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Convexity result and trees with large Balaban index

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Abstract

Balaban index is defined as $J(G) = \frac{m}{m-n+2}\sum \frac{1}{\sqrt{w(u)\cdot w(v)}}$, 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 2011, H. Deng found an interesting property that Balaban index is a convex function in double stars. We show that this holds surprisingly to general graphs by proving that attaching leaves at two vertices in a graph yields a new convexity property of Balaban index. We demonstrate this property by finding, for each n, seven trees with the maximum value of Balaban index, and we conclude the paper with an interesting conjecture.

1 Introduction

In this paper we consider simple and connected graphs. For a graph G, by $V(G)$ and $E(G)$ we denote the vertex and the edge sets of G, respectively. We set $n = |V(G)|$ and $m = |E(G)|$. For vertices $u, v \in V(G)$ we use $\mathrm{dist}_G(u,v)$ to denote the minimal distance from u to v in G, and for $x \in V(G)$, we have $w(x) = \sum_{y\in V(G)} \mathrm{dist}_G(x,y)$.

The *Balaban index* $J(G)$ of a graph G is defined as

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

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where the sum is taken over all edges of G. It was introduced by Balaban in [2, 3] and it was used successfully in QSAR/QSPR modeling [9, 27], see also [5, 15]. Recent papers on mathematical properties of this index include [7, 12, 13, 18, 23]. For further recent topics and open problems in chemical graph theory an interested reader is referred to [1, 6, 17, 19, 25, 28].

It is known, that among graphs on $n \geq 8$ vertices, Balaban index attains its maximum for the star on n vertices S_n, and for graphs on $n \leq 7$ vertices, Balaban index attains its maximum for the complete graph K_n, see [11] and [21]. The problem of finding the minimum value of Balaban index among graphs of given order is much more difficult and it remains open. However, in [16] it was shown that this value is of order $\Theta(n^{-1})$, and the structure of candidates for extremal graphs is discussed. In [18], an upper bound for Balaban index of r-regular graphs on n vertices was given, which led to the observation that the minimum value of Balaban index in the class of graphs on n vertices tends to zero as n increases. The asymptotic behavior of J was discussed in [4] and recently in [20], where it was shown that in fact for an arbitrary positive number r there exists a sequence of graphs whose Balaban index converges to r.

From mathematical aspect, one's aim is to determine the extremal values of indices in various classes of graphs. The class of trees is interesting especially from the point of view of chemists. It was shown by Sun [26], Dong and Guo [10], and Deng [8] that for a tree T on n vertices, $n \geq 2$,

$$J(P_n) \leq J(T) \leq J(S_n)$$

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. Let $D_{n-2,2}$ be a tree obtained from S_{n-1} by subdividing one edge. In [8], Deng proved that $D_{n-2,2}$ has the second maximum value of Balaban index among trees.

Theorem 1. *Let T be a tree with $n \geq 4$ vertices. If T is not a star, then $J(T) \leq J(D_{n-2,2})$ with equality if and only if $J(T) = J(D_{n-2,2})$.*

To prove the above mentioned results, the authors used so called *edge-lifting* and *path-sliding* transformations, which both increase Balaban index.

Theorem 2. *Let G_1 and G_2 be two graphs with n_1 and n_2 vertices, respectively, $n_1, n_2 \geq 2$. If G is the graph obtained from G_1 and G_2 by adding an edge between a vertex u^* of G_1 and a vertex v^* of G_2, G' is the graph obtained by identifying u^* of G_1 to v^* of G_2 and adding a pendant edge to $u^*(v^*)$, then G' is called the edge-lifting transformation of G and we have $J(G) < J(G')$.*

Theorem 3. *Let G_0 be a graph with $n_0 \geq 2$ vertices, and $P = v_1v_2 \ldots v_r$ a path of length $r-1 \geq 2$. If G (resp. G') is the graph obtained by identifying a vertex v^* of G_0 to v_{k-1} (resp. v_k) in P, $2 \leq k \leq \lfloor \frac{r-1}{2} \rfloor$, then G' is called the path-sliding transformation of G and we have $J(G) < J(G')$.*

Using these transformations, together with an interesting convexity property of Balaban index which we prove in the next section, we find trees with the third, fourth, ... and seventh maximum value of Balaban index. We remark that for n big enough, in [14] the authors find first 21 trees with the largest value of Balaban index. However, their proofs are very technical, hard to follow and too many details are left to the reader. Our proofs are much more precise, less technical, we do not restrict ourselves to large n and we conclude the paper with interesting conjectures. Moreover, we expect that the convexity property which we describe in the paper, will appear useful in studying Balaban index in the future.

