

$$J(P_n) \leq J(T) \leq J(S_n), \quad SJ(P_n) \leq SJ(T) \leq SJ(S_n)$$

*with left (or right) equality if and only if $T = P_n$ (or $T = S_n$), where $P_n$ is the path on $n$ vertices and $S_n$ is the star on $n$ vertices.*

In this paper, the unicyclic graphs with the maximum Balaban index and the maximum Sum-Balaban index among all unicyclic graphs on $n$ vertices are characterized, respectively.

## 2. Preliminaries

In this section, we will introduce two transformations which are useful to the proofs of the main results.

**Lemma 2.1** ([7]) *Let $a, a', b, b', w, x, y, z \in R^+$ such that $\frac{b}{x} \geq \frac{a}{w}, \frac{b'}{y} \geq \frac{a'}{z}, w \geq x$ and $z \geq y$. Then $\frac{1}{\sqrt{(w+a)(z+a')}} + \frac{1}{\sqrt{xy}} \geq \frac{1}{\sqrt{wz}} + \frac{1}{\sqrt{(x+b)(y+b')}}$, and the equality holds if and only if $b = a, b' = a', w = x$ and $z = y$.*

**Lemma 2.2** ([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** *Let $x_1, y_1, x_2, y_2 \in R^+$ such that $x_1 > y_1$ and $x_2 - x_1 = y_2 - y_1 > 0$. Then $\frac{1}{\sqrt{x_1}} + \frac{1}{\sqrt{y_2}} < \frac{1}{\sqrt{x_2}} + \frac{1}{\sqrt{y_1}}$.*

**Proof** Let $a = x_2 - x_1 = y_2 - y_1 > 0$ and $f(t) = \frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t+a}}$. It is clear that $f'(t) < 0$, then $f(t)$ is a decreasing function of $t$. So we have $\frac{1}{\sqrt{x_1}} - \frac{1}{\sqrt{x_1+a}} < \frac{1}{\sqrt{y_1}} - \frac{1}{\sqrt{y_1+a}}$ by $x_1 > y_1$, that is to say, $\frac{1}{\sqrt{x_1}} + \frac{1}{\sqrt{y_2}} < \frac{1}{\sqrt{x_2}} + \frac{1}{\sqrt{y_1}}$. $\square$

**The edge-lifting transformation** ([5]) Let $G_1, G_2$ 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 1).

**Lemma 2.4** ([5, 12]) *Let $G'$ be the edge-lifting transformation of $G$. Then $J(G) < J(G')$ and*

$SJ(G) < SJ(G')$.


Figure 1 The edge-lifting transformation

A rooted graph has one of its vertices, called the root, distinguished from the others.

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

Define $G(n, r, 0) = C_n$. For $1 \leq k \leq r \leq n$, define $G(n, r, k)$ to be a unicyclic graph on $n$ vertices obtained from $C_r$, $T_1, T_2, \ldots, T_k$, by attaching $k$ rooted trees $T_1, T_2, \ldots, T_k$ to $k$ distinct vertices of the cycle $C_r$, that is to say, $G(n, r, k)$ is a unicyclic graph on $n$ vertices by identifying some vertex of $C_r$ with the root $u_i$ of $T_i$ for each $i$ $(1 \leq i \leq k)$, where $|V(T_i)| \geq 2$ $(1 \leq i \leq k)$. Clearly, $3 \leq r \leq n - k$.

Let $\mathbb{S} = \{S | S$ is a rooted star and the root is its center$\}$.

Let $\mathbb{G}^*(n, r, k)$ be the set of all unicyclic graphs on $n$ vertices obtained from $C_r$ by attaching $k$ rooted stars in $\mathbb{S}$ to $k$ distinct vertices of $C_r$ (see Figure 2).

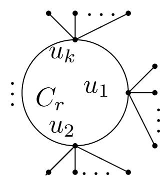



Figure 2 A graph $G^*(n, r, k)$ in the set $\mathbb{G}^*(n, r, k)$

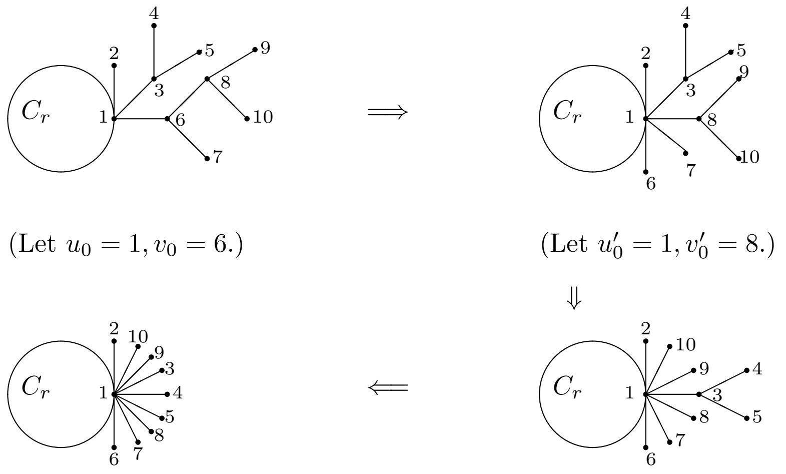
By Lemma 2.4, we can repeat the edge-lifting transformation to the rooted trees of $G(n, r, k)$, and we have

