On the minimum value of sum-Balaban index

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Abstract

We consider extremal values of sum-Balaban index among graphs on n vertices. We determine that the upper bound for the minimum value of the sum-Balaban index is at most 4.47934 when n goes to infinity. For small values of n we determine the extremal graphs and we observe that they are similar to dumbbell graphs, in most cases having one extra edge added to the corresponding extreme for the usual Balaban index. We show that in the class of balanced dumbbell graphs, those with clique sizes $\sqrt[4]{\sqrt{2}\log\left(1+\sqrt{2}\right)\sqrt{n}} + o(\sqrt{n})$ have asymptotically the smallest value of sum-Balaban index. We pose several conjectures and problems regarding this topic.

Keywords: sum-Balaban index; extremal graphs; dumbbell graphs

1 Introduction

In this paper we consider simple and connected graphs. Denote by V(G) and E(G) the vertex and edge sets of a given graph G, respectively. Let

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n = |V(G)| and m = |E(G)|. For vertices $u, v \in V(G)$, by $\operatorname{dist}_G(u, v)$ (or shortly just $\operatorname{dist}(u, v)$) we denote the distance from u to v in G, and by w(u) we denote the transmission (or the distance) of u, defined as $w(u) = \sum_{x \in V(G)} d_G(u, x)$.

Balaban index J(G) of a connected graph G, defined as

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

was introduced in early eighties by Balaban [5, 6]. Later, Balaban et al. [7] (and independently also Deng [10]) proposed a derived measure, namely the sum-Balaban index SJ(G) for a graph G:

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

Similarly as Balaban index, also sum-Balaban was used in various quantitative structure-property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies. Regarding mathematical properties, there are several results known for sum-Balaban index, but they mainly pertain to trees, and graphs containing only one or two cycles.

It was shown by Deng [10] and Xing et al. [24] that for a tree T on n vertices, $n \geq 2$,

$$SJ(P_n) \le SJ(T) \le SJ(S_n)$$

with left (right) equality if and only if $T = P_n$ ($T = S_n$), where P_n is the path on n vertices and S_n is the star on n vertices. The authors in [24] also determined trees with the second-largest, and third-largest as well as the second-smallest, and third-smallest sum-Balaban indices among the n-vertex trees for $n \geq 6$. In [18] alternative proof for the above results and further ranking up to seventh maximum sum-Balaban index was presented. In [25] the authors investigated the maximum sum-Balaban index of trees with given diameter, and in [26] the extremal graph which attains the maximum sum-Balaban index among trees with given vertices and maximum degree were determined.

Unicyclic graphs on n vertices with the maximum sum-Balaban index were considered in [11], and bicyclic graphs were studied in [8, 12]. For various upper and lower bounds of general graphs in terms of some other

parameters (such as the maximum degree, number of edges, etc.) see [10] and [24], and for recent results on r-regular graphs see [21].

Maximal values of Balaban and sum-Balaban index in more general setting were explored in [17]. On the other hand, finding the minimum value of sum-Balaban index among n-vertex graphs is a rather untractable problem. We find it natural to attack this problem in a similar fashion as in the case of Balaban index, so in general we follow the steps of [14]. For small values of n we determine the extremal graphs and we observe that they are similar to dumbbell graphs, in most cases having one extra edge added to the corresponding extreme for the usual Balaban index. We show that in the class of balanced dumbbell graphs, those with clique sizes $\sqrt[4]{\sqrt{2}\log\left(1+\sqrt{2}\right)}\sqrt{n}+o(\sqrt{n})$ have asymptotically the smallest value of sum-Balaban index. Recall that for Balaban index, the coefficient in front of \sqrt{n} is $\sqrt[4]{\pi/2}$, see [14]. Using a computer we find dumbbell-like graphs with slightly smaller sum-Balaban index values. We also pose several conjectures and problems regarding this topic.

2 Two simple lower bounds on sum-Balaban index

We begin by stating two simple lower bounds for sum-Balaban index in the class of graphs on n vertices. Note that these two claims correspond to Theorems 4 and 8 for Balaban index, see [14].

