On the Balaban Index of Trees

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Abstract

Let G be a connected graph with edge set $E(G)$. The Balaban index of G is defined as $J(G) = \frac{m}{\mu+1} \sum_{uv \in E(G)} (D_u D_v)^{-\frac{1}{2}}$, where $m = |E(G)|$, and μ is the cyclomatic number of G, D_u is the sum of distances between vertex u and all other vertices of G. We determine n-vertex trees with the first several largest and smallest Balaban indices.

1 Introduction

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, $d_G(u, v)$ denotes the distance (length of a shortest path) between u and v in G [7]. Let D_u or $D(u|G)$ be the distance sum of vertex u (sum of distances between u and all other vertices) of G, i.e., $D_u = D(u|G) = \sum_{v \in V(G)} d_G(u, v)$.

Let G be a connected graph with n vertices and m edges. The Balaban index of G is defined as [1, 2]

$$J(G) = \frac{m}{\mu + 1} \sum_{uv \in E(G)} (D_u D_v)^{-\frac{1}{2}},$$

where $\mu = m - n + 1$ is the cyclomatic number of G, which is the minimal number of edges that must be removed from G in order to transform it to an acyclic graph.

The Balaban index has been used very successfully for modeling, monitoring, and estimating physicochemical parameters as well as physiological activities of the organic compounds acting as drugs, see, e.g., [3, 8–11, 13, 14]. It also found applications in polymers [4], and transfer RNA of

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Escherichia coli [6]. The discriminating ability and degeneracy of the Balaban index were discussed in [5, 15]. Some combinatorial and algebraic properties of the Balaban index have been established, see [12, 16, 17].

In this paper, we determine n-vertex trees respectively with the largest, the second–largest, the smallest, and the second–smallest Balaban indices for $n \geq 4$, and the third–largest Balaban index for $n \geq 6$. The fact that the star S_n and the path P_n are the unique n-vertex trees with respectively the largest and the smallest Balaban indices has been known in [12], for which we give a different proof here.

2 Preliminaries

For a subgraph H of G, and $u \in V(G)$, let $D_G(u|H) = \sum_{v \in V(H)} d_G(u, v)$. In particular, $D(u|G) = D_G(u|G)$.

Let $M(G) = \sum_{uv \in E(G)} (D_u D_v)^{-\frac{1}{2}}$. If T is a tree, then $\mu = 0$, and thus $J(T) = (n-1)M(T)$.

Let $|G| = |V(G)|$ for a graph G. For $u \in V(G)$, let $N_G(u)$ be the set of neighbors of u in G, and let $G - u$ the graph obtained from G by deleting the vertex u and its incident edges.

3 Trees with large Balaban indices

For a tree T with $uv \in E(T)$, let T_u (T_v, respectively) be the sub-tree obtained by deleting the edge uv containing u (v, respectively). Let $n_u = |T_u|$ and $n_v = |T_v|$. Obviously, $n_u, n_v \geq 1$.

Lemma 3.1. *Let T be a tree with $uv \in E(T)$. Then $D(u|T) + n_u = D(v|T) + n_v$.*

Proof. Note that

$$\begin{aligned} D(u|T) &= D_T(u|T_u) + D_T(u|T_v) = D_T(u|T_u) + D_T(v|T_v) + n_v, \\ D(v|T) &= D_T(u|T_u) + D_T(v|T_v) + n_u. \end{aligned}$$

Then the result follows. □

Lemma 3.2. *Let x be a vertex of a tree T_0 with at least two vertices. For integer $r \geq 1$, let T be the tree obtained from T_0 by attaching a star S_{r+1} at its center y to x, and T' the tree obtained from T_0 by attaching $r+1$ pendant vertices to x, see Fig. 1. Then $J(T) < J(T')$.*

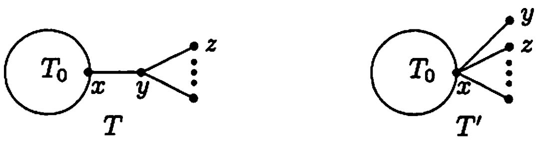

Fig. 1. T and T' in Lemma 3.2.

