On Sum-Balaban Index

Rundan Xing¹, Bo Zhou¹,* Ante Graovac^{2,3}

Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China

²Faculty of Science, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia

³NMR Center, The Rugjer Bošković Institute, P. O. Box 180, HR-10002 Zagreb, Croatia

Abstract

The sum-Balaban index of a connected graph G is defined as

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

where D_u is the sum of distances between vertex u and all other vertices, μ is the cyclomatic number, E(G) is the edge set, and m = |E(G)|. We establish various upper and lower bounds for the sum-Balaban index, and determine the trees with the largest, second-largest, and third-largest as well as the smallest, second-smallest, and third-smallest sum-Balaban indices among the n-vertex trees for $n \geq 6$.

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 a shortest path connecting u and v in G. Let $D_u = D(u|G) = \sum_{v \in V(G)} d_G(u, v)$, which is the distance sum of vertex u in G [4, 8].

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 [12] that $\mu = m - n + 1$.

^{*}Corresponding author. E-mail: zhoubo@scnu.edu.cn

The Balaban index of a connected graph G is defined as [1, 2]

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

It has been used successfully in developing QSAR/QSPR models [11] and in drug design [6]. Mathematical properties of Balaban index may be found in [9, 13]. Balaban et al. [3] proposed the study of the sum-Balaban index of a connected graph G, defined as

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

Note that the idea to change the multiplication to sum was first proposed in the case of the connectivity index in [14].

We establish some mathematical properties, mainly lower and upper bounds for the sum-Balaban index in terms of some other parameters, and determine the trees with the largest, second-largest, and third-largest as well as the smallest, second-smallest, and third-smallest sum-Balaban indices among the n-vertex trees for $n \ge 6$.

2 Sum-Balaban index of connected graphs

For a vertex u of the graph G, the degree of u, denoted by δ_u , is the number of its neighbors, and the eccentricity of u is the maximum distance to other vertices of G. The diameter of G is the maximum eccentricity of vertices of G.

Theorem 2.1. Let G be a connected graph with $n \geq 2$ vertices, m edges, and maximum degree Δ . Then

$${}^{g}\!J(G) \leq \frac{m}{2(\mu+1)} \sqrt{\frac{nm\Delta}{2n-2-\Delta}} \leq \frac{m}{2(\mu+1)} \sqrt{nm}$$

with the first equality if and only if G is a regular graph with diameter at most two, and with the second equality if and only if G is the complete graph.

Proof. By the Cauchy-Schwarz inequality, we have $\sum_{uv \in E(G)} (D_u + D_v)^{-\frac{1}{2}} \leq \sqrt{m \sum_{uv \in E(G)} (D_u + D_v)^{-1}}$ with equality if and only if $D_u + D_v$ is a constant for all edges uv of G. It is easily seen that $(D_u + D_v)^{-1} \leq \frac{D_u + D_v}{4D_u D_v} = \frac{1}{4} \left(\frac{1}{D_u} + \frac{1}{D_v} \right)$ with equality if and only if $D_u = D_v$. Thus

$$\sum_{uv \in E(G)} (D_u + D_v)^{-\frac{1}{2}} \le \sqrt{m \sum_{uv \in E(G)} \frac{1}{4} \left(\frac{1}{D_u} + \frac{1}{D_v}\right)} = \sqrt{\frac{m}{4} \sum_{u \in V(G)} \frac{\delta_u}{D_u}}$$

with equality if and only if D_u is a constant for all vertices u of G.

Note that $D_u \geq 2n - 2 - \delta_u$ with equality if and only if the eccentricity of u is at most two. Since $\frac{x}{2n-2-x}$ is increasing and $\Delta \leq n-1$, we have

$$\sum_{u \in V(G)} \frac{\delta_u}{D_u} \leq \sum_{u \in V(G)} \frac{\delta_u}{2n-2-\delta_u} \leq \frac{n\Delta}{2n-2-\Delta} \leq n$$

with the second equality if and only if G is regular of degree Δ and every vertex has eccentricity at most two, and with the third equality if and only if G is the complete graph. Note that D_u is a constant for all vertices u of G if G is regular of degree Δ and every vertex has eccentricity at most two. It follows that

$$\sum_{uv \in E(G)} (D_u + D_v)^{-\frac{1}{2}} \le \frac{1}{2} \sqrt{\frac{nm\Delta}{2n - 2 - \Delta}} \le \frac{1}{2} \sqrt{nm}$$

with the first equality if and only if G is regular of degree Δ and its diameter is at most two, and with the second equality if and only if G is the complete graph. \Box