**Lemma 2.5** *Let $n, r, k$ be positive integers with $1 \leq k \leq r$ and $3 \leq r \leq n - k$, $G(n, r, k)$ be defined as above, and $G^*(n, r, k) \in \mathbb{G}^*(n, r, k)$ obtained from $G(n, r, k)$ by repeating edge-lifting transformation. Then*

$$J(G(n, r, k)) \leq J(G^*(n, r, k)), \quad SJ(G(n, r, k)) \leq SJ(G^*(n, r, k)),$$

*and the equality holds if and only if $G(n, r, k) \cong G^*(n, r, k)$.*

Figure 3 shows an example how to obtain $G^*(n, r, 1) \in \mathbb{G}^*(n, r, 1)$ by repeating edge-lifting transformation from graph $G(n, r, 1)$.

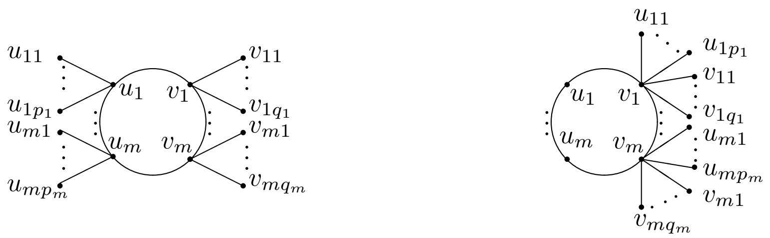



(Let $u_0 = 1, v_0 = 6$.) (Let $u'_0 = 1, v'_0 = 8$.)

$G^*(n, r, 1) \in \mathbb{G}^*(n, r, 1)$ (Let $u''_0 = 1, v''_0 = 3$.)

Figure 3 An example

**Branch transformation** Let $G = G^*(n, r, k) \in \mathbb{G}^*(n, r, k)$ be defined as above. For convenience, let $m = \left\lfloor \frac{r}{2} \right\rfloor$. If $r$ is even, define $C_r = v_1 v_2 \cdots v_m u_m \cdots u_2 u_1 v_1$; if $r$ is odd, define $C_r = v_1 v_2 \cdots v_m v_{m+1} u_m \cdots u_2 u_1 v_1$. Then $G'$ is obtained from $G$ by deleting the pendent edge $u_i w$ and adding the pendent edge $v_i w$ for any $i \in \{1, 2, \ldots, m\}$ (if there exists the pendent edge $u_i w$), where $w \in V(G) \backslash V(C_r)$. We say $G'$ is obtained from $G$ by branch transformation (see Figure 4, where $p_i \geq 0$, $q_i \geq 0$ for any $i \in \{1, 2, \ldots, m\}$).




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

Figure 4 The branch transformation

Let $G$ be a graph and $U (\neq \phi) \subseteq V(G)$. 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 $G[U]$, and for any vertex $u \in V(G)$, we define $D_G(u, U) = \sum_{v \in U} d_G(u, v)$.

**Lemma 2.6** *Let $n, r, k$ be positive integers with $2 \leq k \leq r$, $3 \leq r \leq n - k$, $G = G^*(n, r, k) \in \mathbb{G}^*(n, r, k)$, $G'$ be the graph obtained from $G$ by branch transformation. Then $J(G) < J(G')$.*

**Proof** Let $U_0 = \{u_1, u_2, \ldots, u_m\}$, $U_1 = \{w | u_i w \in E(G), \deg(w) = 1, 1 \leq i \leq m\}$, $V_0 = \{v_1, v_2, \ldots, v_m\}$, and $V_1 = \{w | v_i w \in E(G), \deg(w) = 1, 1 \leq i \leq m\}$ for $r = 2m$ is even, $V_1 = \{w | v_i w \in E(G), \deg(w) = 1, 1 \leq i \leq m + 1\} \cup \{v_{m+1}\}$ for $r = 2m + 1$ is odd.