2 Convexity result for Balaban index

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, see Figure 1 for $D_{n-2,2}$. By symmetry, we may assume that $a > b$. The following result was proved in [8].

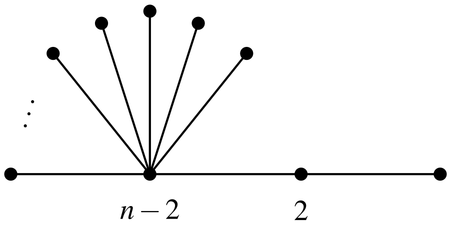

Fig. 1 A double star $D_{n-2,2}$.

Theorem 4. *$J(D_{n-x,x})$, as a function of x, is convex.*

It should be noted that in the proof of Deng the function $J(D_{n-x,x})$ is defined in such a way that it is a continuous function, and the second derivative is used to show that it is convex. In what follows we will show that Theorem 4 can be generalized. For that we need the notion of a discrete convex function. This concept can be introduced in several different ways (an interested reader should consult [24]), but generally a (discrete) function f is *strictly convex* if for every $x_0 < x_1 < x_2$ from the domain of f it holds

$$f(x_1) < \frac{x_2 - x_1}{x_2 - x_0} f(x_0) + \frac{x_1 - x_0}{x_2 - x_0} f(x_2).$$

However, if the domain is the set of integers greater than or equal to b, then the above property is equivalent to

$$2f(x_0+1) < f(x_0) + f(x_0+2)$$

for all $x_0 \geq b$.

Theorem 5. *Let G be a graph with two distinct vertices u^* and v^*. Let $a \geq 2$ and $0 \leq x \leq a$. Attach x pendant edges to u^*, attach $a-x$ pendant edges to v^*, and denote the resulting graph by G_x. Then $J(G_x)$, as a (discrete) function of x, is strictly convex.*

Proof. As mentioned above, it suffices to prove that $J(G_x) + J(G_{x+2}) > 2J(G_{x+1})$ for every x, $0 \leq x \leq a-2$. Therefore, it is sufficient to restrict ourselves to the case $a = 2$ and to prove $J(G_0) + J(G_2) > 2J(G_1)$.

Further, since all the graphs G_x, $0 \leq x \leq 2$, have the same number of vertices and edges, it suffices to prove the strict convexity of $\sum_{uv \in E(G_x)} \frac{1}{\sqrt{w_{G_x}(u) \cdot w_{G_x}(v)}}$. We divide the proof into two claims.

Claim 1. *Let $uv \in E(G)$. Then $\frac{1}{\sqrt{w_{G_x}(u) \cdot w_{G_x}(v)}}$, as a function of x, is strictly convex.*

Denote $c = w_{G_1}(u)$ and $d = w_{G_1}(v)$. Further, denote $\gamma = w_{G_1}(u) - w_{G_0}(u)$ and $\delta = w_{G_1}(v) - w_{G_0}(v)$. Then $w_{G_0}(u) = c - \gamma$ and $w_{G_0}(v) = d - \delta$. Since γ (δ, respectively) is the difference corresponding to removing a pendant edge from v^* and adding it to u^*, we have $w_{G_2}(u) = c + \gamma$ and $w_{G_2}(v) = d + \delta$. Hence, we need to prove

$$\frac{1}{\sqrt{w_{G_0}(u) \cdot w_{G_0}(v)}} + \frac{1}{\sqrt{w_{G_2}(u) \cdot w_{G_2}(v)}} > \frac{2}{\sqrt{w_{G_1}(u) \cdot w_{G_1}(v)}},$$

which is equivalent to

$$\frac{1}{\sqrt{(c-\gamma)(d-\delta)}} + \frac{1}{\sqrt{(c+\gamma)(d+\delta)}} > \frac{2}{\sqrt{cd}}. \tag{1}$$

