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On the Balaban Index of Trees†

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Abstract

In this paper, we give a new proof 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. This corrects some errors of proofs in [H. Dong, X. Guo, Character of graphs with extremal Balaban index, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 799–812] and [L. Sun, Bounds on the Balaban index of trees, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 813–818]. We also characterize the trees with the second minimal and maximal Balaban index, respectively.

For a simple and connected graph G with vertex–set $V(G)$ and edge–set $E(G)$, $d_G(u,v)$ denotes the distance between vertices u and v in G, and $D_G(u) = \sum_{v \in V(G)} d_G(u,v)$ is the distance sum of vertex u in G, i. e., the row sum of distance matrix of G corresponding to u. The Balaban index of G is defined as

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

where m is the number of edges and μ is the cyclomatic number of G, respectively.

The Balaban index was proposed by A. T. Balaban [1,2], which also called the average distance–sum connectivity or J index. It appears to be a very useful molecular descriptor with attractive properties.

Recently, it was showed in [3] that

Theorem 12 ([3]). If T is a tree with $n \geq 2$ vertices, then $J(P_n) \leq J(T) \leq J(S_n)$ with left (or right) equality if and only if $T = P_n$ (or $T = S_n$), where P_n and S_n are the path and the star on n vertices.

The proof of theorem above is dependent on Lemma 6 in [3]. But, the following example 1 shows that Lemma 6 is incorrect.

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Example 1. (see Figure 1) Let $P = p_1p_2p_3$ be a path in a graph G_0, where $G_0 = P$ is the path itself, and $G_j (1 \le j \le 3)$ are the component of $G_0 - E(P)$ containing p_j. $H_1 = u_1u_2u_3$, $H_2 = v_1v_2v_3$, $H_1' = u_1u_2$ and $H_2' = v_1v_2v_3u_3$ are also paths. We have $|V(H_1)| + |V(H_2)| = |V(H_1')| + |V(H_2')|$ and $|V(H_1')| < |V(H_1)| \le |V(H_2)| < |V(H_2')|$. Construct the graph G by identifying p_1 to u_2 in H_1 and p_3 to v_1 in H_2, and the graph G' by identifying p_3 to u_2 in H_1' and p_3 to v_1 in H_2'. Clearly, $|V(G_i)| \le |V(G_{l+1-i})|$ since G_i is an isolated vertex, $l = 3$ and $1 \le i \le \lceil \frac{l}{2} \rceil - 1$. However, we have $J_G(P) > J_{G'}(P)$, where $J_G(P) = \sum\limits_{uv \in E(P)} \frac{1}{\sqrt{D_G(u)D_G(v)}} = \frac{1}{\sqrt{12 \times 11}} + \frac{1}{\sqrt{11 \times 12}}$ and $J_{G'}(P) = \sum\limits_{uv \in E(P)} \frac{1}{\sqrt{D_{G'}(u)D_{G'}(v)}} = \frac{1}{\sqrt{16 \times 13}} + \frac{1}{\sqrt{13 \times 12}}$.

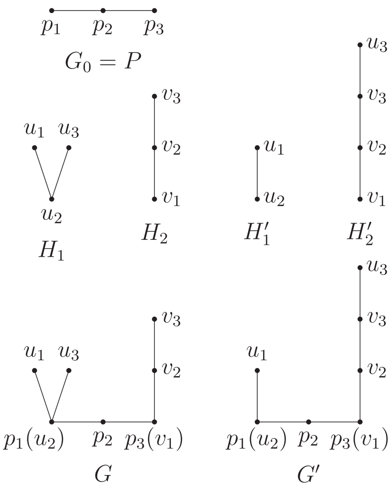

Figure 1.

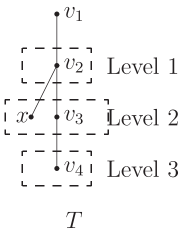

Figure 2.

Also, it was showed in [4] that

Theorem 2.2 ([4]). If T is a tree with $n \ge 2$ vertices, then $J(T) \ge J(P_n)$ with equality if and only if $T = P_n$.

But the following example 2 shows that its proof in [4, lines 1-3 on page 818] is incorrect.