For any $s$ with $1 \leq s \leq m$, it is clear that $u_s \in U_0$ and $v_s \in V_0$, and

$$D_G(u_s) = D_G(u_s, U_0) + D_G(u_s, U_1) + D_G(u_s, V_0) + D_G(u_s, V_1), \tag{2.1}$$

and

$$D_{G'}(v_s) = D_{G'}(v_s, V_0) + D_{G'}(v_s, U_1) + D_{G'}(v_s, U_0) + D_{G'}(v_s, V_1). \tag{2.2}$$

Noting that $G[U_0] \cong G'[V_0]$, $G[V_0] \cong G'[U_0]$ and $G[U_0 \bigcup U_1] \cong G'[V_0 \bigcup U_1]$, so

$$D_G(u_s, U_0) = D_{G'}(v_s, V_0), D_G(u_s, V_0) = D_{G'}(v_s, U_0),$$

and $D_G(u_s, U_1) = D_{G'}(v_s, U_1), D_G(u_s, V_1) > D_{G'}(v_s, V_1)$. Thus we have

$$D_G(u_s) - D_{G'}(v_s) = D_G(u_s, V_1) - D_{G'}(v_s, V_1) > 0. \tag{2.3}$$

Similarly, we have

$$D_G(v_s) = D_G(v_s, U_0) + D_G(v_s, U_1) + D_G(v_s, V_0) + D_G(v_s, V_1), \tag{2.4}$$

and

$$D_{G'}(u_s) = D_{G'}(u_s, V_0) + D_{G'}(u_s, U_1) + D_{G'}(u_s, U_0) + D_{G'}(u_s, V_1). \tag{2.5}$$

Thus

$$D_{G'}(u_s) - D_G(v_s) = D_{G'}(u_s, V_1) - D_G(v_s, V_1) > 0. \tag{2.6}$$

Noting that $D_G(u_s, V_1) = D_{G'}(u_s, V_1)$ and $D_{G'}(v_s, V_1) = D_G(v_s, V_1)$, by (2.3) and (2.6), we have

$$D_G(u_s) - D_{G'}(v_s) = D_{G'}(u_s) - D_G(v_s) = D_G(u_s, V_1) - D_{G'}(v_s, V_1) > 0. \tag{2.7}$$

By (2.1), (2.2), (2.4) and (2.5), we have

$$D_{G'}(u_s) - D_G(u_s) = D_G(v_s) - D_{G'}(v_s) > 0. \tag{2.8}$$

For any edge $u_s u_t \in E(G[U_0])$ and $v_s v_t \in E(G[V_0])$, take $x = D_{G'}(v_s)$, $y = D_{G'}(v_t)$, $w = D_G(u_s)$, $z = D_G(u_t)$, $a = D_{G'}(u_s) - D_G(u_s)$, $a' = D_{G'}(u_t) - D_G(u_t)$, $b = D_G(v_s) - D_{G'}(v_s)$, $b' = D_G(v_t) - D_{G'}(v_t)$. Then $b = a > 0$, $b' = a' > 0$ by (2.8). It is obvious that $a, a', b, b', w, x, y, z \in R^+$, $w > x$, $z > y$ by (2.7). Then $\frac{b}{x} > \frac{a}{w}, \frac{b'}{y} > \frac{a'}{z}$. Thus by Lemma 2.1, we have

$$\frac{1}{\sqrt{D_{G'}(u_s)D_{G'}(u_t)}} + \frac{1}{\sqrt{D_{G'}(v_s)D_{G'}(v_t)}} > \frac{1}{\sqrt{D_G(u_s)D_G(u_t)}} + \frac{1}{\sqrt{D_G(v_s)D_G(v_t)}}. \tag{2.9}$$

Similarly, for any vertex $w \in U_1 \bigcup V_1$, we can show $D_G(w) \geq D_{G'}(w)$, where equality holds if and only if $r = 2m + 1$ is odd, $w = v_{m+1}$ or $r = 2m + 1$ is odd, $w$ is pendent vertex and adjacent to $v_{m+1}$. Then it implies that the following inequalities (2.10)–(2.12) hold.

For any edge $u_s w \in E(G)$ with $u_s \in U_0$ where $1 \leq s \leq m$ and $w \in U_1$, the corresponding edge is $v_s w \in E(G')$, we have

$$\frac{1}{\sqrt{D_{G'}(v_s)D_{G'}(w)}} > \frac{1}{\sqrt{D_G(u_s)D_G(w)}}. \tag{2.10}$$

For any edge $v_sw \in E(G)$ with $v_s \in V_0$ where $1 \le s \le m$ and $w \in V_1$, we have

$$\frac{1}{\sqrt{D_{G'}(v_s)D_{G'}(w)}} > \frac{1}{\sqrt{D_G(v_s)D_G(w)}}. \tag{2.11}$$

When $r = 2m+1$ is odd, then for any edge $v_{m+1}w \in E(G)$ with $w \in V_1$, we have

$$\frac{1}{\sqrt{D_{G'}(v_{m+1})D_{G'}(w)}} = \frac{1}{\sqrt{D_G(v_{m+1})D_G(w)}}. \tag{2.12}$$

For edge $u_1v_1$, by (2.8) and Lemma 2.3, we have

$$\frac{1}{\sqrt{D_{G'}(u_1)D_{G'}(v_1)}} > \frac{1}{\sqrt{D_G(u_1)D_G(v_1)}}. \tag{2.13}$$

From (2.9) to (2.13), we obtain $J(G') > J(G)$ by the definition of Balaban index. $\square$

