The maximum Sum-Balaban index of trees with given diameter *

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Abstract

The Sum-Balaban index defined as

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

where μ is the cyclomatic number of G and $D_G(u) = \sum_{v \in V(G)} d_G(u, v)$. In this paper, we characterize the tree with the maximum Sum-Balaban index among all trees with n vertices and diameter d. We also give a new proof of the result that the star S_n is the graph which has the maximum Sum-Balaban index among all trees with n vertices. Furthermore, we propose a problem for further research.

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 μ of G is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph. It is known that $\mu = m - n + 1$([14]).

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

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

It was proposed by A. T. Balaban [1, 2], which also called the average distance-sum connectivity index or J index. It appear to be a very useful molecular descriptor with attractive properties. It has been used successfully in developing QSAR/QSPR models([13]) and in drug design([10]). Mathematical properties of Balaban index may be found in [4, 6, 7, 8, 11, 12, 16].

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

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

Mathematical properties of Sum-Balaban index may be found in [5, 15].

Theorem 1.1. [5, 15] *If T is a tree with $n \geq 2$ vertices, then $SJ(P_n) \leq SJ(T) \leq SJ(S_n)$ with left* (or *right*) *equality if and only if $T \cong P_n$* (or *$T \cong S_n$*), *where P_n is the path on n vertices and S_n is the star on n vertices.*

In [6, 7], Dong and Guo characterized the tree with the maximum Balaban index among all the trees with n vertices and either given diameter, or the maximum degree, or a given degree sequence, or k pendent vertices, the tree with the minimum Balaban index among all the trees with n vertices and the maximum degree. In [8], they give some order relations of trees about Balaban index among all the trees with n vertices, and they determined at most 21st largest Balaban indices among all the trees with n vertices. In [7], they also proposed to characterize the graphs with maximum Balaban index among graphs with n vertices and given diameter.

In this paper, we characterize the tree with the maximum Sum-Balaban index among all trees with n vertices and diameter d in Section 2. In Section 3, we give a new proof of the result that the star S_n is the graph which has the maximum Sum-Balaban index among all trees with n vertices. Furthermore, we propose a problem for further research in Section 4.

2 The tree with maximum Sum-Balaban index among trees with n vertices and diameter d

In this section, we will introduce two transformations which are important to our main results, and then we will characterize the tree with the maximum Sum-Balaban index among all trees with n vertices and diameter d.

A rooted graph has one of its vertex, called the root, distinguished from the others. Let T be a tree and $V_1 \subseteq V(T)$, then for any vertex $u \in V(T)$, we define $D_T(u, V_1) = \sum_{v \in V_1} d_T(u, v)$. Note that the distance between vertices u and v in a tree T, $d_T(u, v)$, is the length of the path from vertex u to vertex v in T because that the path from u to v in a tree is unique.

2.1 Branch transformation

Branch transformation: Let T be a tree, p, q be positive integers with $p \leq q$, $P = u_p u_{p-1} \cdots u_2 u_1 u_0 v_0 v_1 v_2 \cdots v_q$ be the longest path in T, T_1 and T_2 be the component of $T - u_0 v_0$ rooted at u_0 and v_0, respectively. Let T_{u_i} and T_{v_j} be the component of $T - E(P)$ rooted at u_i and v_j $(0 \leq i \leq p, 0 \leq j \leq q)$, respectively. Then T' is obtained by deleting T_{u_i} except for vertex u_i for $0 \leq i \leq p$ from T and adding T'_{v_i} to the root v_i for $0 \leq i \leq p$, where T'_{v_i} is a rooted tree obtained from T_{u_i} replacing u_i by v_i for any $0 \leq i \leq p$. We call T' is obtained from T by branch transformation (see Fig.1).

Note that P is the longest path in T, so $V(T_{u_p}) = \{u_p\}$ and $V(T_{v_q}) = \{v_q\}$.

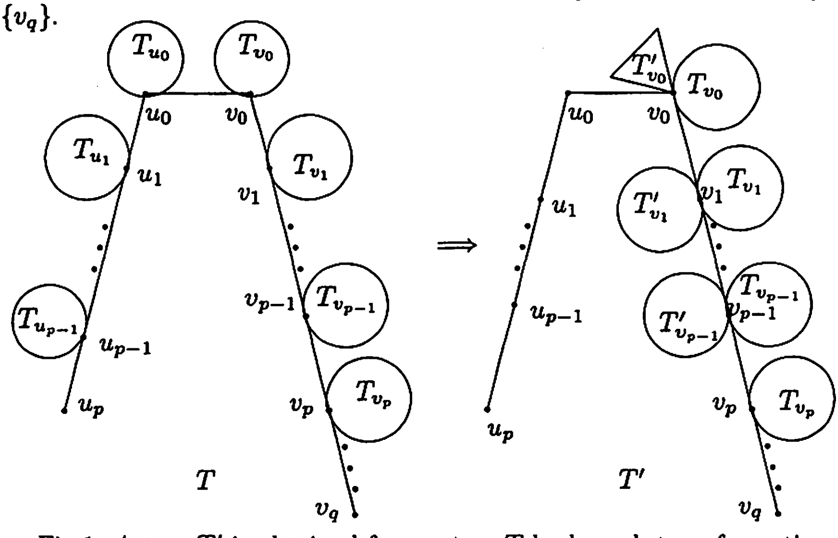


Fig.1: A tree T' is obtained from a tree T by branch transformation.