Proof. Denote by z a pendant neighbor of y in T and a pendant neighbor of x in T' outside T_0. Let $c = |T_0|$. Obviously, $D(u|T') = D(u|T) - r$ for $u \in V(T_0)$, $D(y|T') = D(y|T) + r$, and $D(z|T') = D(z|T) - (c-1)$. For $uv \in E(T_0)$, $D(u|T')D(v|T') < D(u|T)D(v|T)$. By Lemma 3.1, we have $D(x|T) + c = D(y|T) + r + 1$, and thus

$$\begin{aligned} D(x|T')D(y|T') &= (D(x|T) - r)(D(y|T) + r) \\ &= D(x|T)D(y|T) + r(D(x|T) - D(y|T) - r) \\ &= D(x|T)D(y|T) - r(c-1) \\ &< D(x|T)D(y|T), \\ D(x|T')D(z|T') &= (D(x|T) - r)(D(z|T) - c + 1) \\ &= (D(y|T) - c + 1)(D(z|T) - c + 1) \\ &< D(y|T)D(z|T). \end{aligned}$$

Then

$$\begin{aligned} M(T') - M(T) &= \sum_{uv \in E(T_0)} \left(\frac{1}{\sqrt{D(u|T')D(v|T')}} - \frac{1}{\sqrt{D(u|T)D(v|T)}} \right) \\ &\quad + \left(\frac{1}{\sqrt{D(x|T')D(y|T')}} - \frac{1}{\sqrt{D(x|T)D(y|T)}} \right) \\ &\quad + r \left(\frac{1}{\sqrt{D(x|T')D(z|T')}} - \frac{1}{\sqrt{D(y|T)D(z|T)}} \right) \\ &> 0, \end{aligned}$$

i.e., $J(T) < J(T')$. □

By the previous lemma, we have immediately the following.

Theorem 3.1. [12] *Let T be a tree with $n \geq 3$ vertices. Then $J(T) \leq J(S_n)$ with equality if and only if $T = S_n$.*

Let $S_n(a,b)$ be the tree formed by adding an edge between the centers of the stars S_a and S_b, where $a + b = n$ and $2 \leq a \leq \lfloor \frac{n}{2} \rfloor$. We call $S_n(a,b)$ the double star.

Lemma 3.3. *For $2 \leq a \leq \lfloor \frac{n}{2} \rfloor - 1$, $J(S_n(a,b)) > J(S_n(a+1,b-1))$.*

Proof. By direct calculation, we have

$$\begin{aligned} M(S_n(a,b)) &= \frac{1}{\sqrt{(2n-a-2)(n+a-2)}} + \frac{a-1}{\sqrt{(2n-a-2)(3n-a-4)}} \\ &+ \frac{b-1}{\sqrt{(n+a-2)(2n+a-4)}} \\ &= \frac{1}{\sqrt{y_1}} + \frac{a-1}{\sqrt{y_2}} + \frac{n-a-1}{\sqrt{y_3}}, \end{aligned}$$

where $y_1 = (2n-a-2)(n+a-2)$, $y_2 = (2n-a-2)(3n-a-4)$, and $y_3 = (n+a-2)(2n+a-4)$. Note that $y_2 - y_3 = (2n-a-2)(3n-a-4) - (n+a-2)(2n+a-4) = 4n^2 - 6n + (12-8n)a \geq 4n^2 - 6n + (12-8n)\cdot\frac{n}{2} = 0$ and $(n-a-1)(3n+2a-6) - (a-1)(5n-2a-6) = 3n^2 - 4n + (8-6n)a \geq 3n^2 - 4n + (8-6n)\cdot\frac{n}{2} = 0$. Then,

$$\begin{aligned} \frac{d}{da}M(S_n(a,b)) &= -\frac{\frac{dy_1}{da}}{2y_1^{\frac{3}{2}}} + \frac{1}{y_2^{\frac{1}{2}}} - (a-1)\frac{\frac{dy_2}{da}}{2y_2^{\frac{3}{2}}} - \frac{1}{y_3^{\frac{1}{2}}} - (n-a-1)\frac{\frac{dy_3}{da}}{2y_3^{\frac{3}{2}}} \\ &= \frac{1}{y_2^{\frac{1}{2}}} - \frac{1}{y_3^{\frac{1}{2}}} - \frac{n-2a}{2y_1^{\frac{3}{2}}} + \frac{(a-1)(5n-2a-6)}{2y_2^{\frac{3}{2}}} \\ &\quad - \frac{(n-a-1)(3n+2a-6)}{2y_3^{\frac{3}{2}}} \\ &< 0. \end{aligned}$$

