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On the Sum-Balaban Index[1]

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Abstract

We introduce a novel topological index for (molecular) graphs, called sum-Balaban index: $SJ(G) = \frac{m}{\mu+1} \sum_{uv \in E(G)} \frac{1}{\sqrt{D_G(u)+D_G(v)}}$, where $D_G(u)$ is the distance sum of vertex u in G, m is the number of edges and μ is the cyclomatic number of G. We find that the sum-Balaban index is correlated well with some physico-chemical properties and other topological indices of octanes and lower benzenoids. We also give several basic properties for this index and determine the trees with fixed numbers of vertices with the minimum value and the maximum values of the sum-Balaban index of this index, respectively.

1 Introduction

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.

In [3], it was shown that the ordering induced by the Balaban index parallels the ordering induced by the Wiener index for the constitutional isomers of alkanes with 6 through 9 carbon atoms, but reduces the degeneracy of the latter index and provides a much higher discriminating ability.

Several people in view of the successful applications of the Balaban index in QSPR and QSAR gave a physicochemical interpretation of this molecular descriptor [4-6].

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In this report, we first introduce a novel variant topological index that we call the sum-Balaban index and investigate predictive power of this index, then give some basic properties, especially lower and upper bounds in terms of other graph invariants and determine the extremal values of this index among all trees with fixed numbers of vertices.

2 The sum–Balaban index and correlations with some phyisico–chemical properties and other topological index

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.

A novel topological index of (G), that we call the sum-Balaban index, is defined as

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

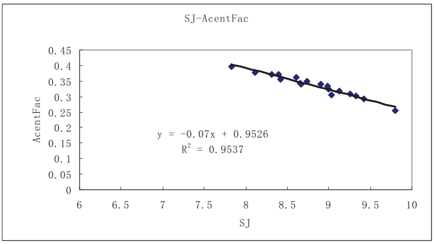
In order to investigate predictive power of the sum-Balaban index, we first use octanes and some of their physico–chemical properties as resource. We find that Acentric factor (AcenFac) and Entropy (S) give good correlations in Table 1. We also compare the sum-Balaban index and other topological indices: Balaban index (J), second Zagreb index (ZM2), Wiener index (W), Schultz molecular topological index (SMTI), Gutman molecular topological index (GMTI), quasi-Wiener index (Kirchhoff number) (QW). Results are presented in Table 2. Then, the π-electronic energies E_π of 30 lower benzenoids is modeled using the sum-Balaban index. It is evident from Table 3 there exists a good linear correlation between SJ and $\log E_\pi$.

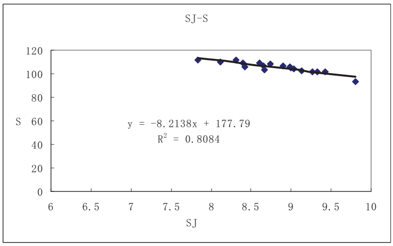
It can be seen from data for correlation coefficients (R) that the sum-Balaban index should be considered in the future QSPR/QSAR researches.

Acentric factor (AcenFac), Entropy (S) and SJ of octanes

Molecule	AcentFac	S	SJ
octane	0.397898	111.67	7.83191
2-methyl-heptane	0.377916	109.84	8.1124
3-methyl-heptane	0.371002	111.26	8.31771
4-methyl-heptane	0.371504	109.32	8.39475
3-ethyl-hexane	0.362472	109.43	8.60722
2,2-dimethyl-hexane	0.339426	103.42	8.66378
2,3-dimethyl-hexane	0.348247	108.02	8.74219
2,4-dimethyl-hexane	0.344223	106.98	8.65128
2,5-dimethyl-hexane	0.35683	105.72	8.42111
3,3-dimethyl-hexane	0.322596	104.74	8.99892
3,4-dimethyl-hexane	0.340345	106.59	8.90176
2-methyl-3-ethyl-pentane	0.332433	106.06	8.9827
3-methyl-3-ethyl-pentane	0.306899	101.48	9.26089
2,2,3-trimethyl-pentane	0.300816	101.31	9.32339
2,2,4-trimethyl-pentane	0.30537	104.09	9.03672
2,3,3-trimethyl-pentane	0.293177	102.06	9.42343
2,3,4-trimethyl-pentane	0.317422	102.39	9.13036
2,2,3,3-tetramethylbutane	0.255294	93.06	9.80213