Lemma 2.1. *Let T' be a graph obtained from T by branch transformation, then $SJ(T') \geq SJ(T)$, and $SJ(T') = SJ(T)$ if and only if $T \cong T'$.*

Proof. Let $U_0 = \{u_0, u_1, u_2, \cdots, u_p\}$, $V_0 = \{v_0, v_1, v_2, \cdots, v_p\}$, $U_1 = V(T_1) \setminus U_0$, and $V_1 = V(T_2) \setminus V_0$. Suppose $T \ncong T'$, then $U_1 \neq \phi$ and $V_1 \neq \phi$.

For any s with $0 \leq s \leq p$, it is clearly that $u_s \in U_0$ and $v_s \in V_0$, and

$$D_T(u_s) = D_T(u_s, U_0) + D_T(u_s, U_1) + D_T(u_s, V_0) + D_T(u_s, V_1), \quad (2.1)$$

and

$$D_{T'}(v_s) = D_{T'}(v_s, V_0) + D_{T'}(v_s, U_1) + D_{T'}(v_s, U_0) + D_{T'}(v_s, V_1). \quad (2.2)$$

Note that $T'[U_0] \cong T[V_0]$ and $T_1 \cong T'[V_0 \bigcup U_1]$, so

$$D_T(u_s, U_0) = D_{T'}(v_s, V_0), D_T(u_s, V_0) = D_{T'}(v_s, U_0),$$

and

$$D_T(u_s, U_1) = D_{T'}(v_s, U_1), D_T(u_s, V_1) > D_{T'}(v_s, V_1).$$

Thus we have

$$D_T(u_s) - D_{T'}(v_s) = D_T(u_s, V_1) - D_{T'}(v_s, V_1) > 0. \quad (2.3)$$

Similarly, we have

$$D_T(v_s) = D_T(v_s, U_0) + D_T(v_s, U_1) + D_T(v_s, V_0) + D_T(v_s, V_1), \quad (2.4)$$

and

$$D_{T'}(u_s) = D_{T'}(u_s, V_0) + D_{T'}(u_s, U_1) + D_{T'}(u_s, U_0) + D_{T'}(u_s, V_1). \quad (2.5)$$

Thus

$$D_{T'}(u_s) - D_T(v_s) = D_{T'}(u_s, V_1) - D_T(v_s, V_1) > 0. \quad (2.6)$$

Note that $D_T(u_s, V_1) = D_{T'}(u_s, V_1)$ and $D_{T'}(v_s, V_1) = D_T(v_s, V_1)$, by (2.3) and (2.6), we have

$$D_T(u_s) - D_{T'}(v_s) = D_{T'}(u_s) - D_T(v_s) = D_T(u_s, V_1) - D_{T'}(v_s, V_1) > 0. \quad (2.7)$$

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

$$D_{T'}(u_s) - D_T(u_s) = D_T(v_s) - D_{T'}(v_s) > 0. \quad (2.8)$$

Let $a = D_{T'}(u_s) - D_T(u_s)$, $a' = D_{T'}(u_t) - D_T(u_t)$, $b = D_T(v_s) - D_{T'}(v_s)$, $b' = D_T(v_t) - D_{T'}(v_t)$ for any s, t with $0 \leq s, t \leq p$. Then

$b = a > 0$, $b' = a' > 0$ by (2.8).

Let $f(x) = \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+a+a'}}$, $f(x)$ is decreasing function of x since $f'(x) < 0$. Note that $D_T(u_s) + D_T(u_t) > D_{T'}(v_s) + D_{T'}(v_t) = D_T(v_s) + D_T(v_t) - a - a'$, we have

$$\frac{1}{\sqrt{D_T(u_s)+D_T(u_t)}} - \frac{1}{\sqrt{D_T(u_s)+D_T(u_t)+a+a'}} < \frac{1}{\sqrt{D_T(v_s)+D_T(v_t)-a-a'}} - \frac{1}{\sqrt{D_T(v_s)+D_T(v_t)}}.$$

Thus

$$\frac{1}{\sqrt{D_{T'}(u_s) + D_{T'}(u_t)}} + \frac{1}{\sqrt{D_{T'}(v_s) + D_{T'}(v_t)}} > \frac{1}{\sqrt{D_T(u_s) + D_T(u_t)}} + \frac{1}{\sqrt{D_T(v_s) + D_T(v_t)}}. \tag{2.9}$$

Similarly, for any vertex $w \in U_1 \bigcup V_1$, we can show $D_T(w) > D_{T'}(w)$. Then it implies that the following inequalities (2.10)-(2.12) hold.