Observe that $c, d > 0$, but γ and δ can be negative. Anyway, since $c - \gamma = w_{G_0}(u) > 0$ and $c + \gamma = w_{G_2}(u) > 0$, we have $c - |\gamma| > 0$. Analogously $d - |\delta| > 0$, and so

$$\begin{aligned} \sqrt{c^2 d^2} &> \sqrt{(c^2-\gamma^2)(d^2-\delta^2)} \\ cd &> \sqrt{(c+\gamma)(c-\gamma)(d+\delta)(d-\delta)} \\ 2\sqrt{(c+\gamma)(c-\gamma)(d+\delta)(d-\delta)} \cdot cd &> 2(c+\gamma)(c-\gamma)(d+\delta)(d-\delta). \end{aligned} \tag{2}$$

Now suppose that $|c\delta| \geq |d\gamma|$. (The case $|d\gamma| \geq |c\delta|$ can be proved analogously since the resulting formula is symmetric, see below.) Then, regardless if $c\delta$ is positive or negative, we have

$$c\delta(c\delta + d\gamma) \geq 0.$$

Since $d^2 - \delta^2 > 0$, see above, we have

$$\begin{aligned}(d^2-\delta^2)\gamma^2 + c\delta(c\delta+d\gamma) &> 0\\ d^2\gamma^2 - \delta^2\gamma^2 + c^2\delta^2 + cd\gamma\delta &> 0\\ 2c^2d^2 + 2cd\gamma\delta &> 2c^2d^2 - 2c^2\delta^2 - 2d^2\gamma^2 + 2\gamma^2\delta^2\\ (c+\gamma)(d+\delta)cd + (c-\gamma)(d-\delta)cd &> 2(c+\gamma)(d+\delta)(c-\gamma)(d-\delta). \end{aligned} \tag{3}$$

Summing (2) and (3) gives

$$\left(\sqrt{(c+\gamma)(d+\delta)}\sqrt{cd} + \sqrt{(c-\gamma)(d-\delta)}\sqrt{cd}\right)^2 > \left(2\sqrt{(c+\gamma)(d+\delta)}\sqrt{(c-\gamma)(d-\delta)}\right)^2,$$

which is equivalent to (1). This establishes the claim.

Claim 2. *Function* $\displaystyle\sum_{uv\in E(G_x)\setminus E(G)} \frac{1}{\sqrt{w_{G_x}(u)\cdot w_{G_x}(v)}}$ *is strictly convex.*

Let $d_G(u^*, v^*) = l$. Denote $c = w_G(u^*)$ and $d = w_G(v^*)$. Then $w_{G_1}(u^*) = c+1+l+1$, $w_{G_2}(u^*) = c+2$, $w_{G_0}(v^*) = d+2$ and $w_{G_1}(v^*) = d+l+2$. Further, denote by u' a pendant vertex attached to u^* and denote by v' a pendant vertex attached to v^*. If $|V(G)| = t$, then $w_{G_1}(u') = c+l+t+2$, $w_{G_2}(u') = c+t+2$, $w_{G_0}(v') = d+t+2$ and $w_{G_1}(v') = d+l+t+2$. Denote $g(x) = \displaystyle\sum_{uv\in E(G_x)\setminus E(G)} \frac{1}{\sqrt{w_{G_x}(u)\cdot w_{G_x}(v)}}$. Then

$$\begin{aligned} g(0) &= \frac{2}{\sqrt{(d+2)(d+t+2)}},\\ g(1) &= \frac{1}{\sqrt{(c+l+2)(c+l+t+2)}} + \frac{1}{\sqrt{(d+l+2)(d+l+t+2)}},\\ g(2) &= \frac{2}{\sqrt{(c+2)(c+t+2)}}. \end{aligned}$$

Since $l \geq 1$, we have

$$\begin{aligned} \frac{2}{\sqrt{(d+2)(d+t+2)}} &> \frac{2}{\sqrt{(d+l+2)(d+l+t+2)}}\\ \frac{2}{\sqrt{(c+2)(c+t+2)}} &> \frac{2}{\sqrt{(c+l+2)(c+l+t+2)}} \end{aligned}$$

and summing the two inequalities above gives $g(0) + g(2) > 2g(1)$ as required. This establishes the claim.