Theorem 2.2. Let G be a connected bipartite graph with m edges. Let Δ_A and Δ_B be the maximum degrees among the partite sets A and B, respectively, where |A| = p and |B| = q. Then

$$\Im(G) \leq \frac{m\sqrt{m}}{2(\mu+1)}\sqrt{\frac{p\Delta_A}{2p+3q-2-\Delta_A} + \frac{q\Delta_B}{2q+3p-2-\Delta_B}}$$

with equality if and only if $q - 2\delta_u = p - 2\delta_v$ for $u \in A$ and $v \in B$, every vertex in A has degree Δ_A , every vertex in B has degree Δ_B , and the diameter of G is at most three.

Proof. By arguments in the proof of Theorem 2.1,

$$\sum_{uv \in E(G)} (D_u + D_v)^{-\frac{1}{2}} \le \sqrt{\frac{m}{4} \sum_{u \in V(G)} \frac{\delta_u}{D_u}}$$

with equality if and only if D_u is a constant for all vertices u of G.

For $u \in A$, $D_u \ge \delta_u + 3(q - \delta_u) + 2(p - 1) = 2p + 3q - 2 - 2\delta_u$ with equality if and only if the eccentricity of u is at most three. For $v \in B$, $D_v \ge \delta_v + 3(p - \delta_v) + 2(q - 1) = 2q + 3p - 2 - 2\delta_v$ with equality if and only if the eccentricity of v is at most three. Thus

$$\sum_{u \in V(G)} \frac{\delta_u}{D_u} \leq \sum_{u \in A} \frac{\delta_u}{2p + 3q - 2 - \delta_u} + \sum_{v \in B} \frac{\delta_v}{2q + 3p - 2 - \delta_v}$$

$$\leq \frac{p\Delta_A}{2p+3q-2-\Delta_A} + \frac{q\Delta_B}{2p+3q-2-\Delta_B}$$

and then

$$\sum_{uv \in E(G)} (D_u + D_v)^{-\frac{1}{2}}$$

$$\leq \sqrt{\frac{m}{4} \sum_{u \in V(G)} \frac{\delta_u}{D_u}}$$

$$\leq \sqrt{\frac{m}{4} \left(\frac{p\Delta_A}{2p + 3q - 2 - \Delta_A} + \frac{q\Delta_B}{2p + 3q - 2 - \Delta_B}\right)}$$

with equalities if and only if $q - 2\delta_u = p - 2\delta_v$ for $u \in A$ and $v \in B$, every vertex in A has degree Δ_B , every vertex in B has degree Δ_B , and the diameter of G is at most three.

For a connected graph G, $D'(G) = \sum_{u \in V(G)} \delta_u D_u$ is the degree distance of G [5], which is also a part of the Schultz molecular topological index [10]. We give a relation between sum-Balaban index and the degree distance.

Theorem 2.3. Let G be a connected graph with n vertices and m edges. Then

$$\Im(G) \ge \frac{m^2 \sqrt{m}}{(\mu+1)\sqrt{D'(G)}}$$

with equality if and only if $D_u + D_v$ is a constant for any $uv \in E(G)$.

Proof. By the Cauchy-Schwarz inequality,

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

$$\sum_{uv \in E(G)} (D_u + D_v)^{\frac{1}{2}} \le \sqrt{m \sum_{uv \in E(G)} (D_u + D_v)} = \sqrt{mD'(G)}$$

with either equality if and only if $D_u + D_v$ is a constant for any $uv \in E(G)$. Thus

$$\sum_{uv \in E(G)} (D_u + D_v)^{-\frac{1}{2}} \ge \frac{m^2}{\sqrt{mD'(G)}} = \frac{m\sqrt{m}}{\sqrt{D'(G)}},$$

and then the result follows easily.

3 Sum-Balaban index of trees

Let T be a tree with n vertices. Then |E(T)| = n - 1, the cyclomatic number of T is 0, and thus ${}^{s}J(G) = (n-1)\sum_{uv \in E(T)} (D_u + D_v)^{-\frac{1}{2}}$.

Let S_n and P_n be the star and the path with n vertices respectively.

First, we determine the first three largest sum-Balaban indices among the *n*-vertex trees, and characterize the trees for which the sum-Balaban indices attain these values.