**Lemma 2.7** *Let $n, r, k$ be positive integers with $2 \le k \le r$ and $3 \le r \le n-k$, $G = G^*(n,r,k) \in \mathbb{G}^*(n,r,k)$, $G'$ be the graph obtained from $G$ by branch transformation. Then $SJ(G) < SJ(G')$.*

**Proof** Let $U_0$, $U_1$, $V_0$, $V_1$, $a, a', b, b'$ be defined as Lemma 2.6. Let $f(x) = \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+a+a'}}$. Then $f(x)$ is a decreasing function of $x$ since $f'(x) < 0$. Noting that $D_G(u_s) + D_G(u_t) > D_{G'}(v_s) + D_{G'}(v_t) = D_G(v_s) + D_G(v_t) - a - a'$, we have

$$\begin{aligned}&\frac{1}{\sqrt{D_G(u_s)+D_G(u_t)}} - \frac{1}{\sqrt{D_G(u_s)+D_G(u_t)+a+a'}}\\ &< \frac{1}{\sqrt{D_G(v_s)+D_G(v_t)-a-a'}} - \frac{1}{\sqrt{D_G(v_s)+D_G(v_t)}}.\end{aligned}$$

Thus

$$\begin{aligned}&\frac{1}{\sqrt{D_{G'}(u_s)+D_{G'}(u_t)}} + \frac{1}{\sqrt{D_{G'}(v_s)+D_{G'}(v_t)}}\\ &> \frac{1}{\sqrt{D_G(u_s)+D_G(u_t)}} + \frac{1}{\sqrt{D_G(v_s)+D_G(v_t)}}.\end{aligned} \tag{2.14}$$

Similarly, for any vertex $w \in U_1 \bigcup V_1$, we can show $D_G(w) \ge D_{G'}(w)$, where equality holds if and only if $r = 2m+1$ is odd, $w = v_{m+1}$ or $r = 2m+1$ is odd, $w$ is pendent vertex and adjacent to $v_{m+1}$. Then it implies that the following inequalities (2.15)–(2.17) hold.

For any edge $u_sw \in E(G)$ with $u_s \in U_0$ where $1 \le s \le m$ and $w \in U_1$, the corresponding edge is $v_sw \in E(G')$, we have

$$\frac{1}{\sqrt{D_{G'}(v_s)+D_{G'}(w)}} > \frac{1}{\sqrt{D_G(u_s)+D_G(w)}}. \tag{2.15}$$

For any edge $v_sw \in E(G)$ with $v_s \in V_0$ where $1 \le s \le m$ and $w \in V_1$, we have

$$\frac{1}{\sqrt{D_{G'}(v_s)+D_{G'}(w)}} > \frac{1}{\sqrt{D_G(v_s)+D_G(w)}}. \tag{2.16}$$

When $r = 2m+1$ is odd, then for any edge $v_{m+1}w \in E(G)$ with $w \in V_1$, we have

$$\frac{1}{\sqrt{D_{G'}(v_{m+1})+D_{G'}(w)}} = \frac{1}{\sqrt{D_G(v_{m+1})+D_G(w)}}. \tag{2.17}$$

For edge $u_1v_1$, by (2.8), we have

$$\frac{1}{\sqrt{D_{G'}(u_1)+D_{G'}(v_1)}}=\frac{1}{\sqrt{D_G(u_1)+D_G(v_1)}}. \tag{2.18}$$

From (2.14) to (2.18), we obtain $SJ(G')>SJ(G)$ by the definition of Sum-Balaban index. $\square$

**Lemma 2.8** *Let $n,r,k$ be positive integers with $1\le k\le r$ and $3\le r\le n-k$, $G=G^*(n,r,k)\in \mathbb{G}^*(n,r,k)$, and $G'$ obtained from $G$ by repeating the branch transformation, and we cannot get other graph from $G'$ by repeating branch transformation. Then*

*(1) $G'\in\mathbb{G}^*(n,r,1)$ (see Figure 5).*

*(2) $J(G)\le J(G')$, and the equality holds if and only if $G\cong G'$.*

*(3) $SJ(G)\le SJ(G')$, and the equality holds if and only if $G\cong G'$.*

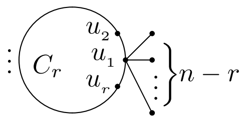



Figure 5 graph $G^*(n,r,1)\in\mathbb{G}^*(n,r,1)$

## 3. The maximum Balaban index of unicyclic graphs

In this section, we will show that $G^*(n,3,1)$ is the graph which has the maximum Balaban index among all unicyclic graphs on $n$ vertices.