Claims 1 and 2 assure that $\sum_{uv\in E(G_x)} \frac{1}{\sqrt{w_{G_x}(u)\cdot w_{G_x}(v)}}$ is a strictly convex function, since the sum of strictly convex functions is a strictly convex function. Thus the claim of the theorem follows.

We remark that the fact that S_n and $D_{n-2,2}$ are trees of order n with the largest and second largest, respectively, Balaban index is a direct consequence of Theorem 5.

Let ν be an invariant on the class of trees. We say that ν is *star-convex*, if for every tree G with two specific vertices u^* and v^* and for every $a \geq 2$, the invariant ν is strictly convex on G_x, which is obtained from G by attaching x pendant edges to u^* and $a-x$ pendant edges to v^*. Further, if $\nu(T') > \nu(T)$ when T' is obtained from T by path-sliding or edge-lifting, and moreover ν is star-convex, then we say that ν has *SLC-property* (which is a short notation for *sliding-lifting-convexity property*). By Theorems 2, 3 and 5, Balaban index has the SLC-property. We remark that also the sum-Balaban index has the SLC-property, see [22].

3 Trees with large Balaban index

In what follows, by T_i^ν we denote a tree which has the i-th greatest value of invariant ν. We omit the superscript ν in the case when ν is the Balaban index. As described in the introduction, $T_1 = S_n$ and $T_2 = D_{n-2,2}$. Here we determine T_3, T_4, T_5, T_6 and T_7. In every case, using the fact that Balaban index has SLC-property we first reduce the class of possible candidates, and then we determine the optimum one.

As we will see later, a double star $D_{n-t,t}$ is one of the candidates in every case. There are four orbits of vertices in $D_{n-t,t}$ with values of w equal to $2n+t-4$, $n+t-2$, $2n-t-2$ and $3n-t-4$, thus the following holds.

Lemma 6. *For $t \geq 2$ we have*

$$J(D_{n-t,t}) = (n-1)\left(\frac{n-t-1}{\sqrt{(2n+t-4)(n+t-2)}} + \frac{1}{\sqrt{(n+t-2)(2n-t-2)}} + \frac{t-1}{\sqrt{(2n-t-2)(3n-t-4)}}\right).$$

A *caterpillar* $H_{a_1,a_2,\ldots,a_{d-1}}$ is 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 $1, a_1, a_2, \ldots, a_{d-1}, 1$. 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 an example.

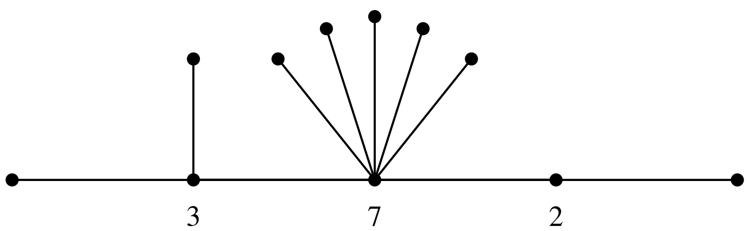

Fig. 2 A caterpillar $H_{3,7,2}$.

First we find T_3. Notice that there is only one tree on 3 vertices and only two trees on 4 vertices. Thus only the cases when $n \geq 5$ are considered when searching for T_3.

Lemma 7. *Let ν be an invariant with SLC-property. If $\{T_1^\nu, T_2^\nu\} = \{S_n, D_{n-2,2}\}$, then $T_3^\nu \in \{D_{n-3,3}, H_{2,n-3,2}\}$.*

Proof. Since edge-lifting reduces the diameter at most by 1, it suffices to consider trees with diameters 3 and 4. Since ν is star-convex, the only candidate among trees of diameter 3 is $D_{n-3,3}$.

As regards trees of diameter 4, due to edge-lifting it suffices to consider those whose vertices of degrees at least 2 form a path, i.e., the caterpillars. Hence, we have to consider caterpillars $H_{a,b,c}$. Observe that all a, b and c are at least 2. However, if at least two from a, b and c are at least 3, then $\nu(H_{a,b,c}) < \nu(D_{n-3,3})$ due to edge-lifting. Moreover, $\nu(H_{n-3,2,2}) < \nu(H_{2,n-3,2})$ due to path-sliding if $n \geq 6$, while if $n = 5$ then $H_{2,n-3,2} = H_{n-3,2,2}$. Therefore, $T_3^\nu \in \{D_{n-3,3}, H_{2,n-3,2}\}$.