Lemma 3.1. Let u be a vertex of a tree Q with at least two vertices. For integer $a \ge 1$, let T_1 be the tree obtained from Q by attaching a star S_{a+1} at its center v to u, and T_2 the tree obtained from Q by attaching a + 1 pendent vertices to u, see Fig. 1. Then ${}^{g}I(T_1) < {}^{g}I(T_2)$.

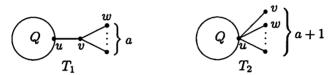


Fig. 1. T_1 and T_2 in Lemma 3.1.

Proof. Let $n=|V(T_1)|=|V(T_2)|$. Denote by w a pendent neighbor of v in T_1 and a pendent neighbor of u in T_2 outside Q. Note that $D(x|T_2)=D(x|T_1)-a\cdot d_{T_1}(x,w)+a\cdot d_{T_2}(x,w)=D(x|T_1)-a$ for any vertex $x\in V(Q)$, and $D(v|T_2)=D(v|T_1)-a\cdot d_{T_1}(v,w)+a\cdot d_{T_2}(v,w)=D(v|T_1)+a$. Then $D(u|T_2)+D(v|T_2)=D(u|T_1)+D(v|T_1)$. Thus

$$\begin{split} &\frac{sJ(T_2) - sJ(T_1)}{n-1} \\ &= \sum_{xy \in E(Q)} \left(\frac{1}{\sqrt{D(x|T_2) + D(y|T_2)}} - \frac{1}{\sqrt{D(x|T_1) + D(y|T_1)}} \right) \\ &+ a \left(\frac{1}{\sqrt{D(u|T_2) + D(w|T_2)}} - \frac{1}{\sqrt{D(v|T_1) + D(w|T_1)}} \right). \end{split}$$

For simplicity, let $D_x = D(x|T_1)$ for $x \in V(T_1)$. Note that $D(w|T_2) = D_w - (|V(Q)| - 1) = D_w - n + a + 2$. For $xy \in E(Q)$, $D(x|T_2) + D(y|T_2) = (D_x - a) + (D_y - a) = D_x + D_y - 2a$, and $D(u|T_2) + D(w|T_2) = (D_u - a) + (D_w - n + a + 2) = D_u + D_w - n + 2$. Note that $D_u = \sum_{x \in V(Q)} d_{T_1}(u, x) + 1 + 2a$ and $D_v = \sum_{x \in V(Q)} d_{T_1}(v, x) + a = \sum_{x \in V(Q)} d_{T_1}(u, x) + 1 + a = \sum_{x \in V(Q)} d_{T_1}(u, x) + n - 1$. Then $D_v = D_u + n - 2a - 2$. Obviously, n - a - 2 > 0. Thus

$$\frac{\Im(T_2)-\Im(T_1)}{n-1}$$

$$= \sum_{xy \in E(Q)} \left(\frac{1}{\sqrt{D_x + D_y - 2a}} - \frac{1}{\sqrt{D_x + D_y}} \right)$$

$$+ a \left(\frac{1}{\sqrt{D_u + D_w - n + 2}} - \frac{1}{\sqrt{D_u + D_w + n - 2a - 2}} \right)$$

$$> 0,$$

from which the result follows.

By the previous lemma, we have immediately the following result.

Theorem 3.1. Let T be a tree with $n \ge 3$ vertices. Then ${}^{s}J(T) \le \frac{(n-1)^2}{\sqrt{3n-4}}$ with equality if and only if $T = S_n$.

For $2 \le a \le \lfloor \frac{n}{2} \rfloor$, let $B_{n,a}$ be the *n*-vertex double star formed by adding an edge to the centers of the stars S_a and S_{n-a} . It is easily seen that

$$=\frac{\frac{3J(B_{n,a})}{n-1}}{\frac{a-1}{\sqrt{(3n-a-4)+(2n-a-2)}}} + \frac{1}{\sqrt{(2n-a-2)+(n+a-2)}} + \frac{n-a-1}{\sqrt{(n+a-2)+(2n+a-4)}}$$

$$=\frac{a-1}{\sqrt{5n-2a-6}} + \frac{1}{\sqrt{3n-4}} + \frac{n-a-1}{\sqrt{3n+2a-6}}.$$

For a function f(x) defined in an interval I, if f''(x) > 0, then by the Lagrange mean-value theorem, f(a) + f(d) > f(b) + f(c) for $a, b, c, d \in I$ with $a < b \le c < d$ and a + d = b + c.