Let $G$ be a unicyclic graph on $n$ vertices. Then $|E(G)|=n$, $\mu=1$, and thus

$$J(G)=\frac{n}{2}\sum_{uv\in E(G)}\frac{1}{\sqrt{D_G(u)D_G(v)}}.$$

**Lemma 3.1** *Let $n,r$ be positive integers with $3\le r\le n$, $G=G^*(n,r,1)\in\mathbb{G}^*(n,r,1)$ (see Figure 5). Then*

$$\frac{2J(G)}{n}=\begin{cases}\frac{n-r}{\sqrt{(\frac{r^2}{4}-r+2n-2)(\frac{r^2}{4}+n-r)}}+\sum\limits_{1\le i\le\frac{r}{2}}\frac{2}{\sqrt{[\frac{r^2}{4}+i(n-r)][\frac{r^2}{4}+(i+1)(n-r)]}}, & r \text{ is even;}\\ \frac{n-r}{\sqrt{(\frac{r^2}{4}-r+2n-\frac{9}{4})(\frac{r^2-1}{4}+n-r)}}+\sum\limits_{1\le i\le\frac{r-1}{2}}\frac{2}{\sqrt{D_G(u_i)D_G(u_{i+1})}}+\frac{1}{\frac{r^2-1}{4}+\frac{r+1}{2}(n-r)}, & r \text{ is odd;}\end{cases} \tag{3.1}$$

*where $D_G(u_i)=\frac{r^2-1}{4}+i(n-r)$ for $r$ is odd and $1\le i\le\frac{r+1}{2}$.*

**Proof** We calculate $D_G(u)$ for any vertex $u\in V(G)$.

**Case 1** $r$ is even.

**Subcase 1.1** $u\in V(G)\backslash V(C_r)$.

$$D_G(u)=2(n-r-1)+(1+2+\cdots+\frac{r}{2})+(2+3+\cdots+\frac{r+2}{2})=\frac{r^2}{4}-r+2n-2.$$

**Subcase 1.2** $u=u_i\in V(C_r)$ where $1\le i\le r$.

Noting that $D_G(u_i) = D_G(u_{r+2-i})$, we only need to calculate $D_G(u_i)$ for $1 \leq i \leq \frac{r+2}{2}$. Clearly, when $1 \leq i \leq \frac{r+2}{2}$, we have

$$D_G(u_i) = (1+2+\cdots+\frac{r}{2}) + (1+2+\cdots+\frac{r-2}{2}) + i(n-r) = \frac{r^2}{4} + i(n-r).$$

**Case 2** $r$ is odd.

**Subcase 2.1** $u \in V(G)\backslash V(C_r)$.

$$D_G(u) = 2(n-r-1) + (1+2+\cdots+\frac{r+1}{2}) + (2+3+\cdots+\frac{r+1}{2}) = \frac{r^2}{4} - r + 2n - \frac{9}{4}.$$

**Subcase 2.2** $u = u_i \in V(C_r)$ where $1 \leq i \leq r$.

Noting that $D_G(u_i) = D_G(u_{r+2-i})$, we only need to calculate $D_G(u_i)$ for $1 \leq i \leq \frac{r+1}{2}$. Clearly, when $1 \leq i \leq \frac{r+1}{2}$, we have

$$D_G(u_i) = (1+2+\cdots+\frac{r-1}{2}) + (1+2+\cdots+\frac{r-1}{2}) + i(n-r) = \frac{r^2-1}{4} + i(n-r).$$

Combine the previous arguments and let $w \in V(G)\backslash V(C_r)$, then we can show (3.1) by the following equation

$$J(G) = \frac{n}{2} \sum_{uv \in E(G)} \frac{1}{\sqrt{D_G(u)D_G(v)}}$$

$$= \begin{cases} \frac{n}{2}(\sum\limits_{1 \leq i \leq \frac{r}{2}} \frac{2}{\sqrt{D_G(u_i)D_G(u_{i+1})}} + \frac{n-r}{\sqrt{D_G(u_1)D_G(w)}}), & r \text{ is even;} \\ \frac{n}{2}(\sum\limits_{1 \leq i \leq \frac{r-1}{2}} \frac{2}{\sqrt{D_G(u_i)D_G(u_{i+1})}} + \frac{1}{\sqrt{D_G(u_{\frac{r+1}{2}})D_G(u_{\frac{r+3}{2}})}} + \frac{n-r}{\sqrt{D_G(u_1)D_G(w)}}), & r \text{ is odd.} \end{cases} \square$$

**Theorem 3.2** *Let $n, r$ be integers with $n \geq 4$, $3 \leq r \leq n$, $G \ncong C_n$ be a connected unicyclic graph on $n$ vertices, the length of unique cycle of $G$ be $r$. Then*

$$J(G) \leq J(G^*(n,3,1)) = \frac{n}{2} \cdot (\frac{1}{2n-4} + \frac{2}{\sqrt{(2n-4)(n-1)}} + \frac{n-3}{\sqrt{(2n-3)(n-1)}}),$$

*where the equality holds if and only if $G \cong G^*(n,3,1)$.*

**Proof** Since $G \ncong C_n$, there exists positive integer $k$ such that $1 \leq k \leq r \leq n$ and $G = G(n,r,k)$. By Lemma 2.5, there exists $G_1$ such that $G_1 \in \mathbb{G}^*(n,r,k)$ and $G_1$ is obtained from $G$ by repeating edge-lifting transformation. Then $J(G) \leq J(G_1)$, where the equality holds if and only if $G = G(n,r,k) \cong G_1$.