For any edge $e = uv \in E(T[U_1]) \bigcup E(T[V_1])$, we have

$$\frac{1}{\sqrt{D_{T'}(u) + D_{T'}(v)}} > \frac{1}{\sqrt{D_T(u) + D_T(v)}}. \tag{2.10}$$

For any edge $u_s w \in E(T_1) \subset E(T)$ with $u_s \in U_0$ where $0 \leq s \leq p$ and $w \in U_1$, the corresponding edge is $v_s w \in E(T')$, we have

$$\frac{1}{\sqrt{D_{T'}(v_s) + D_{T'}(w)}} > \frac{1}{\sqrt{D_T(u_s) + D_T(w)}}. \tag{2.11}$$

For any edge $v_s w \in E(T_2)$ with $v_s \in V_0$ where $0 \leq s \leq p$ and $w \in V_1$, we have

$$\frac{1}{\sqrt{D_{T'}(v_s) + D_{T'}(w)}} > \frac{1}{\sqrt{D_T(v_s) + D_T(w)}}. \tag{2.12}$$

For edge $u_0 v_0$, by (2.8), we have

$$\frac{1}{\sqrt{D_{T'}(u_0) + D_{T'}(v_0)}} = \frac{1}{\sqrt{D_T(u_0) + D_T(v_0)}}. \tag{2.13}$$

From (2.9) to (2.13), we obtain $SJ(T') > SJ(T)$ by the definition of Sum-Balaban index. □

2.2 Edge-lifting transformation

Let $P = v_1 v_2 v_3 \cdots v_r$ be a path of length $r - 1 (\geq 1)$, G_0 be a connected graph with $n_0 (\geq 1)$ vertices and G_1 be a connected graph with $n_1 (\geq 2)$

vertices. Let $x \in V(G_0)$, $y \in V(G_1)$ and $v_k \in V(P)$ where $1 \le k \le r$. G is a graph obtained from G_0, G_1, P by identifying vertex x with vertex v_k and adding an edge $e = xy$. G' is a graph obtained from G_0, G_1, P by identifying vertices x, v_k and y, and adding a pendent edge $e = xw$ to $x(= v_k = y)$. We call G' is obtained from G by edge-lifting transformation (see Fig.2).

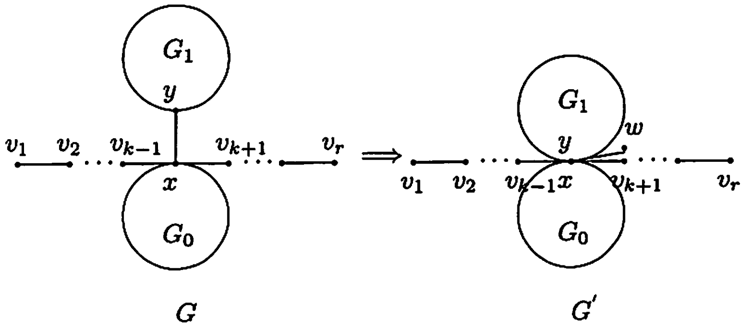


Fig.2: G' is obtained from G by edge-lifting transformation.

Lemma 2.2. *Let P, G_0, G_1, G be connected graphs and defined as above, G' is obtained from G by edge-lifting transformation. Then*

$$D_G(u) = D_{G'}(u) + \begin{cases} n_1 - 1, & u \in V(G_0) \bigcup V(P); \\ n_0 + r - 2, & u \in V(G_1); \end{cases} \tag{2.14}$$

and

$$D_{G'}(w) = D_G(y) + n_1 - 1. \tag{2.15}$$

Proof. In the graph G, note that $v_k = x$ and $d_G(v_k, y) = 1$, then for any $u \in V(G)$, we have

Case 1: $u \in V(G_0)$.

$D_G(u) = \sum_{v \in V(G_0)} d_G(u,v) + \sum_{i=1}^{r} d_G(u, v_i)$
$+ \sum_{v \in V(G_1)} d_G(u,v) - d_G(u,x)$
$= D_{G_0}(u) + \sum_{i=1}^{r} [d_G(u, v_k) + d_G(v_k, v_i)]$
$+ \sum_{v \in V(G_1)} [d_G(u, v_k) + d_G(v_k, y) + d_G(y, v)] - d_G(u,x)$
$= D_{G_0}(u) + D_P(v_k) + D_{G_1}(y) + (n_1 + r - 1) d_G(u,x) + n_1$.

Case 2: $u \in V(G_1)$.

$D_G(u) = \sum_{v \in V(G_0)} d_G(u,v) + \sum_{i=1}^{r} d_G(u, v_i)$
$+ \sum_{v \in V(G_1)} d_G(u,v) - d_G(u,x)$
$= \sum_{v \in V(G_0)} [d_G(u,y) + d_G(y,x) + d_G(x,v)]$
$+ \sum_{i=1}^{r} [d_G(u,y) + d_G(y, v_k) + d_G(v_k, v_i)] + D_{G_1}(u) - [d_G(u,y) + 1]$

$= D_{G_0}(x) + D_P(v_k) + D_{G_1}(u) + (n_0 + r - 1)d_G(u,y) + n_0 + r - 1.$

Case 3: $u \in V(P)$.