Lemma 3.2. For $2 \le a \le \lfloor \frac{n}{2} \rfloor - 1$, ${}^{s}J(B_{n,a+1}) < {}^{s}J(B_{n,a})$.

Proof. Let $f(x) = \frac{x}{\sqrt{5n-2x-8}}$, where $2 \le x \le \lfloor \frac{n}{2} \rfloor - 1$. Then $f'(x) = \frac{5n-8-x}{(5n-2x-8)^{3/2}}$ and thus $f''(x) = \frac{10n-16-x}{(5n-2x-8)^{5/2}} > 0$. We have

$$\begin{split} &\frac{^3\!J(B_{n,a+1})-^3\!J(B_{n,a})}{n-1}\\ =& \left(\frac{a}{\sqrt{5n-2a-8}}+\frac{1}{\sqrt{3n-4}}+\frac{n-a-2}{\sqrt{3n+2a-4}}\right)\\ &-\left(\frac{a-1}{\sqrt{5n-2a-6}}+\frac{1}{\sqrt{3n-4}}+\frac{n-a-1}{\sqrt{3n+2a-6}}\right)\\ =& f(a)-f(a-1)+f(n-a-2)-f(n-a-1)\\ <& 0. \end{split}$$

The result follows.

Theorem 3.2. Let T be a tree with $n \geq 4$ vertices different from S_n . Then ${}^{g}I(T) \leq (n-1)\left(\frac{1}{\sqrt{5n-10}} + \frac{1}{\sqrt{3n-4}} + \frac{n-3}{\sqrt{3n-2}}\right)$ with equality if and only if $T = B_{n,2}$.

Proof. If T has at least two non-pendent edges, then by Lemma 3.1, we can obtain an n-vertex tree with only one non-pendent edge, which is a double star with larger sum-Balaban index than T. Now by Lemma 3.2, the result follows easily.

Let $P_{n+1} = v_0v_1 \dots v_n$. Let $T_{n,a,b}$ be the *n*-vertex tree formed by attaching a,b and n-a-b-3 pendent vertices to v_0, v_1 and v_2 in the path P_3 respectively, where $1 \le a \le \lfloor \frac{n-b}{2} \rfloor - 1$ and $a+b \le n-4$. Then any *n*-vertex tree with exactly two non-pendent edges is of the form $T_{n,a,b}$.

Theorem 3.3. Let T be a tree with $n \ge 6$ vertices different from S_n and $B_{n,2}$. Then ${}^{g}J(T) \le (n-1)\left(\frac{2}{\sqrt{5n-12}} + \frac{1}{\sqrt{3n-4}} + \frac{n-4}{\sqrt{3n}}\right)$ with equality if and only if $T = B_{n,3}$.

Proof. If T has at least two non-pendent edges and is different from $T_{n,1,n-5}$, then by Lemma 3.1, we can obtain an n-vertex tree with only one non-pendent edge, which is a double star different from $B_{n,2}$ with larger sum-Balaban index than T. Thus, if T is different from $T_{n,1,n-5}$, then by Lemma 3.2, ${}^{g}I(T) \leq {}^{g}I(B_{n,3})$ with equality if and only if $T = B_{n,3}$. Let $g(x) = \frac{1}{\sqrt{x}}$ for x > 0. Then g''(x) > 0. Thus

$$\frac{g(B_{n,3}) - g(T_{n,1,n-5})}{n-1}$$

$$= \left(\frac{2}{\sqrt{5n-12}} + \frac{1}{\sqrt{3n-4}} + \frac{n-4}{\sqrt{3n}}\right)$$

$$-\left(\frac{2}{\sqrt{5n-8}} + \frac{2}{\sqrt{3n-2}} + \frac{n-5}{\sqrt{3n}}\right)$$

$$= 2\left(\frac{1}{\sqrt{5n-12}} - \frac{1}{\sqrt{5n-8}}\right) + \frac{1}{\sqrt{3n-4}} + \frac{1}{\sqrt{3n}} - \frac{2}{\sqrt{3n-2}}$$

$$> \frac{1}{\sqrt{3n-4}} + \frac{1}{\sqrt{3n}} - \frac{2}{\sqrt{3n-2}}$$

$$= g(3n-4) + g(3n) - 2g(3n-2)$$

$$> 0,$$

from which the result follows.

In the following, we determine the first three smallest sum-Balaban indices among the *n*-vertex trees, and characterize the trees for which the sum-Balaban indices attain these values.

