# Sum-Balaban index and its properties

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**Abstract**

The sum-Balaban index is defined as $SJ(G) = \frac{m}{m-n+2} \sum \frac{1}{\sqrt{w(u)+w(v)}}$, where the sum is taken over all edges of a connected graph $G$, $n$ and $m$ are the cardinalities of the vertex and the edge set of $G$, respectively, and $w(u)$ (resp. $w(v)$) denotes the sum of distances from $u$ (resp. $v$) to all the other vertices of $G$. In the paper known results on this recently introduced topological index are summarized.

*Keywords*: Balaban index, sum-Balaban index; extremal graphs; molecular descriptor

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## 1.1 Introduction

Topological indices are numerical parameters mathematically derived from the graph structure. They are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity. With respect to the invariant which plays a crucial role in the definition, we usually divide topological indices into three types: degree-based indices, distance-based indices and spectrum-based indices. Sum-Balaban index, the subject of this paper, is one of many distance-based topological indices.

To present its definition, we first need to introduce the basic notions. For a graph $G$, by $V(G)$ and $E(G)$ we denote the vertex and edge sets of $G$, respectively. Let $n = |V(G)|$ and $m = |E(G)|$. For vertices $u, v \in V(G)$, by $\mathrm{dist}_G(u, v)$ (or shortly just $\mathrm{dist}(u, v)$) we denote the distance from $u$ to $v$ in $G$, and by $w(u)$ we denote the *transmission* (or the *status*) of $u$, defined as $w(u) = \sum_{x \in V(G)} d_G(u, x)$. A predecessor of sum-Balaban index, *Balaban index* $J(G)$ of a connected graph $G$, defined as

$$J(G) = \frac{m}{m-n+2} \sum_{e=uv} \frac{1}{\sqrt{w(u) \cdot w(v)}},$$

was introduced in early eighties by Balaban [2, 3]. Later Balaban et al. [4] (and independently also Deng [7]) proposed a derived measure, namely the *sum-Balaban index* $\mathrm{SJ}(G)$ for a connected graph $G$:

$$\mathrm{SJ}(G) = \frac{m}{m-n+2} \sum_{uv \in E(G)} \frac{1}{\sqrt{w(u) + w(v)}}.$$

Since its introduction in 2010 sum-Balaban index was successfully used in QSAR/QSPR modeling, but recently it also attracted attention of mathematicians. In this paper we describe the state of the art on mathematical properties of sum-Balaban index and expose some questions, which stay unanswered.

## 1.2 Sum-Balaban index of trees

To avoid ambiguity we need to mention that throughout this paper we consider simple and connected graphs. In this first section we further restrict to the class of trees, which are especially interesting from the chemists point of view. Deng [7] and Xing et al. [24] considered trees with the given number of vertices.

**Theorem 1** *For a tree $T$ on $n \geq 2$ vertices, we have*

$$\mathrm{SJ}(P_n) \leq \mathrm{SJ}(T) \leq \mathrm{SJ}(S_n)$$

*with left (right, respectively) equality if and only if $T = P_n$ ($T = S_n$, respectively), where $P_n$ is the path on $n$ vertices and $S_n$ is the star on $n$ vertices.*

In [24] also trees with the second-largest, and third-largest (as well as the second-smallest, and third-smallest) sum-Balaban index among the $n$-vertex trees for $n \geq 6$ were determined. Their proof is based on specific transformations, which increase sum-Balaban index. In [19] alternative proof for the above results and tools which enabled the authors to give further ranking up to seventh maximum sum-Balaban index were presented. The results are summarized in Table 1, where $T_k$ denotes the tree with the $k$-th largest sum-Balaban index. In what follows we describe the graphs mentioned in the table.

A double star $D_{a,b}$ is a tree consisting of $a + b$ vertices, two of which have degrees $a$ and $b$, while the remaining ones have degree 1. By symmetry, we may assume that $a \geq b$. In Figure 1 we have the double star $D_{7,2}$.

