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

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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

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

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.

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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.

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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

\[
\frac{1}{\sqrt{(w+a)(z+a')}} + \frac{1}{\sqrt{wz}} \geq \frac{1}{\sqrt{wz}} + \frac{1}{\sqrt{(x+b)(y+b')}}, \quad \text{and the equality holds if and only if } b = a, b' = a', w = x \text{ and } z = y.
\]

**Lemma 2.2** ([7]) Let \( x, y, a \in R^+ \) such that \( x \geq y + a \). Then

\[
\frac{1}{\sqrt{xy}} \geq \frac{1}{\sqrt{(x-a)(y+a)}}, \quad \text{and the equality holds if and only if } x = y + a.
\]

**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

\[
\frac{1}{\sqrt{x_1}} + \frac{1}{\sqrt{x_2}} < \frac{1}{\sqrt{y_1}} + \frac{1}{\sqrt{y_2}}.
\]

**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

\[
\frac{1}{\sqrt{x_1}} - \frac{1}{\sqrt{x_1+a}} < \frac{1}{\sqrt{y_1}} - \frac{1}{\sqrt{y_1+a}} \quad \text{by } x_1 > y_1, \quad \text{that is to say, } \frac{1}{\sqrt{x_1}} + \frac{1}{\sqrt{x_2}} < \frac{1}{\sqrt{y_1}} + \frac{1}{\sqrt{y_2}}.
\]

**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 pendant 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
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 $S = \{ S \mid S$ is a rooted star and the root is its center $\}$. Let $G^*(n, r, k)$ be the set of all unicyclic graphs on $n$ vertices obtained from $C_r$ by attaching $k$ rooted stars in $S$ to $k$ distinct vertices of $C_r$ (see Figure 2).

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 $G^*(n, r, k) \in G^*(n, r, k)$ 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 $G^*(n, r, 1) \in G^*(n, r, 1)$ by repeating edge-lifting transformation from graph $G(n, r, 1)$. 

\[ S J(G) < S J(G') \]

\[ G_1 \quad u_0 \quad G_2 \]

\[ G' \]

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 $S = \{ S \mid S$ is a rooted star and the root is its center $\}$. Let $G^*(n, r, k)$ be the set of all unicyclic graphs on $n$ vertices obtained from $C_r$ by attaching $k$ rooted stars in $S$ to $k$ distinct vertices of $C_r$ (see Figure 2).

\[ G_1 \quad u_0 \quad G_2 \]

\[ G' \]

Figure 2 A graph $G^*(n, r, k)$ in the set $G^*(n, r, k)$
Lemma 2.6 Let $G = G^*(n, r, k) \in \mathcal{G}^*(n, r, k)$ be defined as above. For convenience, let $m = \lceil \frac{n}{2} \rceil$. If $r$ is even, define $C_r = v_1v_2 \cdots v_m u_{m+1} u_m \cdots u_1v_1$; if $r$ is odd, define $C_r = v_1v_2 \cdots v_{m+1} u_{m+1} u_m \cdots u_1v_1$. Then $G'$ is obtained from $G$ by deleting the pendent edge $u_iw$ and adding the pendent edge $v_iw$ for any $i \in \{1, 2, \ldots, m\}$ (if there exists the pendent edge $u_iw$), where $w \in V(G) \setminus V(C_r)$. We say $G'$ is obtained from $G$ by branch transformation (see Figure 4, where $p_i \geq 0$, $q_i \geq 0$ for any $i \in \{1, 2, \ldots, m\}$).

Let $G$ be a graph and $U(\neq \emptyset) \subseteq V(G)$. 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 $2 \leq k \leq r$, $3 \leq r \leq n - k$, $G = G^*(n, r, k) \in \mathcal{G}^*(n, r, k)$, $G'$ be the graph obtained from $G$ by branch transformation. Then $J(G) < J(G')$.

Proof Let $U_0 = \{u_1, u_2, \ldots, u_m\}$, $U_1 = \{w| u_iw \in E(G) \land \deg(w) = 1, 1 \leq i \leq m\}$, $V_0 = \{v_1, v_2, \ldots, v_m\}$, and $V_1 = \{w| v_iw \in E(G) \land \deg(w) = 1, 1 \leq i \leq m\}$ for $r = 2m$ is even, $V_4 = \{w| v_iw \in E(G) \land \deg(w) = 1, 1 \leq i \leq m + 1\}$ \cup $\{v_{m+1}\}$ for $r = 2m + 1$ is odd.