Lemma 3.3. Let x be a vertex of a tree Q with at least two vertices. For integers $a \geq b+1$, let T_1 $(T_2$, respectively) be the tree obtained from Q and the path $P = u_a \dots u_1 u_0 v_0 v_1 \dots v_b$ by identifying x and u_0 (x and v_0 , respectively), see Fig. 2. Then ${}^{\mathfrak{g}}I(T_1) > {}^{\mathfrak{g}}I(T_2)$.

Fig. 2. T_1 and T_2 in Lemma 3.3.

Proof. Let $n=|V(T_1)|=|V(T_2)|$. Then |V(Q)|=n-(a+b+2)+1=n-a-b-1. For $i=0,1,\ldots,a$, $D(u_i|T_2)=D(u_i|T_1)-\sum_{y\in V(Q)\setminus\{x\}}d_{T_1}(u_i,y)+\sum_{y\in V(Q)\setminus\{x\}}d_{T_2}(u_i,y)=D(u_i|T_1)+|V(Q)\setminus\{x\}|=D(u_i|T_1)+n-a-b-2,$ and similarly, for $j=0,1,2,\ldots,b$, $D(v_j|T_2)=D(v_j|T_1)-|V(Q)\setminus\{x\}|=D(v_j|T_1)-(n-a-b-2)$. Then $D(u_0|T_2)+D(v_0|T_2)=D(u_0|T_1)+D(v_0|T_1)$. Thus

$$\frac{{}^{9}I(T_{2}) - {}^{9}J(T_{1})}{n-1}$$

$$= \sum_{yz \in E(Q)} \left(\frac{1}{\sqrt{D(y|T_{2}) + D(z|T_{2})}} - \frac{1}{\sqrt{D(y|T_{1}) + D(z|T_{1})}} \right)$$

$$+ \sum_{i=0}^{a-1} \left(\frac{1}{\sqrt{D(u_{i}|T_{2}) + D(u_{i+1}|T_{2})}} - \frac{1}{\sqrt{D(u_{i}|T_{1}) + D(u_{i+1}|T_{1})}} \right)$$

$$+ \sum_{j=0}^{b-1} \left(\frac{1}{\sqrt{D(v_{j}|T_{2}) + D(v_{j+1}|T_{2})}} - \frac{1}{\sqrt{D(v_{j}|T_{1}) + D(v_{j+1}|T_{1})}} \right).$$

For simplicity, let $D_y = D(y|T_1)$ for $y \in V(T_1)$. Let $w \in V(Q)$. Obviously, for $i = 0, 1, \ldots, a - 1$, $d_{T_2}(w, u_i) = d_{T_1}(w, u_{i+1})$, and for $j = 1, 2, \ldots, b$, $d_{T_2}(w, v_j) = d_{T_1}(w, v_{j-1})$, and then

$$D(w|T_2) - D_w = \left(\sum_{i=0}^a d_{T_2}(w, u_i) - \sum_{i=0}^a d_{T_1}(w, u_i)\right) + \left(\sum_{j=0}^b d_{T_2}(w, v_j) - \sum_{j=0}^b d_{T_1}(w, v_j)\right)$$

$$D_{u_{i}} - D_{u_{i}} = \sum_{y \in V(P)} dT_{1}(u_{i}, y) + \sum_{y \in V(Q) \setminus \{x\}} dT_{1}(u_{i}, y) - \sum_{y \in V(Q) \setminus \{x\}} dT_{1}(u_{i}, y) + \sum_{y \in V(Q) \setminus \{x\}} dT_{1}(u_{i}, y) - \sum_{y \in V(Q) \setminus \{x\}} dT_{1}(u_{i}, y) + \sum_{y \in V(Q) \setminus \{x\}} dT_{1}(u_{i}, y) - \sum_{y \in V(Q) \setminus \{x\}} dT_{2}(u_{i}, y) - \sum_{y \in V(Q)}$$

It is easily seen that

$$+ \frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} - 2(n - a - b - 2)}}{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}} - \frac{\sqrt{D_{v_{i}} + D_{v_{i+1}}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}}$$

$$+ \sum_{i=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}} - \frac{\sqrt{D_{v_{i}} + D_{v_{i+1}}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - 2)}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

$$+ \sum_{j=0}^{l-1} \left(\frac{\sqrt{D_{v_{i}} + D_{v_{i+1}} + 2(n - a - b - b)}}}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} - \frac{1}{\sqrt{D_{v_{i}} + D_{v_{i+1}}}} \right)$$