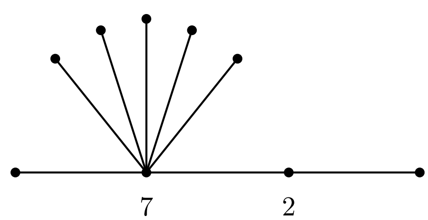


Figure 1: The double star $D_{7,2}$.

By $H_{a_1,a_2,\ldots,a_{d-1}}$ we denote a tree consisting of a diametric path of length $d$ (i.e., with $d + 1$ vertices) and a couple of pendant edges, such that the degrees of vertices of the diametric path are $1, a_1, a_2, \ldots, a_{d-1}, 1$. That is, $H_{a_1,a_2,\ldots,a_{d-1}}$ is a *caterpillar*. Due to symmetry, we may assume that $a_1 \geq a_{d-1}$ in $H_{a_1,a_2,\ldots,a_{d-1}}$, see Figure 2 for $H_{3,7,2}$.

Let $n \geq 7$. By $R_n$ we denote the graph obtained from a star on $n - 3$ vertices by subdividing three distinct edges, see Figure 3 for $R_{11}$.

It was also observed in [19] that for every $k$, the value $\mathrm{SJ}(T_1) - \mathrm{SJ}(T_k)$ is tending to $c_k\sqrt{n}$, where $c_k$ is a constant depending on $k$ but not on $n$.

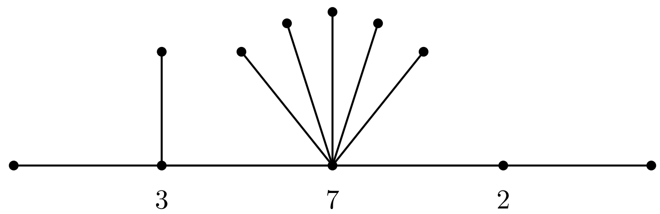


Figure 2: A caterpillar $H_{3,7,2}$.

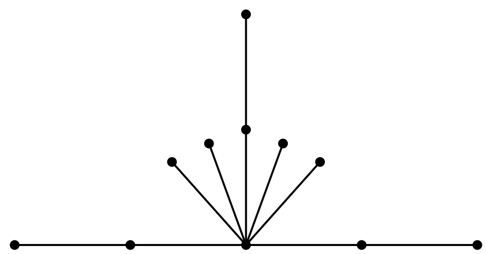

Figure 3: The graph $R_{11}$.

For the maximum value of sum-Balaban index for trees with given diameter the interested reader is referred to [26].

### 1.3 Extremal values for $n$-vertex graphs

In [24] various upper and lower bounds are given for graphs with given parameters such as the maximum degree, number of edges, etc. The authors considered also the special case of bipartite graphs. However, in this section we are interested in extremal values of sum-Balaban index in the case when only the number of vertices is prescribed.

#### 1.3.1 Maximum values

The *cyclomatic number* $\mu$ of $G$, which is the minimum number of edges that must be removed from $G$ in order to transform it to an acyclic graph, equals $m-n+1$. Note that the denominator $m-n+2$ in the definition of Balaban and sum-Balaban index