$$D_G(u) = \sum_{v\in V(G_0)} d_G(u,v) + \sum_{i=1}^{r} d_G(u,v_i)$$
$$+ \sum_{v\in V(G_1)} d_G(u,v) - d_G(u,x)$$
$$= \sum_{v\in V(G_0)}[d_G(u,x) + d_G(x,v)] + D_P(u)$$
$$+ \sum_{v\in V(G_1)}[d_G(u,x) + d_G(x,y) + d_G(y,v)] - d_G(u,x)$$
$$= D_{G_0}(x) + D_P(u) + D_{G_1}(y) + (n_0 + n_1 - 1)d_G(u,v_k) + n_1.$$

In the graph G', note that $v_k = x = y$ and $d_{G'}(x,w) = 1$, then for any $u \in V(G')$, we have

Case 1: $u \in V(G_0)$.

$$D_{G'}(u) = \sum_{v\in V(G_0)} d_{G'}(u,v) + \sum_{i=1}^{r} d_{G'}(u,v_i)$$
$$+ \sum_{v\in V(G_1)} d_{G'}(u,v) - 2d_{G'}(u,x) + d_{G'}(u,w)$$
$$= D_{G_0}(u) + \sum_{i=1}^{r}[d_{G'}(u,v_k) + d_{G'}(v_k,v_i)]$$
$$+ \sum_{v\in V(G_1)}[d_{G'}(u,y) + d_{G'}(y,v)] - 2d_{G'}(u,x)$$
$$+[d_{G'}(u,x) + d_{G'}(x,w)]$$
$$= D_{G_0}(u) + D_P(v_k) + D_{G_1}(y) + (n_1 + r - 1)d_{G'}(u,x) + 1$$
$$= D_{G_0}(u) + D_P(v_k) + D_{G_1}(y) + (n_1 + r - 1)d_G(u,x) + 1.$$

Case 2: $u \in V(G_1)$.

$$D_{G'}(u) = \sum_{v\in V(G_0)} d_{G'}(u,v) + \sum_{i=1}^{r} d_{G'}(u,v_i)$$
$$+ \sum_{v\in V(G_1)} d_{G'}(u,v) - 2d_{G'}(u,x) + d_{G'}(u,w)$$
$$= \sum_{v\in V(G_0)}[d_{G'}(u,x)+d_{G'}(x,v)]+\sum_{i=1}^{r}[d_{G'}(u,v_k)+d_{G'}(v_k,v_i)]$$
$$+D_{G_1}(u) - 2d_{G'}(u,x) + [d_{G'}(u,x) + d_{G'}(x,w)]$$
$$= D_{G_0}(x) + D_P(v_k) + D_{G_1}(u) + (n_0 + r - 1)d_{G'}(u,y) + 1$$
$$= D_{G_0}(x) + D_P(v_k) + D_{G_1}(u) + (n_0 + r - 1)d_G(u,y) + 1.$$

Case 3: $u \in V(P)$.

$$D_{G'}(u) = \sum_{v\in V(G_0)} d_{G'}(u,v) + \sum_{i=1}^{r} d_{G'}(u,v_i)$$
$$+ \sum_{v\in V(G_1)} d_{G'}(u,v) - 2d_{G'}(u,x) + d_{G'}(u,w)$$
$$= \sum_{v\in V(G_0)}[d_{G'}(u,x) + d_{G'}(x,v)] + D_P(u)$$
$$+ \sum_{v\in V(G_1)}[d_{G'}(u,y) + d_{G'}(y,v)] - 2d_{G'}(u,x)$$
$$+[d_{G'}(u,x) + d_{G'}(x,w)]$$
$$= D_{G_0}(x) + D_P(u) + D_{G_1}(y) + (n_0 + n_1 - 1)d_{G'}(u,v_k) + 1$$
$$= D_{G_0}(x) + D_P(u) + D_{G_1}(y) + (n_0 + n_1 - 1)d_G(u,v_k) + 1.$$

Case 4: $u = w$.

$$D_{G'}(w) = \sum_{v\in V(G_0)} d_{G'}(w,v) + \sum_{i=1}^{r} d_{G'}(w,v_i)$$
$$+ \sum_{v\in V(G_1)} d_{G'}(w,v) - 2d_{G'}(w,x) + d_{G'}(w,w)$$
$$= \sum_{v\in V(G_0)}[d_{G'}(w,x)+d_{G'}(x,v)]+\sum_{i=1}^{r}[d_{G'}(w,v_k)+d_{G'}(v_k,v_i)]$$
$$+ \sum_{v\in V(G_1)}[d_{G'}(w,y) + d_{G'}(y,v)] - 2$$
$$= D_{G_0}(x) + D_P(v_k) + D_{G_1}(y) + n_0 + n_1 + r - 2.$$

Combing the above arguments, we obtain (2.14) and (2.15). □

Lemma 2.3. *Let P, G_0, G_1, G be connected graphs and defined as above, G' be a graph obtained from G by edge-lifting transformation. Then $SJ(G') > SJ(G)$.*

Proof. From Lemma 2.2, for any edge $uv \in E(G_0) \bigcup E(G_1) \bigcup E(P)$, we have

$$D_G(u) + D_G(v) > D_{G'}(u) + D_{G'}(v).$$

For edge $xy \in E(G)$, the corresponding edge in $E(G')$ is xw, then we have

$D_G(x) + D_G(y) = [D_{G'}(x) + (n_1 - 1)] + [D_{G'}(w) - (n_1 - 1)] = D_{G'}(x) + D_{G'}(w)$.