Now we can state the result for T_3.

Proposition 8. *The following holds:*

$$T_3 = \begin{cases} P_5, & \text{if } n = 5 \\ D_{n-3,3}, & \text{if } n \geq 6. \end{cases}$$

Proof. Since $\{T_i; 1 \leq i \leq 2\} = \{S_n, D_{n-2,2}\}$ and the Balaban index has SLC-property, it suffices to compare $J(D_{n-3,3})$ and $J(H_{2,n-3,2})$, by Lemma 7. Since for $n = 5$ the graph $D_{n-3,3}$ with $n-3 \geq 3$ does not exist (observe that $D_{n-3,3}$ should be $D_{3,2}$, which is T_2 in this case), we have $T_3 = H_{2,2,2} = P_5$. In what follows we assume $n \geq 6$.

By Lemma 6 we have

$$J(D_{n-3,3}) = (n-1)\left(\frac{2}{\sqrt{(3n-7)(2n-5)}} + \frac{1}{\sqrt{(2n-5)(n+1)}} + \frac{n-4}{\sqrt{(n+1)(2n-1)}}\right).$$

In $H_{2,n-3,2}$ there are also four orbits of vertices with value of w equal to $3n-5$, $2n-3$, $n+1$ and $2n-1$. Therefore

$$J(H_{2,n-3,2}) = (n-1)\left(\frac{2}{\sqrt{(3n-5)(2n-3)}} + \frac{2}{\sqrt{(2n-3)(n+1)}} + \frac{n-5}{\sqrt{(n+1)(2n-1)}}\right).$$

Since $f(x) = \frac{1}{\sqrt{x}}$ is a convex function, we have $\frac{1}{\sqrt{2n-5}} + \frac{1}{\sqrt{2n-1}} > \frac{2}{\sqrt{2n-3}}$, and so

$$\frac{1}{\sqrt{(2n-5)(n+1)}} + \frac{1}{\sqrt{(2n-1)(n+1)}} > \frac{2}{\sqrt{(2n-3)(n+1)}}.$$

Since $\frac{2}{\sqrt{(3n-7)(2n-5)}} > \frac{2}{\sqrt{(3n-5)(2n-3)}}$, we get $J(D_{n-3,3}) > J(H_{2,n-3,2})$. Thus for $n \geq 6$, $D_{n-3,3}$ is a tree with the third maximum value of Balaban index.

In the sequel, we will refer to the following two facts from calculus.

Lemma 9. *Let a, b, c, d, and e, be constants such that $b,d > 0$. Then,*

$$\lim_{n\to\infty} \frac{n+a}{\sqrt{(bn+c)(dn+e)}} = \frac{1}{\sqrt{bd}}. \tag{4}$$

Lemma 10. *Let a, b, c, d, e, and f be constants. Then,*

$$\lim_{n\to\infty}(n+a)\left(\frac{n+b}{\sqrt{(n+c)(2n+d)}} - \frac{n+b}{\sqrt{(n+e)(2n+f)}}\right) = \frac{2(e-c)+(f-d)}{4\sqrt{2}}. \tag{5}$$

Proof. Starting from the left side, we derive

$$\begin{aligned}
&\lim_{n\to\infty}(n+a)\left(\frac{n+b}{\sqrt{(n+c)(2n+d)}} - \frac{n+b}{\sqrt{(n+e)(2n+f)}}\right)\\
&= \lim_{n\to\infty} \frac{(n+a)(n+b)}{\sqrt{(n+c)(2n+d)(n+e)(2n+f)}} \cdot \lim_{n\to\infty}\left(\sqrt{(n+e)(2n+f)} - \sqrt{(n+c)(2n+d)}\right)\\
&= \frac{1}{2}\lim_{n\to\infty} \frac{(n+e)(2n+f)-(n+c)(2n+d)}{\sqrt{(n+e)(2n+f)} + \sqrt{(n+c)(2n+d)}}\\
&= \frac{2(e-c)+(f-d)}{4\sqrt{2}}.
\end{aligned}$$

When searching for T_4, T_5 and T_6, we assume that n is at least 6, since otherwise there are less than 4 non-isomorphic trees and T_4 does not exist.