<table>
<tr><th>$n$</th><th>$T_1$</th><th>$T_2$</th><th>$T_3$</th><th>$T_4$</th><th>$T_5$</th><th>$T_6$</th><th>$T_7$</th></tr>
<tr><td>$2-3$</td><td rowspan="10">$S_n$</td><td></td><td rowspan="2"></td><td rowspan="3"></td><td rowspan="3"></td><td rowspan="3"></td><td rowspan="4"></td></tr>
<tr><td>4</td><td rowspan="9">$D_{n-2,2}$</td></tr>
<tr><td>5</td><td>$P_5$</td></tr>
<tr><td>6</td><td rowspan="7">$D_{n-3,3}$</td><td rowspan="2">$H_{2,n-3,2}$</td><td rowspan="2">$H_{n-3,2,2}$</td><td>$P_6$</td></tr>
<tr><td>7</td><td>$H_{3,3,2}$</td><td>$R_7$</td></tr>
<tr><td>8</td><td>$D_{4,4}$</td><td>$H_{2,5,2}$</td><td rowspan="2">$H_{n-3,2,2}$</td><td rowspan="2">$H_{3,n-4,2}$</td></tr>
<tr><td>9</td><td rowspan="4">$H_{2,n-3,2}$</td><td rowspan="3">$D_{n-4,4}$</td></tr>
<tr><td>$10-11$</td><td>$D_{n-5,5}$</td><td>$H_{n-3,2,2}$</td></tr>
<tr><td>$12-22$</td><td>$H_{n-3,2,2}$</td><td rowspan="2">$H_{3,n-4,2}$</td></tr>
<tr><td>$23-\infty$</td><td>$H_{n-3,2,2}$</td><td>$D_{n-4,4}$</td></tr>
</table>

Table 1: First seven trees with maximal values of sum-Balaban index.

can be expressed as $\mu + 1$. In [20] $n$-vertex graphs which contain at least one cycle were considered.

**Theorem 2** *Let $G$ be a connected graph on $n$ vertices with $\mu \geq 1$. Then* $\mathrm{SJ}(G)$ *is maximum if and only if $G$ is the complete graph $K_n$.*

In [21] we found an erroneous statement that complete graphs attain the maximum sum-Balaban index among all $n$-vertex graphs. However this is true only for small cases of $n$ as proved in [20].

**Theorem 3** *For any connected graph $G$ on $n \geq 2$ vertices, we have*

$$\mathrm{SJ}(G) \leq \begin{cases} \mathrm{SJ}(K_n), & \text{if } n \leq 5 \\ \mathrm{SJ}(S_n), & \text{if } n \geq 6. \end{cases}$$

Moreover, the next theorem implies that for every $k$ and large enough $n$, the first $k$ graphs of order $n$ with the largest value of Balaban index are trees [20].

**Theorem 4** *Let $a$ and $b$ be positive integers such that $a, b \geq 2$, $a + b = n$ and $n \geq 8$. Then* $\mathrm{SJ}(D_{a,b}) > \mathrm{SJ}(K_n)$.

One can observe that Theorems 2 and 3 imply the following:

**Corollary 5** *Let $G$ be a graph with the maximum value of sum-Balaban index in the class of $k$-connected ($k$-edge-connected) graphs of order $n$. Then we have:*

*(1) if $k = 1$ and, $n = 2$ or $n \geq 6$, then $G$ is the star $S_n$;*

*(2) if $k = 1$ and $n \leq 5$, or $k \geq 2$, then $G$ is the complete graph $K_n$.*

### 1.4 Minimum values

As in the case of Balaban index (see [13]) finding the minimum value of sum-Balaban index among $n$-vertex graphs is far more complicated problem. It remains open, however, some insight in the structure of potential candidates was given in [14]. There we have the following results.

**Theorem 6** *Let $G$ be a graph on $n$ vertices, $n \geq 4$. Then*

$$\mathrm{SJ}(G) \geq 2\sqrt{\frac{n}{n-1}}\,.$$

It turns out that for large values of $n$ a better lower bound on the sum-Balaban index can be obtained.