Theorem 1. Let G be a graph on n vertices, $n \geq 4$. Then

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

Proof. Suppose that G has m edges. Since $n \geq 4$, we have

$$\frac{m}{m-n+2} \ge \frac{2n}{m}. (1)$$

For every vertex $v \in V(G)$, it holds $w(v) \leq 1 + 2 + \cdots + (n-1) = \frac{n^2 - n}{2}$. Hence, for every $u, v \in V(G)$ we have

$$\frac{1}{\sqrt{w(u) + w(v)}} \ge \frac{1}{\sqrt{n^2 - n}}.$$
(2)

Since G has m edges, using (1) and (2) we obtain

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

For large values of n we present a better lower bound on the sum-Balaban index.

Theorem 2. Let G be a graph on n vertices, where n is big enough. Then

$$SJ(G) \ge 4 + o(1)$$
.

Proof. Let f(n) be a function that represents the number of edges in extremal graphs on n vertices. Since our graphs are connected, we have $m \ge n - 1$, that is, $f(n) \in \Omega(n)$. Now we split the proof into two cases according to the behaviour of f(n):

• Case 1: $f(n) \notin \Theta(n)$. This means there is a subsequence $\{f(n_i)\}_{i=1}^{\infty}$, such that for every constant k we have $f(n_j) > kn_j$ for all j big enough. From (2), for n's in this subsequence we get

$$SJ(G) \ge \frac{m}{m-n+2} \cdot \frac{m}{\sqrt{n^2-n}} \sim \frac{f(n)}{f(n)} \cdot \frac{f(n)}{n} \sim f(n) \cdot n^{-1}.$$
 (3)

However, Corollary 8 gives a dumbbell graph D on n vertices with sum-Balaban index smaller than 5. Hence $5 > \mathrm{SJ}(D)$ which means that f(n), the function representing the number of edges in extremal graphs, must satisfy $5 > f(n)n^{-1}$ by (3). Hence 5n > f(n). But this contradicts the properties of $\{f(n_i)\}_{i=1}^{\infty}$, and so there is not a subsequence as required in this case.

• Case 2: $f(n) \in \Theta(n)$. This means that there are positive constants c_1 and c_2 , such that for large n we have $c_1 n \leq f(n) \leq c_2 n$. Fix n big enough. Then there is c = c(n) such that $c_1 \leq c \leq c_2$ and f(n) = cn. From (2) we get

$$SJ(G) \ge \frac{m}{m-n+2} \cdot \frac{m}{\sqrt{n^2-n}} \sim \frac{cn}{(c-1)n} \cdot \frac{cn}{n} = \frac{c^2}{c-1}.$$
 (4)

Notice that the right-hand side of (4) is minimal for c = 2. Substituting c = 2 in (4) we obtain $SJ(G) \ge 4 + o(1)$.

By Theorem 2, the asymptotic lower bound for SJ(G) is 4. Let us mention that nanotubes of type (k, l) (regardless if they are open or not) have asymptotic value of sum-Balaban index $\frac{9\sqrt{2}}{2}\sqrt{k+l} \cdot \log(1+\sqrt{2})$, see [1, 3]. However, in the sequel we show that there are graphs with even smaller value of Balaban index.

3 Extremes for small number of vertices

By the proof of Theorem 2, one would expect that a graph with the minimum sum-Balaban index will have $\Theta(n)$ edges and vertices v with big value of w(v). Hence, a path with two complete graphs attached to the end-vertices of the path, so called $dumbbell\ graph$, is a good candidate for an extremal graph. This idea is supported by the list of extremal graphs for $n \leq 10$, see Figure 1, so we devote this section to dumbbell graphs. Some of the graphs on the figure contain a dotted edge. By removing such edge we obtain the graph with the minimum value of Balaban index.

We restrict ourselves to $n \leq 10$ as the realm of graphs is getting huge for bigger n. Perhaps, with a little more powerful computer resources the cases n=11 and 12 could be easily tractable. However, in Figure 2 we present graphs with a potential to be the extremes for $n \in [11, 14]$. These graphs were obtained by restricting the space of graphs of order n (to maximal degree up to 5, for n=11 and n=12 to graphs containing at least n and at most 22 edges, and for n=13 and n=14 to graphs with at least 15 and at most 20 edges).

4 Bounds for balanced dumbbell graphs

Here we consider the lower bound of sum-Balaban index among balanced dumbbell graphs in a similar way as it was done in [14] for Balaban index. Reason for this is that these graphs are simple to define and deal with and in some cases they are extremal, see Figures 1 and 2. We believe that balanced dumbbell graphs asymptotically attain the lower bound.