Then for $yz \in E(Q)$, $D(y|T_2) + D(z|T_2) = D_y + D_z + 2(a-b) > D_y + D_z$ since a > b. Similarly, for $i = 0, 1, \ldots, a-1$, $D(u_i|T_2) + D(u_{i+1}|T_2) = D_{u_i} + D_{u_{i+1}}$, and for $j = 0, 1, \ldots, b-1$, $D_{u_i} + D_{u_{i+1}} + 2(n-a-b-2) > D_{u_i} + D_{u_{i+1}}$, and for $j = 0, 1, \ldots, b-1$, $D(u_j|T_2) + D(u_j|T_2) = D_{u_j} + D_{u_{j+1}} - 2(n-a-b-2)$. Then

$$= d_{T_2}(w, u_0) - d_{T_1}(w, u_0) + d_{T_2}(w, v_0) - d_{T_1}(w, u_0) = 0$$

$$-\left(\sum_{k=1}^{a-i}k + \sum_{k=1}^{b+i+1}k + \sum_{y \in V(Q)\setminus\{x\}}(d_Q(y,x) + i)\right)$$

$$= -\sum_{k=b-i+1}^{a-i}k + \sum_{k=b+i+2}^{a+i+1}k + |V(Q)\setminus\{x\}|$$

$$= 2(a-b)i + n - 2b - 2.$$

Let $a_1 = D_{u_i} + D_{u_{i+1}} + 2(n-a-b-2)$, $a_2 = D_{u_i} + D_{u_{i+1}}$, $a_3 = D_{u_i} + D_{u_{i+1}} + 2(a-b)(2i+1) + 2(n-2b-2) - 2(n-a-b-2)$ and $a_4 = D_{u_i} + D_{u_{i+1}} + 2(a-b)(2i+1) + 2(n-2b-2)$. Note that $a_1 + a_3 = a_2 + a_4$, and since a > b, we have $a_4 > \max\{a_1, a_2, a_3\}$ and $a_2 < \min\{a_1, a_3, a_4\}$. Let $g(x) = \frac{1}{\sqrt{x}}$ for x > 0. Then g''(x) > 0. Thus

$$\frac{sJ(T_2) - sJ(T_1)}{n-1} < \sum_{i=0}^{b-1} \left(\frac{1}{\sqrt{a_1}} - \frac{1}{\sqrt{a_2}} + \frac{1}{\sqrt{a_3}} - \frac{1}{\sqrt{a_4}} \right)$$

$$= \sum_{i=0}^{b-1} (g(a_1) - g(a_2) + g(a_3) - g(a_4))$$

$$< 0,$$

from which the result follows.

By the previously lemma, we have immediately the following result.

Theorem 3.4. Let T be a tree with $n \geq 3$ vertices. Then ${}^gI(T) \geq (n-1)\sum_{i=1}^{n-1} \frac{1}{\sqrt{n^2-2ni+2i^2}}$ with equality if and only if $T = P_n$.

A tree T is said to be starlike if only one vertex of T is of degree more than two. Let $S_n(n_1, n_2, \ldots, n_t)$ be the n-vertex starlike tree obtained by attaching paths $P_{n_1}, P_{n_2}, \ldots, P_{n_t}$ at one of their end vertices to a single vertex respectively, where $n_i \geq 1$ for $1 \leq i \leq t$ and $\sum_{i=1}^t n_i = n-1$. Let $P_n(i,j)$ be the tree obtained from the path $P_{n-2} = v_0v_1\cdots v_{n-3}$ by attaching a pendent vertex to the vertex v_i and v_j respectively, where $1 \leq i \leq \lfloor \frac{n-3}{2} \rfloor$ and $i < j \leq n-4$.

Theorem 3.5. If T is a tree with $n \geq 4$ vertices different from P_n , then ${}^{s}\!J(T) \geq {}^{s}\!J(S_n(1,1,n-3))$ with equality if and only if $T = S_n(1,1,n-3)$. If T is a tree with $n \geq 6$ vertices different from P_n and $S_n(1,1,n-3)$, then ${}^{s}\!J(T) \geq {}^{s}\!J(S_n(1,2,n-4))$ with equality if and only if $T = S_n(1,2,n-4)$.

Proof. Let T be a tree with minimum sum-Balaban index among the trees with $n \geq 4$ vertices different from P_n . By Lemma 3.3, T is a starlike tree, say $T = S_n(n_1, n_2, \ldots, n_t)$ with $t \geq 3$. If $t \geq 4$, then by Lemma 3.3,

we can obtain another starlike tree of maximum degree t-1 with smaller sum-Balaban index, which is a contradiction. Then t=3. By Lemma 3.3, we have $T=S_n(1,1,n-3)$.