**Theorem 7** *Let $G$ be a graph on $n$ vertices, where $n$ is big enough. Then*

$$\mathrm{SJ}(G) \geq 4 + o(1).$$

Let $K_a$ and $K'_{a'}$ be two disjoint complete graphs on $a$ and $a'$ vertices, respectively. We always assume $a \leq a'$. Further, let $P_b$ be a path on $b$ vertices $(v_0, v_1, \ldots, v_{b-1})$ disjoint from the cliques. The *dumbbell graph* $D^0_{a,b,a'}$ is obtained from $K_a \cup P_b \cup K'_{a'}$ by joining all vertices of $K_a$ with $v_0$ and all vertices of $K'_{a'}$ with $v_{b-1}$. Thus, $D^0_{a,b,a'}$ has $a + b + a'$ vertices. In the case when $a = a'$, we call a graph a *balanced dumbbell graph* and we denote it by $B_{a,b}$. A *dumbbell-like graph*, $D^\ell_{a,b,a'}$, is obtained from the dumbbell graph $D^0_{a,b,a'}$ by either inserting $\ell$ edges between $v_1$ and $K_a$ if $\ell > 0$, or by removing $-\ell$ edges between $v_{b-1}$ and $K'_{a'}$ if $\ell < 0$.

In Figure 4 one can find graphs which attain the minimum value of sum-Balaban index among $n$-vertex graphs where $n \leq 10$ (we remark that by removing dotted edges we obtain the corresponding graphs with the minimum value of Balaban index). Observe

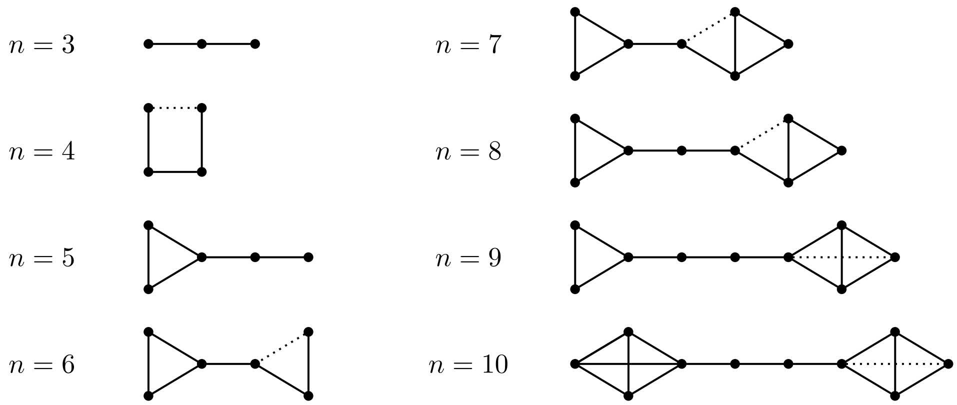


Figure 4: Graphs with the smallest value of sum-Balaban index for $n \in \{3, 4, \ldots, 10\}$.

that all graphs in Figure 4 (with the exception of the case $n = 4$) are dumbbell or dumbbell-like.

In the special case of balanced dumbbell graphs the following statement was obtained in [14].

**Theorem 8** *Let $B_{a,b}$ be a balanced dumbbell graph on $n$ vertices with the smallest possible value of sum-Balaban index. Then $a$ and $b$ are asymptotically equal to $\sqrt[4]{\sqrt{2}\log\left(1+\sqrt{2}\right)}\sqrt{n}$ and $n$, respectively. That is, $a = \sqrt[4]{\sqrt{2}\log\left(1+\sqrt{2}\right)}\sqrt{n} + o(\sqrt{n})$ and $b = n - o(n)$.*

**Corollary 9** *Let $B$ be a balanced dumbbell graph on $n$ vertices, where $n$ is big enough, with the minimum value of sum-Balaban index. Then*

$$\mathrm{SJ}(B) \doteq 4.47934.$$

Comparing Corollary 9 with the lower bound presented in Theorem 7, we see that the asymptotic value of sum-Balaban index for optimum balanced dumbbell graph is only about 1.12 times higher. Hence it can be expected that the optimal balanced dumbbell graph is not much different from the optimal dumbbell graph.

**Conjecture 10** *Among all dumbbell graphs $D^0_{a,b,a'}$ on at least 14 vertices, the minimum value of sum-Balaban index is achieved for one with $a' = a$ or $a' = a + 1$.*

More generally, the following was conjectured in [14].