Figure 3 An example

Figure 4 The branch transformation
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
\[
D_G(u_s) = D_G(u_s, U_0) + D_G(u_s, U_1) + D_G(u_s, V_0) + D_G(u_s, V_1),
\]
(2.1)
and
\[
D_{G'}(v_s) = D_{G'}(v_s, V_0) + D_{G'}(v_s, U_1) + D_{G'}(v_s, V_0) + D_{G'}(v_s, V_1).
\]
(2.2)
Noting that \( G[U_0] \cong G'[V_0] \), \( G[V_0] \cong G'[V_0] \) and \( G[U_0 \cup U_1] \cong G'[V_0 \cup U_1] \), 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
\[
D_G(u_s) - D_{G'}(v_s) = D_G(u_s, V_1) - D_{G'}(v_s, V_1) > 0.
\]
(2.3)
Similarly, we have
\[
D_G(v_s) = D_G(v_s, U_0) + D_G(v_s, U_1) + D_G(v_s, V_0) + D_G(v_s, V_1),
\]
(2.4)
and
\[
D_{G'}(u_s) = D_{G'}(u_s, U_0) + D_{G'}(u_s, U_1) + D_{G'}(u_s, V_0) + D_{G'}(u_s, V_1).
\]
(2.5)
Thus
\[
D_{G'}(u_s) - D_G(u_s) = D_{G'}(u_s, V_1) - D_G(u_s, V_1) > 0.
\]
(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
\[
D_G(u_s) - D_{G'}(v_s) = D_G(u_s, V_1) - D_{G'}(v_s, V_1) > 0.
\]
(2.7)
By (2.1), (2.2), (2.4) and (2.5), we have
\[
D_{G'}(u_s) - D_G(u_s) = D_{G'}(v_s) - D_G(v_s) > 0.
\]
(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 \( x = D_{G'}(v_s), y = D_{G'}(v_t), w = D_G(u_s), z = D_G(u_t), a = D_{G'}(u_s) - D_G(u_s), a' = D_{G'}(u_t) - D_G(u_t), b = D_G(v_s) - D_{G'}(v_t), b' = D_{G'}(v_t) - D_G(v_t) \). Then \( b = a > 0, b' = a' > 0 \) by (2.8). It is obvious that
\[
a, a', b, b', w, x, y, z \in R^+, w > x, z > y \text{ by (2.7). Then } \frac{a}{w}, \frac{a'}{y} > \frac{b'}{z}. \text{ Thus by Lemma 2.1, we have}
\]
\[
\frac{1}{\sqrt{D_{G'}(u_s)D_{G'}(u_t)}} + \frac{1}{\sqrt{D_{G'}(v_s)D_{G'}(v_t)}} > \frac{1}{\sqrt{D_G(u_s)D_G(u_t)}} + \frac{1}{\sqrt{D_G(v_s)D_G(v_t)}}.
\]
(2.9)
Similarly, for any vertex \( w \in U_1 \cup V_1 \), 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
\[
\frac{1}{\sqrt{D_{G'}(v_s)D_{G'}(w)}} > \frac{1}{\sqrt{D_G(u_s)D_G(w)}}.
\]
(2.10)
For any edge $v_sw \in E(G)$ with $v_s \in V_0$ where $1 \leq s \leq m$ and $w \in V_1$, we have
\[
\frac{1}{\sqrt{D_G'(v_s)D_G'(w)}} > \frac{1}{\sqrt{D_G(v_s)D_G(w)}}.
\] (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
\[
\frac{1}{\sqrt{D_G'(v_{m+1})D_G'(w)}} = \frac{1}{\sqrt{D_G(v_{m+1})D_G(w)}}.
\] (2.12)

For edge $u_1v_1$, by (2.8) and Lemma 2.3, we have
\[
\frac{1}{\sqrt{D_G(u_1)D_G(v_1)}} > \frac{1}{\sqrt{D_G'(u_1)D_G'(v_1)}}.
\] (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 $2 \leq k \leq r$ and $3 \leq r \leq n - k$, $G = G^*(n, r, k) \in \mathbb{G}^*(n, r, k)$, $G'$ be the graph obtained from $G$ by branch transformation. Then $SJ(G) < SJ(G')$.