Thus we have $SJ(G') > SJ(G)$ by the definition of Sum-Balaban index. □

2.3 The tree with maximum Sum-Balaban index among trees with n vertices and diameter d

Let T be a tree with n vertices. Then $|E(T)| = n - 1$, $\mu = 0$, and thus

$$SJ(T) = (n-1) \sum_{uv \in E(T)} \frac{1}{\sqrt{D_T(u) + D_T(v)}}.$$

Let n, d, i be positive integers with $n \geq 3$, $2 \leq d \leq n-1$, a path $P_{d+1} = v_1 v_2 \cdots v_{d+1}$. We define $T^*_{n,d}$ is a tree with n vertices and diameter d obtained from S_{n-d} and P_{d+1} by identifying the center vertex v in S_{n-d} to $v_{\lfloor \frac{d}{2} \rfloor + 1}$ in P_{d+1}(see Fig.3).

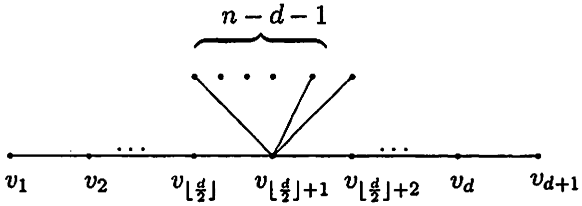


Fig.3: $T^*_{n,d}$

Lemma 2.4. *Let n, d be positive integers with $2 \leq d \leq n-1$. Then*

$$\frac{SJ(T^*_{n,d})}{n-1} = \begin{cases} \sum_{1 \leq i \leq d} \frac{1}{\sqrt{f_i(d)}} + \frac{n-d-1}{\sqrt{\frac{d^2}{2} - d + 3n - \frac{7}{2}}}, & 2 \nmid d\ ; \\ \sum_{1 \leq i \leq \frac{d}{2}} \frac{2}{\sqrt{f_i(d)}} + \frac{n-d-1}{\sqrt{\frac{d^2}{2} - d + 3n - 4}}, & 2 \mid d\ ; \end{cases} \tag{2.16}$$

where

$$f_i(d) = D_{T^*_{n,d}}(v_i) + D_{T^*_{n,d}}(v_{i+1})$$

$$= \begin{cases} (n-1)d + 2n - 1 + 2i^2 - 2ni, & 2 \nmid d, 1 \le i \le \frac{d-1}{2}; \\ \frac{d^2}{2} - 2d + 3n - \frac{5}{2}, & 2 \nmid d, i = \frac{d+1}{2}; \\ (2d+1-n-4i)d + 2n - 1 + (2i - 4 + 2n)i, & 2 \nmid d, \frac{d+3}{2} \le i \le d; \\ (n-2)d + 3n - 2 + 2i^2 - 2ni, & 2 \mid d. \end{cases} \quad (2.17)$$

Proof. Let $k = \lfloor \frac{d}{2} \rfloor + 1$, we calculate $D_{T^*_{n,d}}(u)$ for any vertex $u \in V(T^*_{n,d})$.

Case 1: $u \in V(T^*_{n,d}) \backslash V(P_{d+1})$.

$$\begin{aligned} D_{T^*_{n,d}}(u) &= 2(n-d-2) + (1+2+\cdots+k) + [2+3+\cdots+(d+2-k)] \\ &= \frac{d^2}{2} + \frac{d}{2} + 2n - 2 + k^2 - 2k - dk \\ &= \begin{cases} \frac{d^2}{4} - \frac{d}{2} + 2n - \frac{11}{4}, & 2 \nmid d\ ; \\ \frac{d^2}{4} - \frac{d}{2} + 2n - 3, & 2 \mid d. \end{cases} \end{aligned}$$

Case 2: $u = v_i \in V(P_{d+1})$ where $1 \le i \le d+1$.

Subcase 2.1: d is even.

Note that $D_{T^*_{n,d}}(v_i) = D_{T^*_{n,d}}(v_{d+2-i})$, we only need to calculate $D_{T^*_{n,d}}(v_i)$ for $1 \le i \le k = \frac{d}{2} + 1$. Clearly, when $1 \le i \le k = \frac{d}{2} + 1$, we have

$$\begin{aligned} D_{T^*_{n,d}}(v_i) &= [1+2+\cdots+(i-1)] + [1+2+3+\cdots+(d+1-i)] \\ &\quad +(k-i+1)(n-d-1) \\ &= \frac{(n-2)d}{2} + 2n - 1 + i^2 - (n+1)i. \end{aligned}$$

Subcase 2.2: d is odd.