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 $D_{a,b,a'}$

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, $D_{a,b,a'}$ has a+b+a' vertices. In the case when a=a', we call a graph a balanced dumbbell graph and we denote it by $D_{a,b}$.

Also for Balaban index, balanced dumbbell graphs are close to extremal graphs. However, the cliques and paths in balanced dumbbell graphs achieving the minimum value of Balaban index have different sizes from those, which achieve the minimum value of sum-Balaban index. To derive these sizes, we use a lemma from [14].

Lemma 3. Let u be a vertex of K_a (or K'_a) and let v_i be the i-th vertex of P_b , where K_a , K'_a and P_b are parts of the balanced dumbbell graph $D_{a,b}$ as in the definition. Then

$$w(u) = \frac{b^2}{2} + ab + \frac{b}{2} + 2a - 1,$$
 and
 $w(v_i) = \frac{i^2}{2} + \frac{(b-i)^2}{2} + ab - \frac{b}{2} + i + a.$

Next result gives an upper bound for the minimum value of sum-Balaban index in the class of balanced dumbbell graphs.

Proposition 4. Let c be a positive constant. Further, let $D_{a,b}$ be a balanced dumbbell graph on n vertices, where $a \sim c\sqrt{n}$. Then

$$SJ(D_{a,b}) \in \Theta(1).$$

Proof. Since $a \sim c\sqrt{n}$, we have $b \sim n$. Therefore, $w(u) \sim \frac{b^2}{2} = w^*(u)$ if u is a vertex of K_a or K_a' , while $w(v_i) \sim \frac{i^2}{2} + \frac{(b-i)^2}{2} = w^*(v_i)$ for $v_i \in V(P_b)$, by Lemma 3. Since $\frac{b^2}{4} \leq \frac{i^2}{2} + \frac{(b-i)^2}{2} \leq \frac{b^2}{2}$, for every edge xy we have

$$\frac{b}{\sqrt{2}} \le \sqrt{w^*(x) + w^*(y)} \le b.$$

Hence, for every edge xy there exist $c_{xy}^b \in [\frac{1}{\sqrt{2}}, 1]$ such that $\sqrt{w^*(x) + w^*(y)} = c_{xy}^b b$. Then

$$\frac{1}{\sqrt{w(x) + w(y)}} \sim \frac{1}{c_{xy}^b b}.$$

Since $D_{a,b}$ has $2\binom{a+1}{2} + b - 1$ edges, we have $m = a^2 + a + b - 1 \sim a^2 + b$. Thus, analogously as above we can get

$$\sum_{xy \in E(D_{a,b})} \frac{1}{\sqrt{w(x) + w(y)}} \sim \frac{a^2 + b}{c^b \cdot b},$$

where c^b is some value such that $c^b \in [\frac{1}{\sqrt{2}}, 1]$. Finally, $m - n + 2 = a^2 - a + 1 \sim a^2$. Hence,

$$SJ(D_{a,b}) = \frac{m}{m - n + 2} \sum_{uv \in E(D_{a,b})} \frac{1}{\sqrt{w(u) + w(v)}} \sim \frac{a^2 + b}{a^2} \cdot \frac{a^2 + b}{c^b \cdot b}$$

$$= \frac{1}{c^b} \left[\frac{a^2}{b} + 2 + \frac{b}{a^2} \right], \tag{5}$$

where c^b is a value such that $\frac{1}{\sqrt{2}} \leq c^b \leq 1$. Recall that $a \sim c\sqrt{n}$. Since all terms in brackets of the second line of (5) are in $\Theta(1)$, we conclude $\mathrm{SJ}(D_{a,b}) \in \Theta(1)$.

In what follows we will need the following result from analysis.

Proposition 5. Let b be a positive integer. Then as $b \to \infty$, we have

$$\sum_{i=0}^{b} \frac{1}{\sqrt{i^2 + (b-i)^2}} \sim \sqrt{2} \log \left(1 + \sqrt{2}\right). \tag{6}$$

Proof. Since $g(x) = 1/\sqrt{x^2 + (1-x)^2}$ is a continuous and concave function on the closed interval [0,1], it has the Riemann integral, which implies that

$$\int_0^1 g(x)dx \sim \frac{1}{b} \sum_{i=0}^b \frac{1}{\sqrt{(\frac{i}{b})^2 + (\frac{b-i}{b})^2}} = \sum_{i=0}^b \frac{1}{\sqrt{i^2 + (b-i)^2}}.$$

Since $\int_0^1 g(x)dx = \sqrt{2}\log(1+\sqrt{2})$, we obtain the desired result.