Then the result follows. □

Theorem 3.2. *Let T be a tree with $n \geq 4$ vertices different from S_n. Then $J(T) \leq J(S_n(2, n-2))$ with equality if and only if $T = S_n(2, n-2)$.*

Proof. If T has at least two non-pendant edges, then by Lemma 3.2, we can obtain an n-vertex tree with exactly one non-pendant edge, which is a double star with larger Balaban index than T. Now the result follows from Lemma 3.3. □

Denote $P_{n+1} = v_0v_1\ldots v_n$. Let $S_n(a,b,c)$ be the n-vertex tree formed by attaching $a-1$, $b-1$ and $c-1$ pendant vertices to v_0, v_1 and v_2 in the path P_3, respectively, where $a, c \geq 2$, $b \geq 1$ and $a+b+c = n$. Then any n-vertex tree with exactly two non-pendant edges is of the form $S_n(a,b,c)$.

Theorem 3.3. *Let T be a tree with $n \geq 6$ vertices different from S_n, $S_n(2, n-2)$. Then $J(T) \leq J(S_n(3, n-3))$ with equality if and only if $T = S_n(3, n-3)$.*

Proof. If T has at least two non-pendant edges and different from $S_n(2, n-4, 2)$, then by Lemma 3.2, we can obtain a tree with exactly one non-pendant edge, which is a double star different from $S_n(2, n-2)$ with larger Balaban index than T, and thus we have by Lemma 3.3 that $J(T) \leq J(S_n(3, n-3))$. Let $f(x) = \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+2}}$ for $x > 0$. Then

$$\begin{aligned}
& M(S_n(3,n-3)) - M(S_n(2,n-4,2)) \\
= & \left(\frac{1}{\sqrt{(2n-5)(n+1)}} + \frac{2}{\sqrt{(2n-5)(3n-7)}} + \frac{n-4}{\sqrt{(2n-1)(n+1)}}\right) \\
& - \left(\frac{2}{\sqrt{(2n-3)(n+1)}} + \frac{2}{\sqrt{(2n-3)(3n-5)}} + \frac{n-5}{\sqrt{(2n-1)(n+1)}}\right) \\
= & \frac{1}{\sqrt{n+1}}\left(\frac{1}{\sqrt{2n-5}} + \frac{1}{\sqrt{2n-1}} - \frac{2}{\sqrt{2n-3}}\right) \\
& + \left(\frac{2}{\sqrt{(2n-5)(3n-7)}} - \frac{2}{\sqrt{(2n-3)(3n-5)}}\right) \\
> & \frac{1}{\sqrt{n+1}}(f(2n-5) - f(2n-3)) \\
> & 0,
\end{aligned}$$

from which the result follows, where the last inequality follows because $f(x) = \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+2}}$ is decreasing for $x > 0$. □

4 Trees with small Balaban indices

Lemma 4.1. *Let $P_n = u_a \dots u_1 u_0 v_0 v_1 \dots v_b$, where $a > b$, and $a+b+2 = n$. Then $D(v_i|P_n) = D(u_i|P_n) + (a-b)(2i+1)$ for $i = 0, 1, \dots, b$.*

Proof. Let $D_w = D(w|P_n)$ for $w \in V(P_n)$. Obviously, $D_{v_{b-i}} = D_{u_{a-i}}$ and $D_{u_{a-i}} + (i+1) = D_{u_{a-(i+1)}} + n - (i+1)$ for $i = 0, 1, \dots, b$. Then

$$D_{v_i} = D_{u_{a-(b-i)}},$$

$$D_{u_{a-(b-i+j)}} - D_{u_{a-(b-i+j+1)}} = n - 2(b-i+j+1),$$

where $j = 0, 1, \dots, a-b-1$, and $i = 0, 1, \dots, b$. Thus

$$D_{u_{a-(b-i)}} - D_{u_i} = \sum_{j=0}^{a-b-1} [n - 2(b-i+j+1)] = (a-b)(2i+1),$$

implying that $D_{v_i} = D_{u_i} + (a-b)(2i+1)$ for $i = 0, 1, \dots, b$, as desired. □