Subcase 2.2.1: $1 \le i \le k = \frac{d+1}{2}$.

$$\begin{aligned} D_{T^*_{n,d}}(v_i) &= [1+2+\cdots+(i-1)] + [1+2+3+\cdots+(d+1-i)] \\ &\quad +(k-i+1)(n-d-1) \\ &= \frac{(n-1)d}{2} + \frac{3n}{2} - \frac{1}{2} + i^2 - (n+1)i. \end{aligned}$$

Subcase 2.2.2: $\frac{d+3}{2} \le i \le d+1$.

$$\begin{aligned} D_{T^*_{n,d}}(v_i) &= [1+2+\cdots+(i-1)] + [1+2+3+\cdots+(d+1-i)] \\ &\quad +(i-k+1)(n-d-1) \\ &= d^2 + \frac{3d}{2} - \frac{nd}{2} + \frac{n+1}{2} + i^2 + (n-3-2d)i. \end{aligned}$$

Combing the above arguments, (2.17) holds.

Let $w \in V(T^*_{n,d}) \backslash V(P_{d+1})$, we can show (2.16) by (2.17) and the following formula.

$$\frac{SJ(T^*_{n,d})}{n-1} = \sum_{uv \in E(G)} \frac{1}{\sqrt{D_G(u) + D_G(v)}}$$

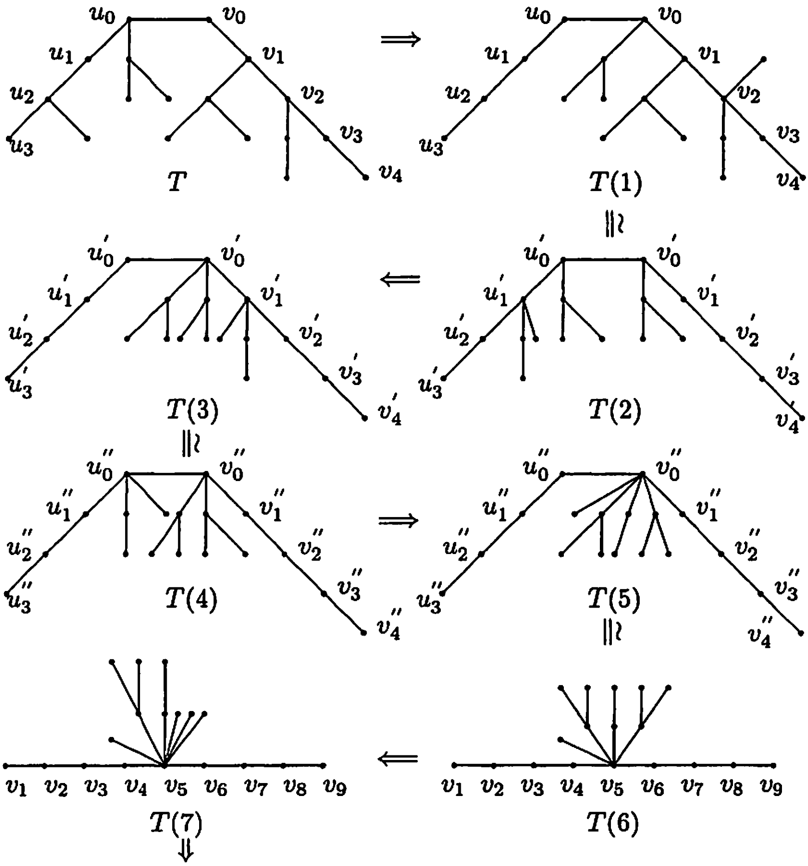
$$= \begin{cases} \sum_{1 \le i \le d} \frac{1}{\sqrt{D_{T^*_{n,d}}(v_i) + D_{T^*_{n,d}}(v_{i+1})}} + \frac{n-d-1}{\sqrt{D_{T^*_{n,d}}(v_{\frac{d+1}{2}}) + D_{T^*_{n,d}}(w)}}, & 2 \nmid d; \\ \sum_{1 \le i \le \frac{d}{2}} \frac{2}{\sqrt{D_{T^*_{n,d}}(v_i) + D_{T^*_{n,d}}(v_{i+1})}} + \frac{n-d-1}{\sqrt{D_{T^*_{n,d}}(v_{\frac{d}{2}+1}) + D_{T^*_{n,d}}(w)}}, & 2 \mid d. \end{cases} \qquad \square$$

Theorem 2.1. *Let n, d be positive integers with $n \geq 4$ and $2 \leq d \leq n-1$, T be a tree with n vertices and diameter d. Then $SJ(T) \leq SJ(T^*_{n,d})$, with equality holds if and only if $T \cong T^*_{n,d}$.*

Proof. It is obvious that d is the length of the longest path of T by the definition of diameter.

Let $P_{d+1} = v_1v_2 \cdots v_dv_{d+1}$ be the longest path in tree T, T_{v_i} be the component of $T - E(P_{d+1})$ rooted at v_i ($i = 2, 3, \cdots, d$). T' is obtained from T by branch transformation repeatedly, where all T_{v_i} are rooted at v_k with $k = \lfloor \frac{d}{2} \rfloor + 1$ by replacing v_i by v_k. Then $T^*_{n,d}$ is obtained from T' by edge-lifting transformation repeatedly.