Lemma 11. *Let ν be an invariant with SLC-property. If $\{T_1^\nu, T_2^\nu, T_3^\nu\} = \{S_n, D_{n-2,2}, D_{n-3,3}\}$, then $T_4^\nu \in \{D_{n-4,4}, H_{2,n-3,2}\}$.*

Proof. Analogously as in Lemma 7, when looking for T_4^ν one has to consider $D_{n-4,4}$ and caterpillars $H_{a,b,c}$. However, if at least two from a,b,c are at least 4, then $\nu(H_{a,b,c}) < \nu(D_{n-4,4})$ due to edge-lifting. Similarly, if $a \geq 4$ and one of b,c is at least 3, then $\nu(H_{a,b,c}) < \nu(D_{n-4,4})$ due to edge-lifting. Therefore it suffices to consider $D_{n-4,4}$, $H_{2,n-3,2}$, $H_{3,n-4,2}$, $H_{3,n-5,3}$ and $H_{n-3,2,2}$. However, $\nu(H_{n-3,2,2}) < \nu(H_{2,n-3,2})$ due to path-sliding. Further, $\nu(D_{4,n-4}) + \nu(H_{3,n-4,2}) > 2\nu(H_{3,n-4,2})$ due to star-convexity, and so $\nu(D_{n-4,4}) > \nu(H_{3,n-4,2})$. Finally, $2\nu(H_{4,n-5,2}) > 2\nu(H_{3,n-5,3})$ due to star-convexity and $\nu(D_{n-4,4}) > \nu(H_{4,n-5,3})$ due to edge-lifting, which means that $\nu(D_{n-4,4}) > \nu(H_{3,n-5,3})$. Therefore, $T_4^\nu \in \{D_{n-4,4}, H_{2,n-3,2}\}$.

Proposition 12. *The following holds:*

$$T_4 = \begin{cases} D_{4,4}, & \textit{if } n = 8 \\ H_{2,n-3,2}, & \textit{if } n \geq 6, n \neq 8. \end{cases}$$

Proof. Since for $n \geq 6$ we have $\{T_i;\ 1 \leq i \leq 3\} = \{S_n, D_{n-2,2}, D_{n-3,3}\}$ and the Balaban index has SLC-property, it suffices to compare $J(H_{2,n-3,2})$ and $J(D_{n-4,4})$, by Lemma 11. As described in the proof of Proposition 8,

$$J(H_{2,n-3,2}) = (n-1)\left(\frac{2}{\sqrt{(3n-5)(2n-3)}} + \frac{2}{\sqrt{(2n-3)(n+1)}} + \frac{n-5}{\sqrt{(n+1)(2n-1)}}\right),$$

and by Lemma 6,

$$J(D_{n-4,4}) = (n-1)\left(\frac{3}{\sqrt{(3n-8)(2n-6)}} + \frac{1}{\sqrt{(2n-6)(n+2)}} + \frac{n-5}{\sqrt{(n+2)2n}}\right).$$

Since there is no $D_{n-4,4}$ for $n \leq 7$, we have $T_4 = H_{2,n-3,2}$ if $6 \leq n \leq 7$. For $n \geq 9$, the following holds:

$$J(H_{2,n-3,2}) > J(D_{n-4,4}), \tag{6}$$

which implies that $T_4 = H_{2,n-3,2}$, for $n \geq 9$. Note that showing (6) analytically would be extremely long and tedious and we would like to omit such a proof here. In order to convince the reader we show that the difference $J(H_{2,n-3,2}) - J(D_{n-4,4})$ tends to a positive constant. By (4) and (5) we have

$$\lim_{n\to\infty}\left(J(H_{2,n-3,2}) - J(D_{n-4,4})\right) = \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{2}} - \frac{3}{\sqrt{6}} - \frac{1}{\sqrt{2}} + \frac{3}{4\sqrt{2}} = \frac{7\sqrt{3}-4}{4\sqrt{6}} \doteq 0.8291885.$$

Let us remark that the difference $J(H_{2,n-3,2}) - J(D_{n-4,4})$ is increasing with n, and we obtain the first four decimals 0.8291 of the above limit when n is of order $8 \cdot 10^4$.