By Lemma 2.8, $G_2 = G^*(n,r,1) \in \mathbb{G}^*(n,r,1)$ can be obtained from $G_1$ by repeating branch transformation such that $J(G_1) \leq J(G_2)$, where the equality holds if and only if $G_1 \cong G_2$.

Now by Lemma 3.1, we will show $J(G^*(n,r,1)) \leq \max\{J(G^*(n,3,1)), J(G^*(n,4,1))\}$ by the following two cases.

**Case 1** $r$ is even.

Let $f(r) = (\frac{r^2}{4} - r + 2n - 2)(\frac{r^2}{4} + n - r)$, and $g_i(r) = [\frac{r^2}{4} + i(n-r)][\frac{r^2}{4} + (i+1)(n-r)]$ for $1 \leq i \leq \frac{r}{2}$.

It is obvious that $f'(r)>0, g_1'(r)>0, g_2'(r)>0,\ldots,$ and $g_{\frac{r}{2}}'(r)>0$. So $J(G^*(n,r,1))=\frac{n}{2}\cdot(\frac{n-r}{\sqrt{f(r)}}+\sum\limits_{1\le i\le\frac{r}{2}}\frac{2}{\sqrt{g_i(r)}})$ is a decreasing function of $r$ when $r$ is even. Thus we have

$$J(G^*(n,4,1))>J(G^*(n,6,1))>\cdots>J(G^*(n,2\lfloor\frac{n-1}{2}\rfloor,1)).$$

**Case 2** $r$ is odd.

Let $f(r)=(\frac{r^2}{4}-r+2n-\frac{9}{4})(\frac{r^2-1}{4}+n-r)$, $g_i(r)=[\frac{r^2-1}{4}+i(n-r)][\frac{r^2-1}{4}+(i+1)(n-r)]$ for $1\le i\le\frac{r-1}{2}$, and $h(r)=\frac{r^2-1}{4}+\frac{r+1}{2}(n-r)$.

It is obvious that $f'(r)>0, g_1'(r)>0, g_2'(r)>0,\ldots,g_{\frac{r-1}{2}}'(r)>0$ and $h'(r)>0$. So $J(G^*(n,r,1))=\frac{n}{2}\cdot(\frac{n-r}{\sqrt{f(r)}}+\sum\limits_{1\le i\le\frac{r-1}{2}}\frac{2}{\sqrt{g_i(r)}}+\frac{1}{h(r)})$ is a decreasing function of $r$ when $r$ is odd. Thus we have $J(G^*(n,3,1))>J(G^*(n,5,1))>\cdots>J(G^*(n,2\lfloor\frac{n-2}{2}\rfloor+1,1))$.

On the other hand, by calaulating, we have

$$\begin{aligned}
&\frac{2}{n}\cdot(J(G^*(n,3,1))-J(G^*(n,4,1)))\\
&=\frac{1}{2n-4}+\frac{2}{\sqrt{(2n-4)(n-1)}}+\frac{n-3}{\sqrt{(2n-3)(n-1)}}-\\
&\quad(\frac{2}{\sqrt{n(2n-4)}}+\frac{2}{\sqrt{(2n-4)(3n-8)}}+\frac{n-4}{\sqrt{n(2n-2)}})\\
&=(\frac{1}{2n-4}-\frac{1}{\sqrt{(2n-4)(3n-8)}})+(\frac{2}{\sqrt{(2n-4)(n-1)}}-\frac{2}{\sqrt{n(2n-4)}})+\\
&\quad(\frac{n-4}{\sqrt{(2n-3)(n-1)}}-\frac{n-4}{\sqrt{n(2n-2)}})+(\frac{1}{\sqrt{(2n-3)(n-1)}}-\frac{1}{\sqrt{(2n-4)(3n-8)}})>0.
\end{aligned}$$

From above arguments, we have

$$J(G)\le J(G_1)\le J(G_2)\le\max\{J(G^*(n,3,1)),J(G^*(n,4,1))\}=J(G^*(n,3,1)).\ \Box$$

If $G=C_n$, then for any vertex $u\in V(C_n)$, $D_G(u)=\frac{n^2}{4}$ for even $n$ and $D_G(u)=\frac{n^2-1}{4}$ for odd $n$. Thus we have

**Proposition 3.3** *Let $n\ge 3$. Then* $J(C_n)=\begin{cases}2, & \text{if } n \text{ is even;}\\ \frac{2n^2}{n^2-1}, & \text{if } n \text{ is odd.}\end{cases}$

**Theorem 3.4** *Let $n,r$ be integers with $n\ge4$, $3\le r\le n$, $G$ be a connected unicyclic graph on $n$ vertices, the length of unique cycle of $G$ be $r$. Then*

$$J(G)\le J(G^*(n,3,1))=\frac{n}{2}\cdot(\frac{1}{2n-4}+\frac{2}{\sqrt{(2n-4)(n-1)}}+\frac{n-3}{\sqrt{(2n-3)(n-1)}}),$$