Thus by Lemmas 2.1 and Lemma 2.3, we have $SJ(T) \leq SJ(T^*_{n,d})$ with equality holds if and only if $T \cong T^*_{n,d}$. □



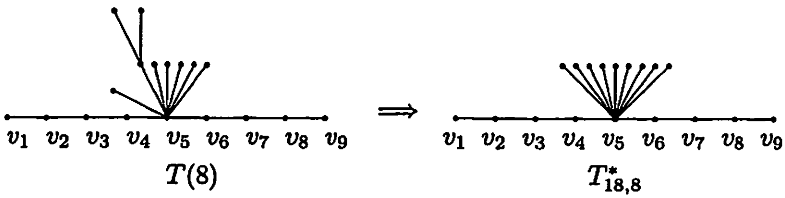


Fig.4: A tree T with 18 vertices and diameter 8 is transformation to a new tree $T(5)$ by three branch transformations and $T(6)(\cong T(5))$ is transformation to tree $T^*_{18,8}$ by three edge-lifting transformations

3 The maximum Sum-Balaban index among all trees on n vertices

In this section, we will give a new proof of the result that the star S_n is the graph which has the maximum Sum-Balaban index among all trees with n vertices.

Theorem 3.1. ([5, 15]) *Let T be a tree with $n \geq 4$ vertices. Then $SJ(T) \leq SJ(S_n)$, with the equality holds if and only if $T \cong S_n$.*

Proof. Note that $T^*_{n,2} = S_n$, so we only need to show $SJ(T^*_{n,d})$ is a monotonically decreasing function of d by Theorem 2.1.

Let n, d, s, t be positive integers with $n \geq 4$, $3 \leq d \leq n-1$, $s+t=d$ and $s=t$ (when d is even) or $s=t+1$ (when d is odd). Let $V_0 = \{v, u_2, u_3, \cdots, u_{n-d-1}\}$, $V_1 = \{v_1, v_2, \cdots, v_s\}$, $V_2 = \{w_1, w_2, \cdots, w_t, v, u_1\}$, G_0, G_1, P be the deduced graph of vertex set V_0, V_1, V_2, respectively. Then we can obtain $T^*_{n,d-1}$ by edge-lifting transformation on $T^*_{n,d}$(see Fig.5).

Thus $SJ(T^*_{n,d}) < SJ(T^*_{n,d-1})$ for $3 \leq d \leq n-1$ by Lemma 2.3. So $SJ(T^*_{n,d})$ is a monotonically decreasing function of d. □

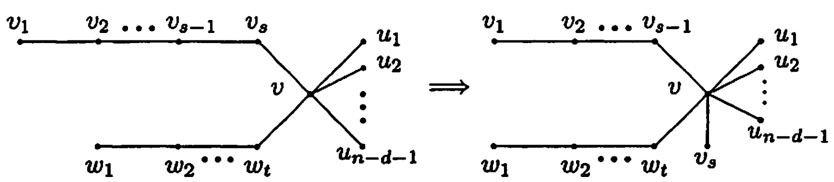


Fig.5: $T^*_{n,d-1}$ is obtained from $T^*_{n,d}$ by edge-lifting transformation

4 Some open problems

In this section, we propose some problems for further research.

By the proof of Theorem 3.1, we know $T^*_{n,3}$ is the graph which has the second largest Sum-Balaban index. So we define the double star $S_n(a,b)$ as follows. In fact, $T^*_{n,3} = S_n(2, n-2) = S_n(n-2, 2)$.

Let $a(\geq 2), b(\geq 2), n$ be positive integers and $a+b=n$, $S_n(a,b)$ be the tree formed by adding an edge between the centers of the stars S_a and S_b. We call $S_n(a,b)$ the double star.

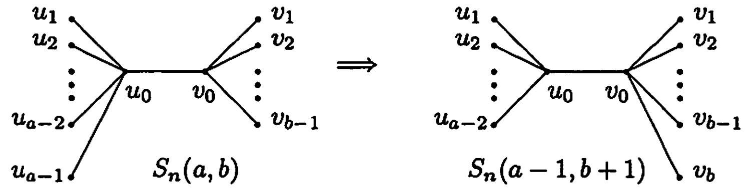


Fig.6: $S_n(a-1,b+1)$ is obtained from $S_n(a,b)$.

Lemma 4.1. *Let $a-b \geq 2$. Then $SJ(S_n(a,b)) > SJ(S_n(a-1,b+1))$.*

Proof. For $a+b=n$, $a \geq 2, b \geq 2$ and $a-b \geq 2$, we have $2 \leq b < \lfloor \frac{n}{2} \rfloor$.