In the next lemma we evaluate the contribution of the edges of the path to the sum-Balaban index.

Lemma 6. For a balanced dumbbell graph $D_{a,b}$ the following holds

$$\sum_{i=0}^{b-2} \frac{1}{\sqrt{w(v_i) + w(v_{i+1})}} \sim \sum_{i=0}^{b} \frac{1}{\sqrt{i^2 + (b-i)^2}}.$$

Proof. Let $v_i v_{i+1}$ be an edge of P_b . Denote $w_i^+ = \max\{w(v_i), w(v_{i+1})\}$ and $w_i^- = \min\{w(v_i), w(v_{i+1})\}$. Then $\frac{1}{\sqrt{2w_i^+}} \le \frac{1}{\sqrt{w(v_i) + w(v_{i+1})}} \le \frac{1}{\sqrt{2w_i^-}}$. Therefore

$$\sum_{i=0}^{b-2} \frac{1}{\sqrt{2w_i^+}} \le \sum_{i=0}^{b-2} \frac{1}{\sqrt{w(v_i) + w(v_{i+1})}} \le \sum_{i=0}^{b-2} \frac{1}{\sqrt{2w_i^-}}.$$

We have

Note that $\sum_{i=0}^{b} \frac{1}{\sqrt{i^2+(b-i)^2}}$ is of order $\Theta(1)$ by Proposition 5. Also notice that the two isolated terms in the above expressions are of order $O(n^{-1})$. Therefore, $\sum_{i=0}^{b-2} \frac{1}{\sqrt{2w_i^+}} \sim \sum_{i=0}^{b} \frac{1}{\sqrt{i^2+(b-i)^2}}$. Analogously we get

$$\sum_{i=0}^{b-2} \frac{1}{\sqrt{2w_i^-}} = \sum_{i=0}^{b} \frac{1}{\sqrt{2w(v_i)}} - \frac{1}{\sqrt{2w(v_0)}} + \frac{1}{\sqrt{2w(v_{\lfloor \frac{b}{2} \rfloor})}} - \frac{1}{\sqrt{2w(v_{b-1})}} - \frac{1}{\sqrt{2w(v_{b-1})}} - \frac{1}{\sqrt{2w(v_b)}} \sim \sum_{i=0}^{b} \frac{1}{\sqrt{i^2 + (b-i)^2}}.$$

This establishes the lemma.

Now we can prove the main result of the paper.

Theorem 7. Let $D_{a,b}$ 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 $\sqrt[4]{\sqrt{2}\log(1+\sqrt{2})}\sqrt{n}$ and n, respectively. That is, $a = \sqrt[4]{\sqrt{2}\log(1+\sqrt{2})}\sqrt{n} + o(\sqrt{n})$ and b = n - o(n).

Proof. Let $D_{a,b}$ be a balanced dumbbell graph on n vertices with the minimum value of sum-Balaban index. By Proposition 4, $SJ(D_{a,b}) \in O(1)$. We study the behaviour of a = a(n) in the following two claims. First notice that since a(n) < n, we have $a \in O(n)$. Therefore if $a \in \Omega(n)$, then $a \in O(n)$.

Claim 1. It holds $a \in o(n)$.

Suppose that the claim is false. Then there is a subsequence $\{a(n_i)\}_{i=1}^{\infty}$ which is in $\Theta(n)$. By Lemma 3, we have $w(u) \sim \frac{b^2}{2} + ab + 2a = w^*(u)$, where u is a vertex of K_a or K_a' , and $w(v_i) \sim \frac{i^2}{2} + \frac{(b-i)^2}{2} + ab + a = w^*(v_i)$ for $v_i \in V(P_b)$. Since $\frac{b^2}{4} \leq \frac{i^2}{2} + \frac{(b-i)^2}{2} \leq \frac{b^2}{2}$, for every vertex x it holds

$$\frac{b^2}{4} + ab + a \le w^*(x) \le \frac{b^2}{2} + ab + 2a.$$

Consequently, for every edge xy we have

$$\sqrt{\frac{b^2}{2} + 2ab + 2a} \le \sqrt{w^*(x) + w^*(y)} \le \sqrt{b^2 + 2ab + 4a}.$$