Lemma 4.2. *Let x be a vertex of a tree T_0 with at least two vertices. For integers $a \geq b+1$, let T (T', respectively) be the tree obtained from T_0 and the path $P_{a+b+2} = u_a \ldots u_1 u_0 v_0 v_1 \ldots v_b$ by identifying x and u_0 (x and v_0, respectively), see Fig. 2. Then $J(T) > J(T')$.*

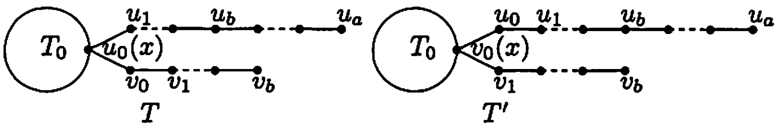

Fig. 2. T and T' in Lemma 4.2.

Proof. For $r, x, y > 0$, let $f_r(x,y) = \frac{1}{\sqrt{x(x+y)}} - \frac{1}{\sqrt{(x+r)(x+r+y)}}$. Since

$$\begin{aligned} \frac{\partial f_r(x,y)}{\partial x} &= -\frac{2x+y}{2x(x+y)\sqrt{x(x+y)}} \\ &\quad + \frac{2(x+r)+y}{2(x+r)(x+r+y)\sqrt{(x+r)(x+r+y)}}, \end{aligned}$$

we have

$$\begin{aligned} s \cdot \frac{\partial f_r(x,y)}{\partial x} &= -(2x+y)(x+r)(x+r+y)\sqrt{(x+r)(x+r+y)} \\ &\quad +(2x+2r+y)x(x+y)\sqrt{x(x+y)} \\ &< 0, \end{aligned}$$

where $s = 2x(x+y)(x+r)(x+r+y)\sqrt{x(x+y)(x+r)(x+r+y)} > 0$. Then $\frac{\partial f_r(x,y)}{\partial x} < 0$. Similarly, $\frac{\partial f_r(x,y)}{\partial y} < 0$. It follows that $f_r(x,y)$ is decreasing for x and y.

Now we are ready to prove our result. Let $c = |T_0|$. Let $D_w = D(w|T)$ for $w \in V(T)$ and $D'_w = D(w|T')$ for $w \in V(T')$.

Obviously, for $u \in V(T_0 - x)$, we have $D'_u = D_u + a - b$, and thus for $uv \in E(T_0 - x)$, we have $D'_u D'_v = (D_u + a - b)(D_v + a - b) > D_u D_v$.

For $u_i \in V(P_{a+1})$ with $i = 0, 1, \ldots, a$, we have $D'_{u_i} = D_{u_i} + c - 1$, and for $v_i \in V(P_{b+1})$ with $i = 0, 1, \ldots, b$, we have $D'_{v_i} = D_{v_i} - c + 1$. Then

$$\begin{aligned} D'_{u_i} D'_{u_{i+1}} &> D_{u_i} D_{u_{i+1}} \quad \text{for } i = 0, 1, \ldots, a-1, \\ D'_{v_j} D'_{v_{j+1}} &< D_{v_j} D_{v_{j+1}} \quad \text{for } j = 0, 1, \ldots, b-1. \end{aligned}$$

By Lemma 3.1, we have $D_{v_0} + b + 1 = D_{u_0} + c + a$, and then

$$\begin{aligned} D'_{u_0} D'_{v_0} &= (D_{u_0} + c - 1)(D_{v_0} - c + 1) \\ &= D_{u_0} D_{v_0} + (c-1)(a-b) > D_{u_0} D_{v_0} \end{aligned}$$

$$\begin{aligned} D'_x D'_y &= (D_{v_0} - c + 1)(D_y + a - b) \\ &= (D_{u_0} + a - b)(D_y + a - b) > D_x D_y \end{aligned}$$

for $y \in N_{T_0}(x)$.

For $i = 0, 1, \ldots, b$, we have $D_{v_i} = D_{u_i} + (a-b)(2i+1) + c - 1$, and for $i = 0, 1, \ldots, a-1$, we have $D_{u_{i+1}} = D_{u_i} + c + 2i - a + b + 1$. Since

$$\begin{aligned} D_{v_i} &= D(v_i|P_{a+b+2}) + D(v_i|T_0 - x) \\ &= D(v_i|P_{a+b+2}) + (i+1)(c-1) + D(x|T_0), \\ D_{u_i} &= D(u_i|P_{a+b+2}) + D(u_i|T_0 - x) \\ &= D(u_i|P_{a+b+2}) + i(c-1) + D(x|T_0), \end{aligned}$$

we have $D_{v_i} = D_{u_i} + (a-b)(2i+1) + c - 1$ for $i = 0, 1, \ldots, b$. Note also that $D_{u_{i+1}} = D_{u_i} + c + a + b + 1 - (a-i) - (a-i) = D_{u_i} + 2i + c - a + b + 1$ for $i = 0, 1, \ldots, a-1$.