**Conjecture 11** *Dumbbell-like graphs $D^{\ell}_{a,b,a'}$ attain the minimum value of sum-Balaban index.*

## 1.5 Accumulation points of sum-Balaban index

In [18] it is shown that for every nonnegative real number $r$ there exists a sequence of graphs $\{G_{r,i}\}_{i=1}^{\infty}$ such that the number of vertices of $G_{r,i}$ tends to infinity as $i \to \infty$ and $\lim_{i\to\infty} J(G_{r,i}) = r$. An analogous result was proved for sum-Balaban index [20]. Denote $Q = \sqrt{2}\ln(1+\sqrt{2})$. Observe that $Q \doteq 1.24650$ and $1+Q+2\sqrt{Q} \doteq 4.47934$. We have the following statement.

**Theorem 12** *Let $r \geq 1+Q+2\sqrt{Q}$. Further, let $\{B_{a_i,b_i}\}_{i=1}^{\infty}$ be a sequence of balanced dumbbell graphs on $n_i = 2a_i + b_i$ vertices such that $n_i \to \infty$ and*

$$\lim_{i\to\infty} \frac{a_i}{\sqrt{n_i}} = \frac{1}{\sqrt{2}}\sqrt{r-1-Q+\sqrt{(r-1-Q)^2-4Q}}.$$

*Then* $\lim_{i\to\infty} \mathrm{SJ}(B_{a_i,b_i}) = r$.

Although we conjecture that for graphs $G$ on large number of vertices $\mathrm{SJ}(G) \geq 1+Q+2\sqrt{Q}$ (see Corollary 9), it is proved only that $\mathrm{SJ}(G) \geq 4+o(1)$ (see Theorem 7). Hence, if the conjecture is false, then the problem of accumulation points of sum-Balaban index for values in the interval $[4, 4.47934)$ remains open.

## 1.6 Unicyclic and bicyclic graphs

Unicyclic graphs on $n$ vertices with the maximum sum-Balaban index were considered in [25]. Let $S_n^+$ denote the graph, obtained from the star $S_n$ by adding an edge between two nonadjacent vertices of the star.

**Theorem 13** *Let $G$ be a connected unicyclic graph on $n \geq 4$ vertices. Then*

$$\mathrm{SJ}(G) \leq \frac{n}{2}\left(\frac{1}{\sqrt{4n-8}} + \frac{2}{\sqrt{3n-5}} + \frac{n-3}{\sqrt{3n-4}}\right),$$

*where the equality holds if and only if $G = S_n^+$.*

A connected graph on $n$ vertices is said to be *bicyclic* if it contains exactly $n+1$ edges. Denote by $S_n^{++}$ the bicyclic graph obtained from the star $S_n$ by adding two edges with a common vertex (see Figure 5 where $S_7^{++}$ is depicted).

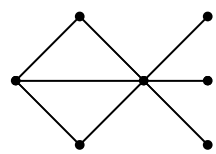

Figure 5: The graph $S_7^{++}$.

Maximum values of sum-Balaban index were first examined in [6]. However, Fang et al. [11] found some flaws in this paper and proved the following.

**Theorem 14** *The graph $S_n^{++}$ has the largest sum-Balaban index among all $n$-vertex bicyclic graphs.*

## 1.7 Regular graphs

Folowing the results of [15], Lei et al. [21] proved that for an $r$-regular graph $G$ on $n$ vertices with $r \geq 3$ it holds

$$\mathrm{SJ}(G) \leq \frac{r^2(r-1)n^{\frac{1}{2}}}{2(r-2)^{\frac{3}{2}}\sqrt{2\left\lfloor \log_{r-1}\left(\frac{(r-2)n+2}{r}\right)\right\rfloor}}.$$

They also considered fullerenes, and proved that if they contain at least 60 vertices, then $\mathrm{SJ}(G) \leq \frac{9n}{\sqrt{n\sqrt{n}}}$.

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