Now let T be a tree with minimum sum-Balaban index among the trees with $n \geq 6$ vertices different from P_n and $S_n(1, 1, n-3)$. First suppose that T is a starlike tree, say $T = S_n(n_1, n_2, \ldots, n_t)$ with $t \geq 3$. By Lemma 3.3, if $t \geq 4$, then ${}^{s}J(T) \geq {}^{s}J(S_{n}(1,1,1,n-4)) > {}^{s}J(S_{n}(1,2,n-4))$, and if t=3, then $^s\!J(T) \geq ^s\!J(S_n(1,2,n-4))$ with equality if and only if $T = S_n(1,2,n-4)$. Now suppose that T is not starlike and $T \neq P_n(1, n-4)$. Then there exist at least two vertices of degree more than one in T. If there are at least three vertices of degree more than one in T, then by using Lemma 3.3 to the two vertices, both of degree at least two, which are with maximal distance among all pairs of vertices of degree more than one, we can get a starlike tree with smaller sum-Balaban index, which is a contradiction. If there are exactly two vertices of degree more than one in T, then by Lemma 3.3, T is of the form $P_n(i,j)$. Since $T \neq P_n(1,n-4)$ and by Lemma 3.3, ${}^s\!J(T) \geq {}^s\!J(S_n(1,2,n-4))$ with equality if and only if $T = S_n(1,2,n-4)$. It follows that T is the tree $S_n(1,2,n-4)$ or $P_n(1,n-4)$ with smaller sum-Balaban index. Let $E_i = \sum_{j=1}^{i-1} j + \sum_{j=1}^{n-2-i} j = \frac{i(i-1)+(n-1-i)(n-2-i)}{2}$. Then

$$= \frac{\frac{\mathcal{Y}(S_n(1,2,n-4))}{n-1}}{\frac{1}{\sqrt{2E_1+n+4}} + \frac{1}{\sqrt{E_1+E_3+n}} + \frac{1}{\sqrt{E_1+E_3+n+2}}} + \frac{1}{\sqrt{E_1+E_3+n+2}} + \frac{1}{\sqrt{2E_1+3n-8}} + \frac{1}{\sqrt{E_1+E_2+2(n-3)}} + \sum_{i=3}^{n-4} \frac{1}{\sqrt{E_i+E_{i+1}+2(n-3)}},$$

$$\frac{3(P_n(1,n-4))}{n-1} = \frac{4}{\sqrt{E_1 + E_2 + 2(n-2)}} + \sum_{i=2}^{n-4} \frac{1}{\sqrt{E_i + E_{i+1} + 2(n-3)}},$$

and thus

$$\frac{{}^{3}J(S_{n}(1,2,n-4)) - {}^{3}J(P_{n}(1,n-4))}{n-1}$$

$$= \frac{1}{\sqrt{2E_{1}+n+4}} + \frac{1}{\sqrt{E_{1}+E_{3}+n}} + \frac{1}{\sqrt{E_{1}+E_{3}+n+2}} + \frac{1}{\sqrt{2E_{1}+3n-8}} + \frac{1}{\sqrt{E_{1}+E_{2}+2(n-3)}}$$

$$+\sum_{i=3}^{n-4} \frac{1}{\sqrt{E_i + E_{i+1} + 2(n-3)}}$$

$$-\left(\frac{4}{\sqrt{E_1 + E_2 + 2(n-2)}} + \sum_{i=2}^{n-4} \frac{1}{\sqrt{E_i + E_{i+1} + 2(n-3)}}\right)$$

$$= \frac{1}{\sqrt{2E_1 + n + 4}} + \frac{1}{\sqrt{E_1 + E_3 + n}} + \frac{1}{\sqrt{E_1 + E_3 + n + 2}}$$

$$+ \frac{1}{\sqrt{2E_1 + 3n - 8}} + \frac{1}{\sqrt{E_1 + E_2 + 2(n-3)}}$$

$$-\frac{4}{\sqrt{E_1 + E_2 + 2(n-2)}} - \frac{1}{\sqrt{E_2 + E_3 + 2(n-3)}}.$$

By direct calculation, we have $E_1 = \frac{n^2 - 5n + 6}{2}$, $E_2 = \frac{n^2 - 7n + 14}{2}$ and $E_3 = \frac{n^2 - 9n + 26}{2}$. Let $g(x) = \frac{1}{\sqrt{x}}$ for x > 0. Then g''(x) > 0. Thus