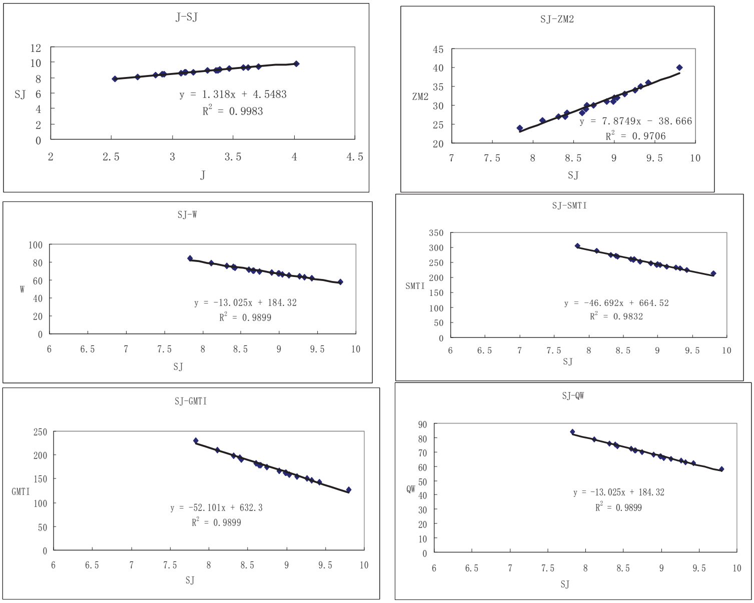
Table 1. Graphs showsing correlations between SJ and Acentric factor (AcenFac) and Entropy (S)





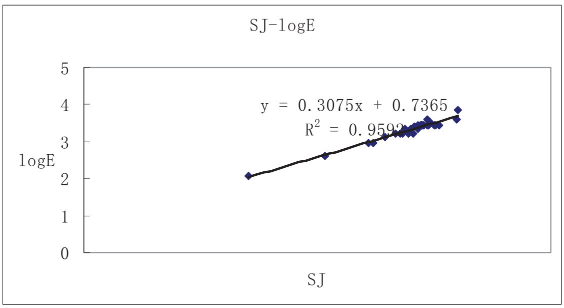
Correlation coefficients (R)	
Acentric factor (AcenFac)	-0.976567
Entropy (S)	-0.899111

Table 2. Graphs showsing correlations between SJ and other topological indices



Balaban index (J)	0.99515
second Zagreb index (ZM2)	0.98519
Wiener index (W)	-0.994937
Schultz molecular topological index (SMTI)	-0.991564
Gutman molecular topological index (GMTI)	-0.994937
quasi-Wiener index (Kirchhoff number) (QW)	-0.994937

Table 3. Graph showsing correlation between SJ and Π-electronic energies



R=0.979

The π-electronic energies E_π, the sum-Balaban indices of 30 lower benzenoids

Benzenoid	E_π	SJ
benzene	8.000	4.24264
naphthalene	13.683	6.20765
anthracene	19.314	7.30883
phenanthrene	19.448	7.42898
tetracene	24.931	8.0046
benzo[c]phenanthrene	25.188	8.34866
benzo[a]anthracene	25.101	8.13053
chrysene	25.129	8.1988
triphenylene	25.275	8.46906
pyrene	22.506	7.73777
pentacene	30.544	8.48211
benzo[a]tetracene	30.726	8.59097
dibenzo[a,h]anthracene	30.881	8.6698
dibenzo[a,j]anthracene	30.880	8.73831
pentaphene	30.763	8.63351
benzo[g]chrysene	30.999	9.12277
pentahelicene	30.936	9.02814
benzo[c]chrysene	30.943	8.86537
picene	30.943	8.71449
benzo[b]chrysene	30.839	8.67326
dibenzo[a,c]anthracene	30.942	8.99313
dibenzo[b,g]phenanthrene	30.834	8.82403
perylene	28.245	8.57805
benzo[e]pyrene	28.336	8.41465
benzo[a]pyrene	28.222	8.23812
hexahelicene	36.681	9.59642
benzo[ghi]perylene	31.425	8.7322
hexacene	36.156	8.82958
coronene	34.572	8.87291
ovalene	46.497	9.59924

3 Mathematical properties of the sum-Balaban index

In this section we establish some basic mathematical properties of the sum-Balaban index.

Proposition 1. Let $G = (V, E)$ be a connected graph with order $n \geq 3$. Then $SJ(G) \geq J(G)$ with equality if and only if $G = K_3$.