**Proof** Let $U_0$, $U_1$, $V_0$, $V_1$, $a, a', b, b'$ be defined as Lemma 2.6. Let $f(x) = \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+1}}$. 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
\[
\frac{1}{\sqrt{D_G(u_s) + D_G(u_t)}} \cdot \frac{1}{\sqrt{D_G(v_s) + D_G(v_t)}} > \frac{1}{\sqrt{D_G(u_s) + D_G(u_t) + a + a'}} \cdot \frac{1}{\sqrt{D_G(v_s) + D_G(v_t)}}.
\]

Thus
\[
\frac{1}{\sqrt{D_G(u_s) + D_G(u_t)} + \sqrt{D_G'(v_s) + D_G'(v_t)}} > \frac{1}{\sqrt{D_G(u_s) + D_G(u_t)} + \sqrt{D_G'(v_s) + D_G'(v_t)}}.
\] (2.14)

Similarly, for any vertex $w \in U_1 \cup V_1$, 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 pendant vertex and adjacent to $v_{m+1}$. Then it implies that the following inequalities (2.15)–(2.17) 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
\[
\frac{1}{\sqrt{D_G'(v_s) + D_G'(w)}} > \frac{1}{\sqrt{D_G(v_s) + D_G(w)}}.
\] (2.15)

For any edge $v_s w \in E(G)$ with $v_s \in V_0$ where $1 \leq s \leq m$ and $w \in V_1$, we have
\[
\frac{1}{\sqrt{D_G(v_s) + D_G(w)}} > \frac{1}{\sqrt{D_G'(v_s) + D_G'(w)}}.
\] (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
\[
\frac{1}{\sqrt{D_G'(v_{m+1}) + D_G'(w)}} = \frac{1}{\sqrt{D_G(v_{m+1}) + D_G(w)}}.
\] (2.17)
For edge $u_1v_1$, by (2.8), we have

$$\frac{1}{\sqrt{D_{G^*}(u_1)+D_{G^*}(v_1)}} = \frac{1}{\sqrt{D_G(u_1)+D_G(v_1)}}.$$ (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 $1 \leq k \leq r$ and $3 \leq r \leq n - k$, $G = G^*(n, r, k) \in \mathbb{G}^*(n, r, k)$, 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. $J(G) \leq J(G')$, and the equality holds if and only if $G \cong G'$.
3. $SJ(G) \leq SJ(G')$, and the equality holds if and only if $G \cong G'$.

![Figure 5](image)

**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

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

**Lemma 3.1** 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

$$\frac{2J(G)}{n} = \begin{cases} \frac{n-r}{\sqrt{\frac{r}{2}(2n-r+2n-1)(2n-r)}} + \sum_{i=1}^{r-1} \frac{2}{\sqrt{\left\lfloor \frac{r}{2} + i(n-r) \right\rfloor} \left\lfloor \frac{r}{2} + (i+1)(n-r) \right\rfloor}} & r \text{ is even}; \\
\frac{2}{\sqrt{\frac{r}{2} - 2n-1}} + \sum_{i=1}^{r-1} \frac{2}{\sqrt{D_G(u_i)D_G(u_{i+1})}} \cdot \frac{r-i+1}{2n-r-1} & r \text{ is odd}; \end{cases}$$

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

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

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

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

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

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

Noting that $D_G(u_i) = D_G(u_{r+2-i})$, we only need to calculate $D_G(u_i)$ for $1 \leq i \leq \frac{r+2}{2}$. 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** $u \in V(G) \setminus V(C_r)$.

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

**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 $w \in V(G) \setminus V(C_r)$, then we can show (3.1) by the following equation

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

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

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

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

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

**Proof** Since $G \not\cong G_n$, 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 $G_1 \in G^*(n, r, k)$ 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 $G = G(n, r, k) \equiv G_1$.

By Lemma 2.8, $G_2 = G^*(n, r, 1) \in G^*(n, r, 1)$ 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 $G_1 \equiv G_2$.

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 \( g'_2(r) > 0. \) So \( J(G^*(n,r,1)) = \frac{2}{n} \cdot \left( \frac{n-r}{\sqrt{f(r)}} + \sum_{1 \leq i \leq \frac{r}{2}} \frac{2}{\sqrt{g_i(r)}} \right) \) is a decreasing function of \( r \) when \( r \) is even. Thus we have

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

**Case 2** \( r \) is odd.

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

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 \( J(G^*(n,r,1)) = \frac{2}{n} \cdot \left( \frac{n-r}{\sqrt{f(r)}} + \sum_{1 \leq i \leq \frac{r-1}{2}} \frac{2}{\sqrt{g_i(r)}} + \frac{1}{h(r)} \right) \) is a decreasing function of \( r \) when \( r \) is odd.