$$\frac{{}^{3}\!J(S_{n}(1,2,n-4)) - {}^{3}\!J(P_{n}(1,n-4))}{n-1}$$

$$= \frac{1}{\sqrt{n^{2}-4n+10}} + \frac{1}{\sqrt{n^{2}-6n+16}} + \frac{1}{\sqrt{n^{2}-6n+18}} + \frac{1}{\sqrt{n^{2}-2n-2}} + \frac{1}{\sqrt{n^{2}-4n+4}} - \frac{4}{\sqrt{n^{2}-4n+6}} - \frac{1}{\sqrt{n^{2}-6n+14}}$$

$$= g(n^{2}-6n+16) + g(n^{2}-4n+4) - g(n^{2}-4n+6) - g(n^{2}-6n+14) + \frac{1}{\sqrt{n^{2}-4n+10}} + \frac{1}{\sqrt{n^{2}-6n+18}} + \frac{1}{\sqrt{n^{2}-2n-2}} - \frac{3}{\sqrt{n^{2}-4n+6}}$$

$$< \frac{1}{\sqrt{n^{2}-4n+10}} + \frac{1}{\sqrt{n^{2}-6n+18}} + \frac{1}{\sqrt{n^{2}-2n-2}} - \frac{3}{\sqrt{n^{2}-4n+6}} .$$

By Matlab 7.0, the right-most function of the above inequality is negative for $n \ge 6$. Thus ${}^{g}J(S_{n}(1,2,n-4)) < {}^{g}J(P_{n}(1,n-4))$.

As a corollary of Theorems 3.1 and 3.4, the sum-Balaban index satisfies the basic requirement to be a branching index in that it has the minimum value for the path and the maximum value for the star among trees [7] with given number of vertices.

Acknowledgement. This work was supported by the National Natural Science Foundation of China (Grant No. 11071089) and the Ministry of Science, Education and Sports of Republic of Croatia (Grants No. 098-0982929-2940 and No. 177-0000000-0884).

References

- [1] A.T. Balaban, Distance connectivity index, Chem. Phys. Lett. 89 (1982) 399-404.
- [2] A.T. Balaban, Topological indices based on topological distances in molecular graphs, Pure Appl. Chem. 55 (1983) 199-206.
- [3] A.T. Balaban, P.V. Khadikar, S. Aziz, Comparison of topological indices based on iterated 'sum' versus 'product' operations, Iranian J. Math. Chem. 1 (2010) 43-67.
- [4] F. Buckley, F. Harary, Distance in Graphs, Addison-Wesley, Reading, MA, 1990.
- [5] A.A. Dobrynin, A.A. Kochetova, Degree distance of a graph: A degree analogue of the Wiener index, J. Chem. Inf. Comput. Sci. 34 (1994) 1082–1086.
- [6] G. Grassy, B. Calas, A. Yasri, R. Lahana, J. Woo, S. Iyer, M. Kaczorek, R. Floc'h, R. Buelow, Computer-assisted rational design of immunosuppressive compounds, Nature Biotechnol. 16 (1998) 748-752.
- [7] O. Ivanciuc, T. Ivanciuc, D. Cabrol-Bass, A.T. Balaban, Investigation of alkane branching (and resulting partial ordering) by topological indices, MATCH Commun. Math. Comput. Chem. 42 (2000) 155-180.
- [8] D. Janežić, A. Miličević, S. Nikolić, N. Trinajstić, Graph Theoretical Matrices in Chemistry, Univ. Kragujevac, Kragujevac, 2007.
- [9] S. Li, B. Zhou, On the Balaban index of trees, Ars Combin. 100 (2011), in press.
- [10] W.R. Müller, K. Szymanski, J.V. Knop, N. Trinajstić, Molecular topological index, J. Chem. Inf. Comput. Sci. 30 (1990) 160-163.
- [11] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.
- [12] R.J. Wilson, Introduction to Graph Theory, Oliver & Boyd, Edinburgh, 1972.
- [13] B. Zhou, N. Trinajstić, Bounds on the Balaban index, Croat. Chem. Acta 81 (2008) 319–323.
- [14] B. Zhou, N. Trinajstić, On a novel connectivity index, J. Math. Chem. 46 (2009) 1252-1270.