Example 2. (see Figure 2) Let $P = v_1v_2v_3v_4$ be a longest path in T, and v_1 the root of T. Then the other vertices of T can be divided into levels by the distance on v_1. Let L_i be the set of vertices in level i $(1 \le i \le 3)$, where $L_1 = \{v_2\}$, $L_2 = \{v_3, x\}$ and $L_3 = \{v_4\}$. However, for $x \in L_2$, $D_x = D_T(x) = 8$, and $D_3 = 6$ since $D_i = \frac{(n-i+1)(n-i)}{2} + \frac{(i-1)i}{2}$ and

$n = 5$. We have $D_x > D_3$.

Now, we will give a new proof of the results above.

The path-sliding transformation. Let G_0 be a graph with $n_0 \geq 2$ vertices, and $P = v_1 v_2 \cdots v_r$ a path of length $r - 1 \geq 2$. If G (resp. G') is the graph obtained by identifying a vertex v_0 in G_0 to v_k (resp. v_{k-1}) in P, $2 \leq k \leq \frac{r}{2}$, then G' is called the path-sliding transformation of G (see Figure 3).

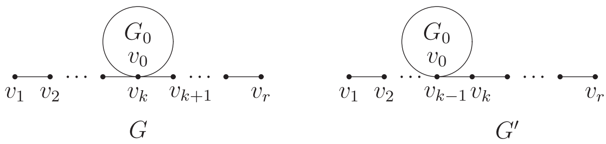

Figure 3. The path-sliding transformation.

For any $u \in V(G_0)$,

$$\begin{aligned} D_G(u) = & \sum_{v \in V(G_0)} d_G(u,v) + \sum_{i=1}^{r} d_G(u,v_i) - d_G(u,v_0) \\ = & \ D_{G_0}(u) + \sum_{i=1}^{r} [d_G(u,v_0) + d_G(v_k,v_i)] - d_G(u,v_0) \\ = & \ D_{G_0}(u) + D_P(v_k) + (r-1) d_{G_0}(u,v_0) \end{aligned} \tag{1}$$

and

$$\begin{aligned} D_G(v_t) = & \sum_{v \in V(G_0)} d_G(v_t,v) + \sum_{i=1}^{r} d_G(v_t,v_i) - d_G(v_t,v_0) \\ = & \sum_{v \in V(G_0)} [d_G(v_t,v_0) + d_G(v_0,v)] + D_P(v_t) - d_G(v_t,v_0) \\ = & \ D_{G_0}(v_0) + D_P(v_t) + (|V(G_0)| - 1) d_G(v_t,v_0) \\ = & \ D_{G_0}(v_0) + D_P(v_t) + (n_0 - 1)|k - t| \ . \end{aligned} \tag{2}$$

Similarly,

$$D_{G'}(u) = D_{G_0}(u) + D_P(v_{k-1}) + (r-1) d_{G_0}(u,v_0) \tag{3}$$

and

$$D_{G'}(v_t) = D_{G_0}(v_0) + D_P(v_t) + (n_0 - 1)|k - 1 - t|. \tag{4}$$

where $D_P(v_t) = \frac{(r-t+1)(r-t)}{2} + \frac{(t-1)t}{2}$, $t = 1, 2, \cdots, r$.

Note that $D_p(v_1), D_P(v-2), \cdots, D_P(v_r)$ is symmetric and $D_P(v_1) > D_P(v_2) > \cdots > D_P(v_{\lfloor \frac{r}{2} \rfloor}) = D_P(v_{\lceil \frac{r}{2} \rceil}) < D_P(v_{\lceil \frac{r}{2} \rceil + 1}) < \cdots < D_P(v_r)$.

Lemma 1. If G' is the path-sliding transformation of G, then $J(G) > J(G')$.

Proof. From (1) and (3), $\forall e = uv \in E(G_0)$, $D_G(u) < D_{G'}(u)$ and $D_G(v) < D_{G'}(v)$ since $D_P(v_k) < D_P(v_{k-1})$ for $2 \le k \le \frac{r}{2}$. Thus

$$\frac{1}{\sqrt{D_G(u)D_G(v)}} > \frac{1}{\sqrt{D_{G'}(u)D_{G'}(v)}} \tag{5}$$

From (2) and (4),

$$D_G(v_t) - D_{G'}(v_t) = \begin{cases} (n_0 - 1), & 1 \le t \le k-1; \\ \\ -(n_0 - 1), & k \le t \le r. \end{cases}$$

(i) For $t = 1, 2, \cdots, k-1$, because $k \le \frac{r}{2}$, $D_P(v_t) > D_P(v_{2k-t-1})$ and $D_P(v_{t-1}) > D_P(v_{2k-t})$. By (2), $D_G(v_{2k-t}) < D_G(v_{t-1}) - (n_0 - 1)$ and $D_G(v_{2k-t-1}) < D_G(v_t) - (n_0 - 1)$.