*where the equality holds if and only if $G\in\mathbb{G}^*(n,3,1)$.*

**Proof** By Theorem 3.2 and Proposition 3.3, we only need to show $J(G^*(n,3,1))>J(C_n)$.

**Case 1** $n=4$.

$$J(G^*(4,3,1))-J(C_4)=2(\frac{1}{4}+\frac{2}{\sqrt{12}}+\frac{1}{\sqrt{15}})-2>0.$$

**Case 2** $n\ge5$.

Then $(\frac{n^2-1}{4})^2-(2n-3)(n-1)=\frac{n^4-34n^2+80n-47}{16}=\frac{(n+5)^2(n-5)^2}{16}+(n+\frac{5}{2})^2-\frac{772}{16}>0$. So

$$J(G^*(n,3,1))-J(C_n)\geq\frac{n}{2}\cdot(\frac{1}{2n-4}+\frac{2}{\sqrt{(2n-4)(n-1)}}+\frac{n-3}{\sqrt{(2n-3)(n-1)}})-\frac{2n^2}{n^2-1}$$
$$=\frac{n}{2}\cdot(\frac{1}{2n-4}+\frac{2}{\sqrt{(2n-4)(n-1)}}+\frac{n-3}{\sqrt{(2n-3)(n-1)}}-\frac{n}{\frac{n^2-1}{4}})$$
$$=\frac{n}{2}\cdot[(\frac{1}{2n-4}-\frac{1}{\frac{n^2-1}{4}})+(\frac{2}{\sqrt{(2n-4)(n-1)}}-\frac{2}{\frac{n^2-1}{4}})+(\frac{n-3}{\sqrt{(2n-3)(n-1)}}-\frac{n-3}{\frac{n^2-1}{4}})]>0.$$

Combining the above two cases, we complete the proof. □

## 4. The maximum Sum-Balaban index of unicyclic graphs

In this section, we will show that $G^*(n,3,1)$ is the graph which has the maximum Sum-Balaban index among all unicyclic graphs on $n$ vertices.

Let $G$ be a unicyclic graph on $n$ vertices. Then $|E(G)|=n$, $\mu=1$, and thus

$$SJ(G)=\frac{n}{2}\sum_{uv\in E(G)}\frac{1}{\sqrt{D_G(u)+D_G(v)}}.$$

Similarly to Section 3, we can obtain the following results immediately.

**Lemma 4.1** *Let $n,r$ be positive integers with $3\leq r\leq n$, $G=G^*(n,r,1)\in\mathbb{G}^*(n,r,1)$ (see Figure 5). Then*

$$\frac{2SJ(G)}{n}=\begin{cases}\frac{n-r}{\sqrt{\frac{r^2}{2}-2r+3n-2}}+\sum\limits_{1\leq i\leq\frac{r}{2}}\frac{2}{\sqrt{\frac{r^2}{2}+(2i+1)(n-r)}}, & r \text{ is even;}\\ \frac{n-r}{\sqrt{\frac{r^2}{2}-2r+3n-\frac{5}{2}}}+\sum\limits_{1\leq i\leq\frac{r-1}{2}}\frac{2}{\sqrt{\frac{r^2-1}{2}+(2i+1)(n-r)}}+\frac{1}{\sqrt{nr-\frac{r^2+1}{2}+n-r}}, & r \text{ is odd;}\end{cases}$$

**Theorem 4.2** *Let $n,r$ be integers with $n\geq 4$, $3\leq r\leq n$, $G\ncong C_n$ be a connected unicyclic graph on $n$ vertices, the length of unique cycle of $G$ be $r$. Then*

$$SJ(G)\leq SJ(G^*(n,3,1))=\frac{n}{2}\cdot(\frac{1}{\sqrt{4n-8}}+\frac{2}{\sqrt{3n-5}}+\frac{n-3}{\sqrt{3n-4}}),$$

*where the equality holds if and only if $G\cong G^*(n,3,1)$.*

**Proof** Note that

$$\begin{aligned}&SJ(G^*(n,3,1))-SJ(G^*(n,4,1))\\&=\frac{n}{2}\cdot[(\frac{1}{\sqrt{4n-8}}+\frac{2}{\sqrt{3n-5}}+\frac{n-3}{\sqrt{3n-4}})-(\frac{2}{\sqrt{3n-4}}+\frac{2}{\sqrt{5n-12}}+\frac{n-4}{\sqrt{3n-2}})]\\&=\frac{n}{2}\cdot[(\frac{1}{\sqrt{4n-8}}-\frac{1}{\sqrt{5n-12}})+(\frac{2}{\sqrt{3n-5}}-\frac{2}{\sqrt{3n-4}})+\\&\quad(\frac{n-4}{\sqrt{3n-4}}-\frac{n-4}{\sqrt{3n-2}})+(\frac{1}{\sqrt{3n-4}}-\frac{1}{\sqrt{5n-12}})]>0.\end{aligned}$$