Proof. Since $G = (V, E)$ is a connected graph with order $n \geq 3$, $D_G(u) \geq 2$ for any vertex $u \in V$, and $D_G(u)D_G(v) \geq 2(D_G(u) + D_G(v)) - 4 \geq D_G(u) + D_G(v)$ for any edge

$uv \in E$. Thus $SJ(G) \geq J(G)$ with equality if and only if $D_G(u)D_G(v) = D_G(u) + D_G(v)$ for every edge uv of G, i. e., $D_G(u) = D_G(v) = 2$ for every edge uv of G and thus $G = K_3$.

Let $d_G(u)$ be the degree of vertex u and $D'(G) = \sum_{u \in V(G)} d_G(u)D_G(u)$ the degree distance of G ([7,8]).

Proposition 2. Let G be a connected graph with order $n \geq 2$. Then $SJ(G) \geq \frac{m^2\sqrt{m}}{(\mu+1)\sqrt{D'(G)}}$ with equality if and only if $D_G(u) + D_G(v)$ is a constant for every edge uv of G.

Proof. Since $x^{-1/2}$ is a strictly convex function for $x > 0$, we have

$$\sum_{uv \in E(G)} \frac{(D_G(u) + D_G(v))^{-1/2}}{m} \geq \left(\sum_{uv \in E(G)} \frac{D_G(u) + D_G(v)}{m} \right)^{-1/2}$$

and then

$$SJ(G) \geq \frac{m^2}{\mu+1} \left(\sum_{uv \in E(G)} \frac{D_G(u) + D_G(v)}{m} \right)^{-1/2} = \frac{m^2\sqrt{m}}{(\mu+1)\sqrt{D'(G)}}$$

with equality if and only if $D_G(u) + D_G(v)$ is a constant for every edge uv of G.

In the following, we will investigate the extremal value of trees respect to the sum-Balaban index.

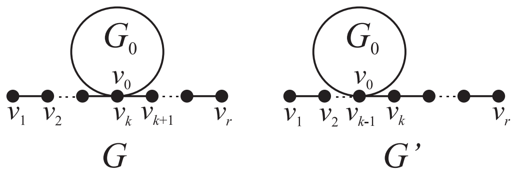


Figure 1. The path-sliding transformation.

The path-sliding transformation [9]. Let G_0 be a graph with $n_0 \geq 2$ vertices, and $P = v_1v_2 \cdots v_r$ 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 1).

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

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

Proof. From (1) and (3), $\forall e = uv \in E(G_0)$,

$$\begin{aligned} & [D_{G'}(u) + D_{G'}(v)] - [D_G(u) + D_G(v)] \\ = \ & 2(D_P(v_{k-1}) - D_P(v_k)) \\ = \ & 2(r - 2k + 2) > 0 \ . \end{aligned} \tag{5}$$

From (2) and (4),

$D_G(v_1) + D_G(v_2) = 2D_{G_0}(v_0) + D_P(v_1) + D_P(v_2) + (2k-3)(n_0-1)$
$D_G(v_2) + D_G(v_3) = 2D_{G_0}(v_0) + D_P(v_2) + D_P(v_3) + (2k-5)(n_0-1)$
$\cdots$
$D_G(v_{k-2}) + D_G(v_{k-1}) = 2D_{G_0}(v_0) + D_P(v_{k-2}) + D_P(v_{k-1}) + 3(n_0-1)$
$\mathbf{D_G(v_{k-1}) + D_G(v_k) = 2D_{G_0}(v_0) + D_P(v_{k-1}) + D_P(v_k) + (n_0-1)}$
$D_G(v_k) + D_G(v_{k+1}) = 2D_{G_0}(v_0) + D_P(v_k) + D_P(v_{k+1}) + (n_0-1)$
$D_G(v_{k+1}) + D_G(v_{k+2}) = 2D_{G_0}(v_0) + D_P(v_{k+1}) + D_P(v_{k+2}) + 3(n_0-1)$
$\cdots$
$D_G(v_{r-2}) + D_G(v_{r-1}) = 2D_{G_0}(v_0) + D_P(v_{r-2}) + D_P(v_{r-1}) + (2r-2k-3)(n_0-1)$
$D_G(v_{r-1}) + D_G(v_r) = 2D_{G_0}(v_0) + D_P(v_{r-1}) + D_P(v_r) + (2r-2k-1)(n_0-1)$