For $i = 0, 1, \ldots, b-1$, we have

$$\begin{aligned} D_{u_i} D_{u_{i+1}} &= D_{u_i}(D_{u_i} + 2i + c - a + b + 1) = x_1(x_1 + y_1), \\ D'_{u_i} D'_{u_{i+1}} &= (D_{u_i} + c - 1)(D_{u_{i+1}} + c - 1) \\ &= (D_{u_i} + c - 1)(D_{u_i} + c - 1 + 2i + c - a + b + 1) \\ &= (x_1 + r)(x_1 + r + y_1), \\ D'_{v_i} D'_{v_{i+1}} &= (D_{v_i} - c + 1)(D_{v_{i+1}} - c + 1) \\ &= [D_{u_i} + (a-b)(2i+1)][D_{u_{i+1}} + (a-b)(2i+3)] \\ &= [D_{u_i} + (a-b)(2i+1)][D_{u_i} + (a-b)(2i+1) \\ &\quad +2i + c + a - b + 1] \\ &= x_2(x_2 + y_2), \\ D_{v_i} D_{v_{i+1}} &= [D_{u_i} + (a-b)(2i+1) + c - 1] \\ &\quad \cdot[D_{u_{i+1}} + (a-b)(2i+3) + c - 1] \\ &= [D_{u_i} + (a-b)(2i+1) + c - 1] \\ &\quad \cdot[D_{u_i} + (a-b)(2i+1) + c - 1 + 2i + c + a - b + 1] \\ &= (x_2 + r)(x_2 + r + y_2), \end{aligned}$$

where $x_1 = D_{u_i}$, $y_1 = 2i + c - a + b + 1$, $x_2 = D_{u_i} + (a-b)(2i+1) > x_1$, $y_2 = 2i + c + a - b + 1 > y_1$, and $r = c - 1$. For $i = 0, 1, \ldots, b$, let $A_i = (D'_{u_i} D'_{u_{i+1}})^{-\frac{1}{2}} + (D'_{v_i} D'_{v_{i+1}})^{-\frac{1}{2}}$, and $B_i = (D_{u_i} D_{u_{i+1}})^{-\frac{1}{2}} + (D_{v_i} D_{v_{i+1}})^{-\frac{1}{2}}$. Then

$$\begin{aligned} A_i - B_i &= \left((D'_{v_i} D'_{v_{i+1}})^{-\frac{1}{2}} - (D_{v_i} D_{v_{i+1}})^{-\frac{1}{2}}\right) \\ &\quad - \left((D_{u_i} D_{u_{i+1}})^{-\frac{1}{2}} - (D'_{u_i} D'_{u_{i+1}})^{-\frac{1}{2}}\right) \end{aligned}$$

$$= \quad f_r(x_2, y_2) - f_r(x_1, y_1) < 0.$$

Thus

$$\begin{aligned}
M(T') - M(T) &= \sum_{uv \in E(T')} (D'_u D'_v)^{-\frac{1}{2}} - \sum_{uv \in E(T)} (D_u D_v)^{-\frac{1}{2}} \\
&= \left(\sum_{uv \in E(T_0 - x)} (D'_u D'_v)^{-\frac{1}{2}} - \sum_{uv \in E(T_0 - x)} (D_u D_v)^{-\frac{1}{2}} \right) \\
&\quad + \left(\sum_{y \in N_{T_0}(x)} (D'_x D'_y)^{-\frac{1}{2}} - \sum_{y \in N_{T_0}(x)} (D_x D_y)^{-\frac{1}{2}} \right) \\
&\quad + \left(\sum_{i=b}^{a-1} (D'_{u_i} D'_{u_{i+1}})^{-\frac{1}{2}} - \sum_{i=b}^{a-1} (D_{u_i} D_{u_{i+1}})^{-\frac{1}{2}} \right) \\
&\quad + \left(\sum_{i=0}^{b-1} A_i - \sum_{i=0}^{b-1} B_i \right) \\
&\quad + \left((D'_{u_0} D'_{v_0})^{-\frac{1}{2}} - (D_{u_0} D_{v_0})^{-\frac{1}{2}} \right) \\
&< 0,
\end{aligned}$$

i.e., $J(T) > J(T')$. □

By the previous lemma, we have immediately the following.