Thus similarly to the proof of Theorem 3.2, we have

$$SJ(G)\leq SJ(G_1)\leq SJ(G_2)\leq\max\{SJ(G^*(n,3,1)),SJ(G^*(n,4,1))\}=SJ(G^*(n,3,1)).\ \square$$

**Proposition 4.3** *Let $n \geq 3$. Then* $SJ(C_n) = \begin{cases} \frac{\sqrt{2}n}{2}, & \text{if } n \text{ is even;} \\ \frac{\sqrt{2}n^2}{2\sqrt{n^2-1}}, & \text{if } n \text{ is odd.} \end{cases}$

**Theorem 4.4** *Let $n, r$ be integers with $n \geq 4$, $3 \leq r \leq n$, $G$ be a connected unicyclic graph on $n$ vertices, the length of unique cycle of $G$ be $r$. Then*

$$SJ(G) \leq SJ(G^*(n,3,1)) = \frac{n}{2} \cdot (\frac{1}{\sqrt{4n-8}} + \frac{2}{\sqrt{3n-5}} + \frac{n-3}{\sqrt{3n-4}}),$$

*where the equality holds if and only if $G \in \mathbb{G}^*(n,3,1)$.*

**Proof** By Theorem 4.2 and Proposition 4.3, we only need to show $SJ(G^*(n,3,1)) > SJ(C_n)$.

**Case 1** $n = 4$.

$$SJ(G^*(4,3,1)) - SJ(C_4) = 2(\frac{2}{\sqrt{8}} + \frac{2}{\sqrt{7}}) - 2\sqrt{2} = \frac{4\sqrt{7}}{7} - \sqrt{2} > 0.$$

**Case 2** $n \geq 5$.

$$\begin{aligned} SJ(G^*(n,3,1)) - SJ(C_n) &\geq \frac{n}{2} \cdot (\frac{1}{\sqrt{4n-8}} + \frac{2}{\sqrt{3n-5}} + \frac{n-3}{\sqrt{3n-4}}) - \frac{\sqrt{2}n^2}{2\sqrt{n^2-1}} \\ &= \frac{n}{2} \cdot [(\frac{1}{\sqrt{4n-8}} - \frac{1}{\sqrt{\frac{n^2-1}{2}}}) + (\frac{2}{\sqrt{3n-5}} - \frac{2}{\sqrt{\frac{n^2-1}{2}}}) + (\frac{n-3}{\sqrt{3n-4}} - \frac{n-3}{\sqrt{\frac{n^2-1}{2}}})] > 0. \end{aligned}$$

Combining the above two cases, we complete the proof. □

**Acknowledgements** The authors would like to thank the referees for their valuable comments, corrections, and suggestions, which lead to an improvement of the original paper.

## References

[1] R. J. WILSON. *Introduction to Graph Theory*. Oliver & Boyd, Edinburgh, 1972.
[2] A. T. BALABAN. *Highly discriming distance-based topological index*. Chem. Phys. Lett., 1982, **89**: 399–404.
[3] A. T. BALABAN. *Topological indices based on topological distances in molecular graphs*. Pure Appl. Chem., 1983, **55**: 199–206.
[4] A. T. BALABAN, P. V. KHADIKAR, S. AZIZ. *Comparison of topological indices based on iterated 'sum' versus 'product' operations*. Iranian J. Math. Chem., 2010, **1**: 43–67.
[5] Hanyuan DENG. *On the Balaban index of trees*. MATCH Commun. Math. Comput. Chem., 2011, **66**(1): 253–260.
[6] Hawei DONG, Xiaofeng GUO. *Character of graphs with extremal Balaban index*. MATCH Commun. Math. Comput. Chem., 2010, **63**(3): 799–812.
[7] Hawei DONG, Xiaofeng GUO. *Character of trees with extreme Balaban index*. MATCH Commun. Math. Comput. Chem., 2011, **66**(1): 261–272.
[8] Shuxian LI, Bo ZHOU. *On the Balaban index of trees*. Ars Combin., 2011, **101**: 503–512.
[9] Lingli SUN. *Bounds on the Balaban index of trees*. MATCH Commun. Math. Comput. Chem., 2010, **63**(3): 813–818.
[10] Lihua YOU, Han HAN. *The maximum Balaban index (Sum-Balaban index) of trees with given diameter*. Ars Combin., 2013, **112**: 115–128.
[11] Bo ZHOU, N. TRINAJSTIĆ. *Bounds on the Balaban index*. Croat. Chem. Acta, 2008, **81**: 319–323.
[12] Hanyuan DENG. *On the Sum-Balaban index*. MATCH Commun. Math. Comput. Chem., 2011, **66**(1): 273–284.
[13] Rundang XING, Bo ZHOU, A. GROVAC. *On sum-Balaban index*. Ars Combin., 2012, **104**: 211–223.