Thus we have \( J(G^*(n,3,1)) > J(G^*(n,5,1)) > \cdots > J(G^*(n,2\left\lfloor \frac{n-2}{2} \right\rfloor + 1,1)). \)

On the other hand, by calculation, we have

\[
\frac{2}{n} \cdot (J(G^*(n,3,1)) - J(G^*(n,4,1)))
= \frac{1}{2n-4} + \frac{2}{\sqrt{(2n-4)(n-1)}} + \frac{n-3}{\sqrt{(2n-3)(n-1)}} - \left( \frac{2}{\sqrt{n(2n-4)}} + \frac{2}{\sqrt{(2n-4)(3n-8)}} + \frac{n-4}{\sqrt{n(2n-2)}} \right)
= \frac{1}{2n-4} - \frac{1}{\sqrt{(2n-4)(3n-8)}} + \frac{2}{\sqrt{(2n-4)(n-1)}} - \frac{2}{\sqrt{n(2n-4)}} + \left( \frac{n-4}{\sqrt{(2n-3)(n-1)}} - \frac{1}{\sqrt{n(2n-2)}} \right) > 0.
\]

From above arguments, we have

\[
J(G) \leq J(G_1) \leq J(G_2) \leq \max\{J(G^*(n,3,1)), J(G^*(n,4,1))\} = J(G^*(n,3,1)). \quad \square
\]

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 \( n \geq 3 \). Then \( J(C_n) = \left\{ \begin{array}{ll} 2, & \text{if } n \text{ is even;} \\ 2n^2, & \text{if } n \text{ is odd.} \end{array} \right. \)

**Theorem 3.4** 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

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

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

**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** \( n \geq 5. \)
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 \( 3 \leq r \leq n \), \( G = G^*(n, r, 1) \in G^*(n, r, 1) \) (see Figure 5). Then

\[
\frac{2SJ(G)}{n} = \begin{cases} 
\frac{n-r}{2\sqrt{r^2 - 2r + 3n - 2}} + \sum_{1 \leq i \leq \frac{n-r}{2}} \frac{2}{\sqrt{r^2 + (2i+1)(n-r)}} & \text{if } r \text{ is even;} \\
\frac{n-r}{2\sqrt{r^2 - 2r + 3n - 2}} + \sum_{1 \leq i \leq \frac{n-r}{2}} \frac{2}{\sqrt{r^2 + (2i+1)(n-r)}} + \frac{1}{\sqrt{n^2 - 2r + 3n - 2}} & \text{if } r \text{ is odd.}
\end{cases}
\]

**Theorem 4.2** Let \( n, r \) be integers with \( n \geq 4, 3 \leq r \leq n \), \( G \not\cong C_n \) be a connected unicyclic graph on \( n \) vertices, the length of unique cycle of \( G \) be \( r \). Then

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

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

**Proof** Note that

\[
SJ(G^*(n, 3, 1)) - SJ(G^*(n, 4, 1)) = \frac{n}{2} \cdot \left[ \left( \frac{1}{\sqrt{4n-8}} + \frac{2}{\sqrt{3n-5}} + \frac{n-3}{\sqrt{3n-4}} \right) - \left( \frac{2}{\sqrt{3n-4}} + \frac{2}{\sqrt{5n-12}} + \frac{n-4}{\sqrt{3n-2}} \right) \right] = \frac{n}{2} \cdot \left[ \left( \frac{1}{\sqrt{4n-8}} - \frac{1}{\sqrt{5n-12}} \right) + \left( \frac{2}{\sqrt{3n-4}} - \frac{2}{\sqrt{3n-2}} \right) + \left( \frac{n-4}{\sqrt{3n-4}} - \frac{n-4}{\sqrt{3n-2}} \right) \right] > 0.
\]

Thus similarly to the proof of Theorem 3.2, we have

\[
SJ(G) \leq SJ(G_1) \leq SJ(G_2) \leq \max\{SJ(G^*(n, 3, 1)), SJ(G^*(n, 4, 1))\} = SJ(G^*(n, 3, 1)). \quad \Box
\]
Proposition 4.3 Let $n \geq 3$. Then $SJ(C_n) = \begin{cases} \sqrt{\frac{2n}{n^2}}, & \text{if } n \text{ is even;} \\ \sqrt{\frac{2n^2}{n^2-1}}, & \text{if } n \text{ is odd.} \end{cases}$

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

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

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

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

Case 1 $n = 4$.

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

Case 2 $n \geq 5$.

$$SJ(G^*(n, 3, 1)) - SJ(C_n) \geq \frac{n}{2} \cdot \left( \frac{1}{\sqrt{4n} - 8} + \frac{2}{\sqrt{3n} - 5} + \frac{n - 3}{\sqrt{3n} - 4} \right) - \frac{\sqrt{2n^2}}{2\sqrt{n^2 - 1}}$$

$$= \frac{n}{2} \cdot \left[ \frac{1}{\sqrt{4n} - 8} - \frac{1}{\sqrt{n^2 - 1}} \right] + \left( \frac{2}{\sqrt{3n} - 5} - \frac{2}{\sqrt{n^2} - 2} \right) + \left( \frac{n - 3}{\sqrt{3n} - 4} - \frac{n - 3}{\sqrt{n^2} - 2} \right] > 0.$$

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

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