Hence, for every edge xy there exist values $c_{xy}^b \in [\frac{1}{2}, 1]$ and $c_{xy}^a \in [2, 4]$ such that $\sqrt{w^*(x) + w^*(y)} = \sqrt{c_{xy}^b b^2 + 2ab + c_{xy}^a a}$. Then

$$\frac{1}{\sqrt{w(x) + w(y)}} \sim \frac{1}{\sqrt{c_{xy}^b b^2 + 2ab + c_{xy}^a a}},$$

and analogously as in the proof of Proposition 4 we get

$$\sum_{xy \in E(D_{a,b})} \frac{1}{\sqrt{w(x) + w(y)}} \sim \frac{a^2 + b}{\sqrt{c^b b^2 + 2ab + c^a a}},$$

where c^b and c^a are some values such that $c^b \in [\frac{1}{2}, 1]$ and $c^a \in [2, 4]$. Estimating m/(m-n+2) analogously as in (5) we get

$$SJ(D_{a,b}) \sim \frac{a^2 + b}{a^2} \cdot \frac{a^2 + b}{\sqrt{c^b b^2 + 2ab + c^a a}}.$$
 (7)

Since $b \leq n$, the numerator in (7) is of order n^4 , while the denominator is of order at most n^3 . This gives that for our sequence of n's, $\{n_i\}_{i=1}^{\infty}$,

 $J(D_{a,b}) \to \infty$. However, by Proposition 4, for the very same subsequence $\{n_i\}_{i=1}^{\infty}$ we have already derived that $J(D_{a,b}) \in O(1)$, which is a contradiction that establishes the claim.

With the next claim we go further and determine the asymptotic order of a(n).

Claim 2. It holds $a \in \Theta(\sqrt{n})$.

By Claim 1, for every positive constant k we have a(n) < kn for all n big enough. Since 2a + b = n, we get b > n - 2kn for all n big enough and consequently $b \in \Theta(n)$. We proceed analogously as in Case 1. By the property of $\{a(n)\}_{n=1}^{\infty}$, we get $w(u) = \frac{b^2}{2} + ab + \frac{b}{2} + 2a - 1 \sim \frac{b^2}{2}$ if u is a vertex of K_a or K'_a , while $w(v_i) = \frac{i^2}{2} + \frac{(b-i)^2}{2} + ab - \frac{b}{2} + i + a \sim \frac{i^2}{2} + \frac{(b-i)^2}{2}$ for $v_i \in V(P_b)$. Hence, analogously as in the proof of Proposition 4 we get

$$SJ(D_{a,b}) \sim \frac{a^2 + b}{a^2} \cdot \frac{a^2 + b}{c^b \cdot b} = \frac{1}{c^b} \left[\frac{a^2}{b} + 2 + \frac{b}{a^2} \right], \tag{8}$$

where c^b is a value such that $\frac{1}{\sqrt{2}} \leq c^b \leq 1$. Recall that a = a(n). Then the terms in brackets of (8) are in $\Theta\left(\frac{a^2(n)}{n}\right)$, $\Theta(1)$, $\Theta\left(\frac{n}{a^2(n)}\right)$, respectively, and the order of $\mathrm{SJ}(D_{a,b})$ is the maximum order of these three terms. Since the second term is in $\Theta(1)$, we have $\mathrm{SJ}(D_{a,b}) \in \Omega(1)$. But in the case $J(D_{a,b}) \in \Theta(1)$ we have $a^2(n) \in O(n)$ from the first term and $a^2(n) \in \Omega(n)$ from the third term. This gives $a(n) \in \Theta(\sqrt{n})$, which establish the claim.

By Claim 2, there are positive constants c_1 and c_2 such that $c_1\sqrt{n} \le a \le c_2\sqrt{n}$ for each large enough n. Hence, for n big enough $a = c\sqrt{n}$, where c = c(n) is in $[c_1, c_2]$, and $b \sim n$. In the rest of the proof we determine c = c(n). In order to do this, we need a more precise calculation of $\mathrm{SJ}(D_{a,b})$.