Theorem 4.1. [12] *Let T be a tree with $n \geq 3$ vertices. Then $J(T) \geq J(P_n)$ with equality if and only if $T = P_n$.*

Let $P_{n-1,i}$ be the tree obtained by attaching a pendant vertex to vertex v_i of the path $P_{n-1} = v_1 v_2 \cdots v_{n-1}$, $1 \leq i \leq \lfloor \frac{n-1}{2} \rfloor$. Clearly, $P_n = P_{n-1,1}$.

Theorem 4.2. *Let T be a tree with $n \geq 4$ vertices different from P_n. Then $J(T) \geq J(P_{n-1,2})$ with equality if and only if $T = P_{n-1,2}$.*

Proof. Let d be the diameter of T. Then $d \leq n-2$. If $d < n-2$, then by Lemma 4.2, we can obtain an n-vertex tree with diameter $n-2$, which is of the form $P_{n-1,i}$ with smaller Balaban index than T.

Suppose that $T = P_{n-1,i}$. Denote by x the pendant vertex incident with v_i outside P_{n-1}. By Lemma 4.2 with $T_0 = xv_i$, we have

$$J(P_{n-1,i}) > J(P_{n-1,i-1}) > \cdots > J(P_{n-1,3}) > J(P_{n-1,2})$$

for $3 \leq i \leq \lfloor \frac{n-1}{2} \rfloor$. The result follows. □

Let $P_{n-2}(i,j)$ $(2 \leq i \leq j \leq n-3)$ be the n-vertex tree formed by attaching a pendant vertex at v_i and v_j of the path $P_{n-2} = v_1 v_2 \ldots v_{n-2}$, respectively. In particular, $P_{n-2}(i,i)$ is tree formed by attaching two pendant vertices at v_i of the path P_{n-2}.

Suppose that T is an n-vertex tree with diameter $d < n-3$. If the number of pendant vertices of T is three, then by Lemma 4.2, we can obtain an n-vertex tree T' of diameter $n-3$ and a P_2 attached to some vertex v_j of the diameter-achieving path, say $P_{n-2} = v_1v_2 \ldots v_{n-2}$, where $3 \leq j \leq n-4$, with smaller Balaban index than T. It is easily seen that $J(T) > J(T') > J(P_{n-1,3})$. If the number of pendant vertices of T at least four, then by Lemma 4.2, we can obtain an n-vertex tree with $n-3$, which is of the form $P_{n-2}(i,j)$ with smaller Balaban index than T.

Suppose that $T = P_{n-2}(i,j)$ different from $P_{n-2}(2, n-3)$. It is easily seen that $J(P_{n-2}(2,2)) > J(P_{n-1,3})$. Suppose without loss of generality that $3 \leq i \leq \lfloor \frac{n-1}{2} \rfloor$. Denote by x the pendant neighbor of v_j outside the diameter-achieving path P_{n-2} in T. By Lemma 4.2 with T_0 being the component containing v_j of the tree obtained from $P_{n-2}(i,j)$ by deleting edges v_jv_{j+1} and v_jx, we have a tree $P_{n-1,i}$, for which

$$J(P_{n-2}(i,j)) > J(P_{n-1,i}) \geq J(P_{n-1,3}).$$

Thus we have: If T is a tree with $n \geq 6$ vertices different from P_n and $P_{n-1,2}$, then $J(T) \geq \min\{J(P_{n-1,3}), J(P_{n-2}(2, n-3))\}$ with equality if and only if G is $P_{n-1,3}$ or $P_{n-2}(2, n-3)$ with smaller Balaban index [After computing by Matlab, we find that $J(P_{n-1,3}) < J(P_{n-2}(2, n-3))$ though their difference tends to zero as $n \to \infty$, and thus $J(T) \geq J(P_{n-1,3})$ with equality if and only if G is $P_{n-1,3}$].

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