$$
\begin{array}{l}
D_{G'}(v_1) + D_{G'}(v_2) = 2D_{G_0}(v_0) + D_P(v_1) + D_P(v_2) + (2k-5)(n_0-1) \\
D_{G'}(v_2) + D_{G'}(v_3) = 2D_{G_0}(v_0) + D_P(v_2) + D_P(v_3) + (2k-7)(n_0-1) \\
\cdots \\
D_{G'}(v_{k-2}) + D_{G'}(v_{k-1}) = 2D_{G_0}(v_0) + D_P(v_{k-2}) + D_P(v_{k-1}) + (n_0-1) \\
\mathbf{D_{G'}(v_{k-1}) + D_{G'}(v_k) = 2D_{G_0}(v_0) + D_P(v_{k-1}) + D_P(v_k) + (n_0-1)} \\
D_{G'}(v_k) + D_{G'}(v_{k+1}) = 2D_{G_0}(v_0) + D_P(v_k) + D_P(v_{k+1}) + 3(n_0-1) \\
D_{G'}(v_{k+1}) + D_{G'}(v_{k+2}) = 2D_{G_0}(v_0) + D_P(v_{k+1}) + D_P(v_{k+2}) + 5(n_0-1) \\
\cdots \\
D_{G'}(v_{r-2}) + D_{G'}(v_{r-1}) = 2D_{G_0}(v_0) + D_P(v_{r-2}) + D_P(v_{r-1}) + (2r-2k-1)(n_0-1) \\
D_{G'}(v_{r-1}) + D_{G'}(v_r) = 2D_{G_0}(v_0) + D_P(v_{r-1}) + D_P(v_r) + (2r-2k+1)(n_0-1)\ .
\end{array}
$$

Note that

$$D_P(v_1) > D_P(v_2) > \cdots > D_P(v_{\lfloor \frac{r}{2} \rfloor}) = D_P(v_{\lceil \frac{r}{2} \rceil}) < D_P(v_{\lceil \frac{r}{2} \rceil + 1}) < \cdots < D_P(v_r)\ .$$

We have

$$(D_G(v_{k-2}) + D_G(v_{k-1})) - (D_{G'}(v_{k-2}) + D_{G'}(v_{k-1})) = 2(n_0-1)$$

$$(D_G(v_k) + D_G(v_{k+1})) - (D_{G'}(v_k) + D_{G'}(v_{k+1})) = -2(n_0-1)$$

$$(D_G(v_{k-2}) + D_G(v_{k-1})) > (D_{G'}(v_k) + D_{G'}(v_{k+1}))\ .$$

Since $f(x) = \dfrac{1}{\sqrt{x}} - \dfrac{1}{\sqrt{x + (n_0+1)}}$ is decreasing,

$$
\begin{aligned}
& \frac{1}{\sqrt{D_G(v_k) + D_G(v_{k+1})}} - \frac{1}{\sqrt{D_{G'}(v_k) + D_{G'}(v_{k+1})}} \\
> \ & \frac{1}{\sqrt{D_{G'}(v_{k-2}) + D_{G'}(v_{k-1})}} - \frac{1}{\sqrt{D_G(v_{k-2}) + D_G(v_{k-1})}}\ .
\end{aligned}
$$

Thus

$$
\begin{aligned}
& \frac{1}{\sqrt{D_G(v_{k-2}) + D_G(v_{k-1})}} - \frac{1}{\sqrt{D_{G'}(v_{k-2}) + D_{G'}(v_{k-1})}} \\
+ \ & \frac{1}{\sqrt{D_G(v_k) + D_G(v_{k+1})}} - \frac{1}{\sqrt{D_{G'}(v_k) + D_{G'}(v_{k+1})}} > 0\ .
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
& \frac{1}{\sqrt{D_G(v_{t-1}) + D_G(v_t)}} - \frac{1}{\sqrt{D_{G'}(v_{t-1}) + D_{G'}(v_t)}} \\
+ \ & \frac{1}{\sqrt{D_G(v_{2k-t}) + D_G(v_{2k-t-1})}} - \frac{1}{\sqrt{D_{G'}(v_{2k-t}) + D_{G'}(v_{2k-t-1})}} > 0 \qquad (6)
\end{aligned}
$$

where $t = 1, 2, \cdots, k-2$. Again, since $D_G(v_{k+t-1})+D_G(v_{k+t}) < D_{G'}(v_{k+t-1})+D_{G'}(v_{k+t})-2(n_0-1) < D_{G'}(v_{k+t-1}) + D_{G'}(v_{k+t})$ for $t = k-1, k, \cdots, r-k$,

$$\frac{1}{\sqrt{D_G(v_{k+t-1}) + D_G(v_{k+t})}} - \frac{1}{\sqrt{D_{G'}(v_{k+t-1}) + D_{G'}(v_{k+t})}} > 0 \tag{7}$$