Let uv be an edge of $D_{a,b}$. Then it is either in one of the two complete graphs on a+1 vertices, in which case $w(u) \sim w(v) \sim \frac{b^2}{2}$, or it is an edge of the path P_b , say $u=v_i$ and $v=v_{i+1}$, in which case $w(v_i) \sim \frac{1}{2}[i^2+(b-i)^2]$ and $w(v_{i+1}) \sim \frac{1}{2}[(i+1)^2+(b-i-1)^2]$. There are $2\binom{a+1}{2}$ edges of the first type and they contribute $(a^2+a)\cdot \frac{1}{b} \sim \frac{a^2}{b}$ to $\sum_{uv\in E(D_{a,b})} \frac{1}{\sqrt{w(u)+w(v)}}$. By Lemma 6 and Proposition 5, the contribution of edges of P_b is

$$\sum_{i=0}^{b-2} \frac{1}{\sqrt{w(v_i) + w(v_{i+1})}} \sim \sqrt{2} \log (1 + \sqrt{2}).$$

Denote $Q = \sqrt{2} \log \left(1 + \sqrt{2}\right)$. Since $m \sim a^2 + b$ and $m - n + 2 \sim a^2$, we get $\mathrm{SJ}(D_{a,b}) \sim \frac{a^2 + b}{a^2} \left(\frac{a^2}{b} + Q\right)$.

Recall that $a \sim c\sqrt{n}$ while $b \sim n$. Hence,

$$SJ(D_{a,b}) \sim \frac{c^2 + 1}{c^2} \cdot (c^2 + Q) = c^2 + 1 + Q + \frac{Q}{c^2}.$$
 (9)

Now setting $c^2 = x$ and differentiating the above expression we see that $SJ(D_{a,b})$ is minimum if $c^2 = \sqrt{Q}$, that is if $c = \sqrt[4]{\sqrt{2}\log(1+\sqrt{2})}$.

Observe that for Balaban index we have an analogue of Theorem 7, but the value of c is different. Balanced dumbbell graphs with the minimum value of Balaban index have $a \sim c\sqrt{n}$, where $c = \sqrt[4]{\pi/2} \doteq 1.1195$, see [14], while those with the minimum value of sum-Balaban index have $a \sim c\sqrt{n}$, where $c \doteq 1.0566$, by Theorem 7.

Substituting $c = \sqrt[4]{\sqrt{2} \log (1 + \sqrt{2})}$ in (9), Theorem 7 yields the following corollary.

Corollary 8. Let D be a balanced dumbbell graph on n vertices, where n is big enough, with the minimum value of sum-Balaban index. Then

$$SJ(D) \doteq 4.47934.$$

Comparing Corollary 8 with the lower bound presented in Theorem 2, we see that the asymptotic value of sum-Balaban index for optimum balanced dumbbell graph is only about 1.12 times higher than our lower bound. Our expectation is that the optimal balanced dumbbell graph is not much different from the optimal dumbbell graph. Namely, we have the following conjectures.

Conjecture 9. Among all dumbbell graphs $D_{a,b,a'}$ on at least 14 vertices, the minimum value of sum-Balaban index is achieved for one with a' = a or a' = a + 1.

The reason for the assumption that $n \geq 14$ in the above conjecture is that $D_{2,7,4}$ has the lowest sum-Balaban index among all dumbbell graphs on 13 vertices.

Conjecture 10. Among all dumbbell graphs $D_{a,b,a'}$ on n vertices, the minimum is achieved for one with $a = \sqrt[4]{\sqrt{2}\log(1+\sqrt{2})}\sqrt{n} + o(\sqrt{n})$, $a' = \sqrt[4]{\sqrt{2}\log(1+\sqrt{2})}\sqrt{n} + o(\sqrt{n})$ and b = n - o(n).

5 Dumbbell-like graphs

Dumbbell-like graph are obtained from dumbbell graphs by removing or attaching some edges from or to the cliques. As shown in [14], they may have slightly smaller Balaban index, so we are using the same approach with sum-Balaban index to see if this is true also for sum-Balaban index.