Note that $f(x, y) = \frac{1}{\sqrt{xy}} - \frac{1}{\sqrt{(x+(n_0+1))(y+(n_0+1))}}$ is a decreasing function of x and y since $\frac{\partial f}{\partial x} < 0$ and $\frac{\partial f}{\partial y} < 0$.

$$\begin{aligned} &\frac{1}{\sqrt{D_G(v_{2k-t})D_G(v_{2k-t-1})}} - \frac{1}{\sqrt{(D_G(v_{2k-t}) + (n_0-1))(D_G(v_{2k-t-1}) + (n_0-1))}} \\ > \quad &\frac{1}{\sqrt{(D_G(v_{t-1}) - (n_0-1))(D_G(v_t) - (n_0-1))}} - \frac{1}{\sqrt{D_G(v_{t-1})D_G(v_t)}}, \end{aligned}$$

i.e.,

$$\begin{aligned} &\frac{1}{\sqrt{D_G(v_{2k-t})D_G(v_{2k-t-1})}} - \frac{1}{\sqrt{D_{G'}(v_{2k-t})D_{G'}(v_{2k-t-1})}} \\ > \quad &\frac{1}{\sqrt{D_{G'}(v_{t-1})D_{G'}(v_t)}} - \frac{1}{\sqrt{D_G(v_{t-1})D_G(v_t)}} \end{aligned}$$

and

$$\begin{aligned} &\left[\frac{1}{\sqrt{D_G(v_{t-1})D_G(v_t)}} - \frac{1}{\sqrt{D_{G'}(v_{t-1})D_{G'}(v_t)}}\right] \\ +&[\frac{1}{\sqrt{D_G(v_{2k-t})D_G(v_{2k-t-1})}} - \frac{1}{\sqrt{D_{G'}(v_{2k-t})D_{G'}(v_{2k-t-1})}}] > 0\ . \end{aligned} \tag{6}$$

(ii) For $t = 2k-1, 2k, \cdots, r$, we have $D_G(v_t) < D_{G'}(v_t)$ and

$$\frac{1}{\sqrt{D_G(v_t)D_G(v_{t+1})}} > \frac{1}{\sqrt{D_{G'}(v_t)D_{G'}(v_{t+1})}} \tag{7}$$

for $t = 2k-1, \cdots, r-1$.

(iii) By (2) and (4), $D_G(v_{k-1}) + D_G(v_k) = D_{G'}(v_{k-1}) + D_{G'}(v_k)$, and

$$D_G(v_k) < D_{G'}(v_{k-1}) < D_G(v_{k-1}), \quad D_G(v_k) < D_{G'}(v_k) < D_G(v_{k-1})$$

since $D_P(v_k) < D_P(v_{k-1})$. We have $D_G(v_{k-1})D_G(v_k) < D_{G'}(v_{k-1})D_{G'}(v_k)$. So,

$$\frac{1}{\sqrt{D_G(v_{k-1})D_G(v_k)}} > \frac{1}{\sqrt{D_{G'}(v_{k-1})D_{G'}(v_k)}} \tag{8}$$