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

From (5)–(7), we have

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

Using Lemma 1 and the path-sliding transformation repeatedly, we can easily obtain:

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

$$SJ(G) \geq SJ(P_n) = (n-1) \sum_{i=1}^{n-1} (n^2 - 2i)^{-1/2}$$

$$J(G) \geq J(P_n) = 2(n-1) \sum_{i=1}^{n-1} [(n^2 - 2in + 2i^2 + n - 2i)(n^2 - 2in + 2i^2 - n + 2i)]^{-1/2}$$

$$D'(G) \leq D'(P_n) = \sum_{i=1}^{n-1} (n^2 - 2in + 2i^2)$$

with equality if and only if $T = P_n$ is the path with n vertices.

The edge-lifting transformation([9]). 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 2).

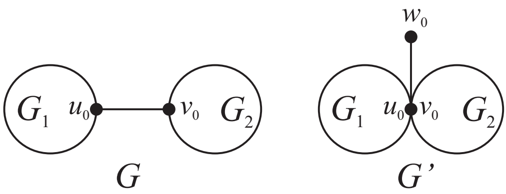


Figure 2. The edge-lifting transformation.

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

$$\begin{aligned} D_G(u) &= \sum_{v\in V(G_1)} d_G(u,v) + \sum_{v\in V(G_2)} d_G(u,v) \\ &= D_{G_1}(u) + \sum_{v\in V(G_2)} [d_G(u,u_0) + 1 + d_G(v_0,v)] \\ &= D_{G_1}(u) + D_{G_2}(v_0) + [d_G(u,u_0)+1]n_2 \ . \end{aligned} \tag{8}$$

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

$$D_G(u) = D_{G_1}(u_0) + D_{G_2}(u) + [d_G(u,v_0)+1]n_1 \ . \tag{9}$$

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

$$\begin{aligned} D_{G'}(u) &= \sum_{v\in V(G_1)} d_G(u,v) + \sum_{v\in V(G_2)} d_G(u,v) - d_G(u,u_0) + d_G(u,v_0) \\ &= D_{G_1}(u) + \sum_{v\in V(G_2)} [d_G(u,u_0) + d_G(u_0,v)] + 1 \\ &= D_{G_1}(u) + D_{G_2}(v_0) + n_2 d_G(u,u_0) + 1 \ . \end{aligned} \tag{10}$$

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

$$D_{G'}(u) = D_{G_1}(u_0) + D_{G_2}(u) + n_1 d_G(u,v_0) + 1 \tag{11}$$

and

$$D_{G'}(w_0) = D_{G_1}(u_0) + D_{G_2}(v_0) + n_1 + n_2 - 1 \tag{12}$$

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

Proof. From (8)–(12), 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

$$D_G(u) + D_G(v) > D_{G'}(u) + D_{G'}(v) \quad , \quad D_G(u)D_G(v) > D_{G'}(u)D_{G'}(v)$$

$$D_G(u_0) + D_G(v_0) = D_{G'}(u_0) + D_{G'}(w_0) \ .$$

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

Using Lemma 2 and the edge-lifting transformation repeatedly, we easily obtain:

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

$$SJ(T) \leq (n-1)^2\,(3n-4)^{-1/2}$$

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

Another Simpler Proof of Theorem 2. Since T is a tree with n vertices, we have $m = n-1$ and $\mu = 0$. Thus $SJ(T) = (n-1) \sum\limits_{uv \in E(G)} \frac{1}{\sqrt{D_u + D_v}}$.

For any edge $e = uv$ of T,

$$D_u \geq d_u + 2(n-1-d_u) = 2n-2-d_u$$

$$D_v \geq d_v + 2(n-1-d_u) = 2n-2-d_v$$

and $d_u + d_v \leq n$. We have

$$D_u + D_v \geq 4n-4-(d_u+d_v) \geq 3n-4$$

with equality if and only if $d_u + d_v = n$. So,

$$SJ(T) \leq (n-1)^2(3n-4)^{-1/2}$$

with equality if and only if $d_u + d_v = n$ for every edge uv of T, i. e., $T = S_n$.

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