By direct calculation, we have

$$\begin{aligned}
&\frac{SJ(S_n(a,b))}{n-1}\\
&= \frac{1}{\sqrt{(n+b-2)+(2n-b-2)}} + \frac{b-1}{\sqrt{(2n-b-2)+(3n-b-4)}} + \frac{n-b-1}{\sqrt{(n+b-2)+(2n+b-4)}}\\
&= \frac{1}{\sqrt{3n-4}} + \frac{b-1}{\sqrt{5n-2b-6}} + \frac{n-b-1}{\sqrt{3n+2b-6}}.
\end{aligned}$$

Let $h(x) = \frac{1}{\sqrt{3n-4}} + \frac{x-1}{\sqrt{5n-2x-6}} + \frac{n-x-1}{\sqrt{3n+2x-6}}$ where $2 \leq x < \lfloor \frac{n}{2} \rfloor$. Then

$$\begin{aligned}
h'(x) &= \frac{5n-x-7}{\sqrt{(5n-2x-6)^3}} + \frac{-4n-x+7}{\sqrt{(3n+2x-6)^3}}\\
&= \frac{(5n-2x-6)+(x-1)}{\sqrt{(5n-2x-6)^3}} + \frac{-(3n+2x-6)-n+x+1}{\sqrt{(3n+2x-6)^3}}\\
&= \frac{1}{\sqrt{5n-2x-6}} - \frac{1}{\sqrt{3n+2x-6}} + \frac{x-1}{\sqrt{(5n-2x-6)^3}} - \frac{n-x-1}{\sqrt{(3n+2x-6)^3}}.
\end{aligned}$$

Note that $5n-2x-6-(3n+2x-6) = 2n-4x > 0$. It implies that $\frac{x-1}{\sqrt{(5n-2x-6)^3}} - \frac{n-x-1}{\sqrt{(3n+2x-6)^3}} < \frac{-n+2x}{\sqrt{(3n+2x-6)^3}} < 0$ and $\frac{1}{\sqrt{5n-2x-6}} - \frac{1}{\sqrt{3n+2x-6}} < 0$. Thus $h'(x) < 0$ when $2 \leq x < \lfloor \frac{n}{2} \rfloor$ and $SJ(S_n(a,b)) > SJ(S_n(a-1,b+1))$. □

Corollary 4.1. *Let $n \geq 4$ be an integer. Then*

$$\begin{aligned}
SJ(S_n) &> SJ(T^*_{n,3}) = SJ(S_n(n-2,2)) = SJ(S_n(2,n-2))\\
&> SJ(S_n(n-3,3)) = SJ(S_n(3,n-3))\\
&> \cdots\\
&> SJ(S_n(\lceil \tfrac{n}{2} \rceil + 1, \lfloor \tfrac{n}{2} \rfloor - 1)) = SJ(S_n(\lfloor \tfrac{n}{2} \rfloor - 1, \lceil \tfrac{n}{2} \rceil + 1))\\
&> SJ(S_n(\lceil \tfrac{n}{2} \rceil, \lfloor \tfrac{n}{2} \rfloor)) = SJ(S_n(\lfloor \tfrac{n}{2} \rfloor, \lceil \tfrac{n}{2} \rceil)).
\end{aligned}$$

Let $n, a(\geq 2), b(\geq 2), l$ be positive integers and $a+b+l = n+1$, $S_n(a,b,l)$ be the tree formed by adding a path with length l between the centers of the stars S_a and S_b. We call $S_n(a,b,l)$ the like double star.

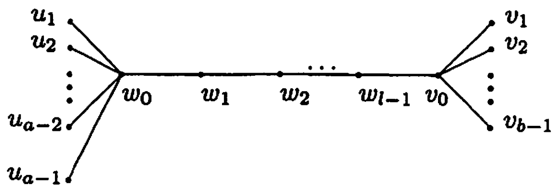


Fig.7: The like double star $S_n(a,b,l)$.

It is known that P_n is the tree with the smallest Sum-Balaban index among all trees with n vertices. Now we propose a conjecture about the smallest Sum-Balaban index with given vertices and given diameter.

Conjecture 4.1. *Let n, d be positive integers with $n \geq 4$ and $2 \leq d \leq n-1$, T be a tree with n vertices and diameter d. Then*

$$SJ(T) \geq SJ(S_n(\lfloor\frac{n-d+3}{2}\rfloor, \lceil\frac{n-d+3}{2}\rceil, d-2)),$$

with equality holds if and only if $T \cong S_n(\lfloor\frac{n-d+3}{2}\rfloor, \lceil\frac{n-d+3}{2}\rceil, d-2)$.

Let n, i be positive integers with $n \geq 4$, and $2 \leq i \leq n-2$, a path $P_{n-1} = v_1v_2\cdots v_{n-1}$. We define $T_n(i)$ is a tree with n vertices obtained from P_{n-1} by adding an edge v_iw where $w \notin \{v_1, v_2, \cdots, v_{n-1}\}$.

Clearly, $T_n(i)$ is a tree with n vertices and diameter $n-2$. By branch transformation and Lemma 2.1, we can show

$$SJ(P_n) < SJ(T_n(2)) < SJ(T_n(3)) < \cdots < SJ(T_n(\lfloor\frac{n}{2}\rfloor)).$$

In [8], the authors ordered the first 21st largest Balaban indices among all trees with n vertices. Naturely, we can propose the following problems:

Problem 1. Order the largest Sum-Balaban indices among all trees with n vertices.

Problem 2. Order the smallest Sum-Balaban indices among all trees with n vertices.

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