From (5)-(8), we can obtain

$$\begin{aligned}
&J(G) - J(G') \\
&= (n-1)\left[\sum_{uv\in E(G)} \frac{1}{\sqrt{D_G(u)D_G(v)}} - \sum_{uv\in E(G')} \frac{1}{\sqrt{D_{G'}(u)D_{G'}(v)}}\right] \\
&= (n-1)\left(\sum_{uv\in E(G_0)} \left[\frac{1}{\sqrt{D_G(u)D_G(v)}} - \frac{1}{\sqrt{D_{G'}(u)D_{G'}(v)}}\right]\right. \\
&+ \frac{1}{\sqrt{D_G(v_{k-1})D_G(v_k)}} - \frac{1}{\sqrt{D_{G'}(v_{k-1})D_{G'}(v_k)}} \\
&+ \sum_{t=2}^{k-1}\left[\frac{1}{\sqrt{D_G(v_{t-1})D_G(v_t)}} - \frac{1}{\sqrt{D_{G'}(v_{t-1})D_{G'}(v_t)}}\right. \\
&+ \left.\frac{1}{\sqrt{D_G(v_{2k-t})D_G(v_{2k-t-1})}} - \frac{1}{\sqrt{D_{G'}(v_{2k-t})D_{G'}(v_{2k-t-1})}}\right] \\
&+ \left.\sum_{t=2k-2}^{r-1}\left[\frac{1}{\sqrt{D_G(v_t)D_G(v_{t+1})}} - \frac{1}{\sqrt{D_{G'}(v_t)D_{G'}(v_{t+1})}}\right]\right) > 0\,.
\end{aligned}$$

Using the path-sliding transformation repeatedly, we can easily obtain the following result by Lemma 1.

Theorem 1. If T is a tree with $n \geq 2$ vertices, then

$$J(T) \geq J(P_n) = (n-1)\sum_{i=1}^{n-1}(D_iD_{i+1})^{-\frac{1}{2}}$$

with equality if and only if $T = P_n$ is the path with n vertices, where $D_i = \frac{(n-i+1)(n-i)}{2} + \frac{(i-1)i}{2}$.

For a tree T with $n \geq 4$ vertices, if T is not a path, then T can be changed into a tree of diameter $n-2$ by a series of path-sliding transformations. Moreover, using the path-sliding transformation, any tree with n vertices and diameter $n-2$ can be changed into the tree T_0, which is obtained by attaching a pendant vertex v_n to v_2 of the path $v_1v_2\cdots v_{n-1}$ (see Figure 5). So, we can characterize the tree with the second minimal Balaban index by Lemma 1.

Theorem 2. Let T be a tree with $n \geq 4$ vertices. If T is not a path, then $J(T) \geq J(T_0)$ with equality if and only if $T = T_0$.

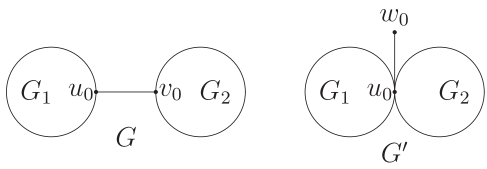

Figure 4. The edge-lifting transformation.

The edge-lifting transformation. Let G_1 and 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 4).

In the graph G, if $u \in V(G_1)$, then

$$\begin{aligned} D_G(u) &= \sum_{v \in V(G_1)} d_G(u,v) + \sum_{v \in V(G_2)} d_G(u,v) \\ &= D_{G_1}(u) + \sum_{v \in V(G_2)} [d_G(u,u_0) + 1 + d_G(v_0,v)] \\ &= D_{G_1}(u) + D_{G_2}(v_0) + [d_{G_1}(u,u_0) + 1]n_2 \end{aligned} \tag{9}$$

Similarly, if $u \in V(G_2)$, then

$$D_G(u) = D_{G_1}(u_0) + D_{G_2}(u) + [d_{G_2}(u,v_0) + 1]n_1 \tag{10}$$

In the graph G', if $u \in V(G_1)$, then

$$\begin{aligned} D_{G'}(u) &= \sum_{v \in V(G_1)} d_{G'}(u,v) + \sum_{v \in V(G_2)} d_{G'}(u,v) - d_{G'}(u,u_0) + d_{G'}(u,w_0) \\ &= D_{G_1}(u) + \sum_{v \in V(G_2)} [d_{G'}(u,u_0) + d_{G'}(u_0,v)] \\ &- d_{G'}(u,u_0) + d_{G'}(u,u_0) + d_{G'}(u_0,w_0) \\ &= D_{G_1}(u) + D_{G_2}(v_0) + n_2 d_{G_1}(u,u_0) + 1 \end{aligned} \tag{11}$$

Similarly, if $u \in V(G_2)$, then

$$D_{G'}(u) = D_{G_1}(u_0) + D_{G_2}(u) + n_1 d_{G_2}(u,v_0) + 1 \tag{12}$$

And

$$D_{G'}(w_0) = D_{G_1}(u_0) + D_{G_2}(v_0) + n_1 + n_2 - 1 \tag{13}$$

Lemma 2. If G' is the edge-lifting transformation of G, then $J(G) < J(G')$.