We start with a precise definition. A dumbbell-like graph, $D_{a,b,a'}^{\ell}$, is obtained from the dumbbell graph $D_{a,b,a'}$ by either inserting ℓ edges between v_1 and K_a if $\ell > 0$, or by removing $-\ell$ edges between v_{b-1} and $K'_{a'}$ if $\ell < 0$. Note that we assume $a \leq a'$, so we always add edges to the smaller clique and remove them from the bigger one. In [14] it was conjectured that dumbbell-like graphs $D_{a,b,a'}^{\ell}$ attain the minimum value of Balaban index. Experiments show that this happens in the cases a = a' or a = a' + 1, $a \in \Theta(\sqrt{n})$.

This approach together with Conjecture 9 suggests the following two-step process for finding graphs with the minimum sum-Balaban index.

- (i) For a given n find parameters a, b, a', where a + b + a' = n and $a \le a' \le a + 1$, such that $D_{a,b,a'}$ has the smallest sum-Balaban index.
- (ii) Find ℓ such that $D_{a,b,a'}^{\ell}$ has the smallest value of sum-Balaban index.

The outcome of the two-step process for n satisfying $190 \le n \le 210$ is presented in Table 1. In this table we present also the values of sum-Balaban index for optimal dumbbell and dumbbell-like graphs.

With the exception of n = 13, for all $n \le 210$ the smallest value of sum-Balaban index for optimal dumbbell graph is obtained when $a \le a' \le a + 1$. Case n = 13 is special, since $D_{2,7,4}$ has indeed lower sum-Balaban index than $D_{3,6,4}$. But even in this case our two-step process finds the optimal dumbbell-like graph on 13 vertices.

We conclude the paper with the following conjecture, which is supported by our computer experiments.

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

For further recent topics and open problems in chemical graph theory an interested reader is referred to [2, 9, 13, 16, 19, 22]. The quantitative graph measures are used also elsewhere, for example, in nowadays popular large networks, some results of the authors in that direction one can find in [23].

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6 Figures

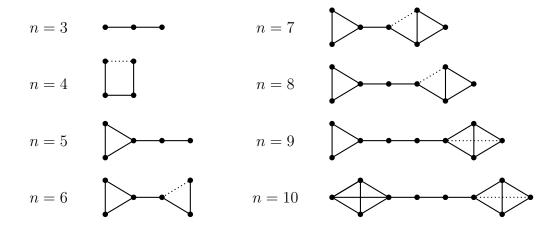


Figure 1: Graphs with the smallest value of sum-Balaban index for $n \in \{3, 4, \dots, 10\}$.

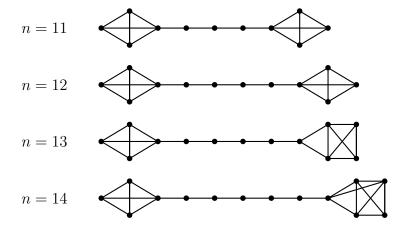


Figure 2: Candidates for the smallest value of sum-Balaban index for $n \in \{11, 12, 13, 14\}$.

7 Tables

n	a	a'	b	$J(D_{a,b,a'})$	ℓ	$J(D_{a,b,a'}^{\ell})$
190	14	15	161	4.6411	-5	4.6405
191	14	15	162	4.6405	-3	4.6401
192	14	15	163	4.6399	-2	4.6397
193	14	15	164	4.6394	-1	4.6393
194	14	15	165	4.6389	0	4.6389
195	14	15	166	4.6386	1	4.6385
196	14	15	167	4.6383	2	4.6381
197	14	15	168	4.6381	3	4.6377
198	14	15	169	4.6379	4	4.6373
199	14	15	170	4.6379	6	4.6369
200	14	15	171	4.6379	7	4.6365
201	15	15	171	4.6372	-6	4.6361
202	15	15	172	4.6364	-5	4.6357
203	15	15	173	4.6357	-4	4.6353
204	15	15	174	4.6351	-3	4.6349
205	15	15	175	4.6346	-2	4.6345
206	15	15	176	4.6341	0	4.6341
207	15	15	177	4.6337	0	4.6337
208	15	15	178	4.6334	0	4.6334
209	15	15	179	4.6331	1	4.6331
210	15	15	180	4.6329	3	4.6328

Table 1: The optimal dumbbell graph $D_{a,b,a'}$ on $n \in [190,210]$ vertices, and its improvement $D_{a,b,a'}^{\ell}$ in the class of dumbbell-like graphs.