Proof. From (9)-(13), we have

$$D_G(u) = D_{G'}(u) + \begin{cases} n_2 - 1, & u \in V(G_1); \\ \\ n_1 - 1, & u \in V(G_2) \end{cases}$$

and $\forall uv \in E(G_1) \cup E(G_2)$,

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

$$D_G(u_0)D_G(v_0) = D_{G'}(u_0)D_{G'}(w_0) + (n_1 - 1)(n_2 - 1) > D_{G'}(u_0)D_{G'}(w_0).$$

By the definitions of $J(G)$, we have $J(G) < J(G')$.

Using Lemma 2 and the edge-lifting transformation repeatedly on a tree T, we can obtain

Theorem 3. If T is a tree with $n \geq 2$ vertices, then

$$J(T) \leq J(S_n) = (n-1)^{3/2}(2n-3)^{-1/2}$$

with equality if and only if $T = S_n$ is the star with n vertices.

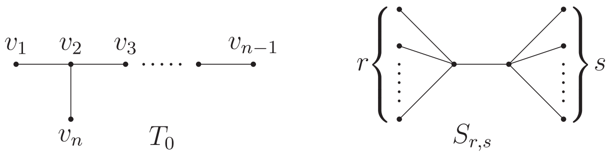

Figure 5.

Finally, we characterize the tree with the second maximal Balaban index.

If a tree T with $n \geq 4$ vertices is not a star, then T can be changed into a tree of diameter 3 by a series of edge-lifting transformations. Moreover, any tree of diameter 3 with n vertices is a double-star $S_{r,s}$ with $r \geq 1$, $s \geq 1$ and $r + s = n - 2$ (see Figure 5). By Lemma 2, we only need to find the tree with the maximal Balaban index among all double-star with $n \geq 4$ vertices.

It can be computed that the Balaban index of $S_{r,s}$ is

$$\begin{aligned} J(S_{r,s}) = & \frac{r}{\sqrt{(1+2r+3s)(1+r+2s)}} + \frac{1}{\sqrt{(1+r+2s)(1+s+2r)}} \\ & + \frac{s}{\sqrt{(1+s+2r)(1+2s+3r)}} \end{aligned}$$

Let $a = n - 2$. Then $s = a - r$ and $1 \le r \le a - 1$.

$$\begin{aligned} f(r) = \;& J(S_{r,s}) \\ = \;& \frac{r}{\sqrt{1+5a+6a^2-2r-5ar+r^2}} + \frac{a-r}{\sqrt{1+3a+2a^2+2r+3ar+r^2}} \\ + \;& \frac{1}{\sqrt{1+3a+2a^2+ar-r^2}} \end{aligned}$$

It can be easily computed that

$$4f''(r) = \frac{A_1(r)}{A(r)} + \frac{B_1(r)}{B(r)} + \frac{C_1(r)}{C(r)}$$

where

$$\begin{aligned} A(r) &= (1+5a+6a^2-2r-5ar+r^2)^{5/2}\,, \\ B(r) &= (1+3a+2a^2+2r+3ar+r^2)^{5/2}\,, \\ C(r) &= (1+3a+2a^2+ar-r^2)^{5/2}\,, \\ A_1(r) &= 8+60a+148a^2+120a^3-16r-80ar-97a^2r+8r^2+20ar^2\,, \\ B_1(r) &= 8+44a+76a^2+43a^3+16r+64ar+57a^2r+8r^2+20ar^2\,, \\ C_1(r) &= 4+12a+11a^2-8ar+8r^2 \quad . \end{aligned}$$

Note that $1 \le r \le a-1$, we have $f''(r) > 0$, i.e., $f(r)$ is concave for $1 \le r \le a-1$. So, $f(r) \le \max\{f(1), f(a-1)\} = f(1) = f(a-1)$, i.e., $J(S_{r,s}) \le J(S_{1,a-1})$ with equality if and only if $r = 1, s = a-1$ or $r = a-1, s = 1$.

Theorem 4. Let T be a tree with $n \ge 4$ vertices. If T is not a star, then $J(T) \le J(S_{n-1,1})$ with equality if and only if $T = S_{1,n-3}$.

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