Finally, (6) does not hold for $n = 8$, so for this order $T_4 = D_{4,4}$.

Let $n \geq 7$. Then 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}. Now we determine T_5.

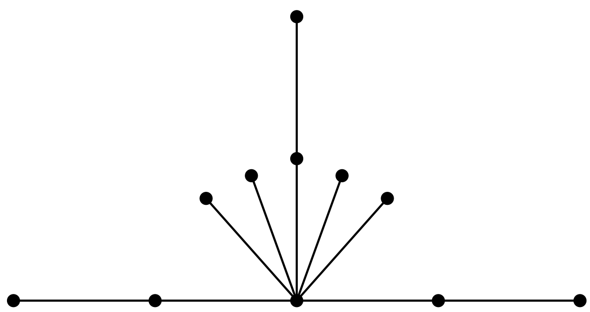

Fig. 3 The graph R_{11}.

Lemma 13. *Let v be an invariant with SLC-property. If $\{T_i^v;\ 1 \leq i \leq 4\} = \{S_n, D_{n-2,2}, D_{n-3,3}, H_{2,n-3,2}\}$, then $T_5^v \in \{D_{n-4,4}, H_{n-3,2,2}\}$.*

Proof. Notice that T_5^v must be of diameter 3, 4 or 5, since $H_{2,n-3,2}$ has diameter 4. So, first consider trees of diameter 5. If T_5^v has diameter 5, it must have the property that every edge-lifting of T_5^v results in $H_{2,n-3,2}$.

Consequently, T_5^ν has a unique vertex of degree at least 3 and even in this case one can choose edge-lifting resulting in a tree of diameter 4 other than $H_{2,n-3,2}$. Hence, it suffices to consider $D_{n-4,4}$ and trees of diameter 4.

If T_5^ν has diameter 4 and is a caterpillar, then analogously as in Lemma 11 the candidates are $H_{3,n-4,2}$, $H_{3,n-5,3}$ and $H_{n-3,2,2}$. However, in Lemma 11 we have shown that $\nu(D_{n-4,4}) > \nu(H_{3,n-4,2})$ and $\nu(D_{n-4,4}) > \nu(H_{3,n-5,3})$. If T_5^ν has diameter 4 and is not a caterpillar, then the central vertex of a diametric path of T_5^ν is adjacent with three distinct vertices of degree at least 2, and every edge-lifting of T_5^ν must result in $H_{2,n-3,2}$. So T_5^ν is R_n. We have $\nu(H_{3,n-4,2}) + \nu(H_{3,n-4,2}) > 2\nu(R_n)$ by star-convexity. Since $\nu(D_{n-4,4}) > \nu(H_{3,n-4,2})$, we have $\nu(D_{n-4,4}) > \nu(R_n)$. Therefore, $T_5^\nu \in \{D_{n-4,4}, H_{n-3,2,2}\}$.

Proposition 14. *The following holds:*

$$T_5 = \begin{cases} H_{2,5,2}, & \text{if } n = 8 \\ D_{n-4,4}, & \text{if } 9 \leq n \leq 17 \\ H_{n-3,2,2}, & \text{if } n \in \{6,7\} \text{ or } n \geq 18. \end{cases}$$

Proof. Since for $n \geq 6$ and $n \neq 8$ we have $\{T_i;\, 1 \leq i \leq 4\} = \{S_n, D_{n-2,2}, D_{n-3,3}, H_{2,n-3,2}\}$ and the Balaban index has SLC-property, it suffices to compare $J(H_{n-3,2,2})$ and $J(D_{n-4,4})$ if $n \neq 8$, by Lemma 13. In $H_{n-3,2,2}$ there are five orbits of vertices with value of w equal to $4n-10$, $3n-8$, $2n-4$, $n+2$ and $2n$. Therefore

$$J(H_{n-3,2,2}) = (n-1)\left(\frac{1}{\sqrt{(4n-10)(3n-8)}} + \frac{1}{\sqrt{(3n-8)(2n-4)}} + \frac{1}{\sqrt{(2n-4)(n+2)}} + \frac{n-4}{\sqrt{(n+2)2n}}\right).$$

We already know that

$$J(D_{n-4,4}) = (n-1)\left(\frac{3}{\sqrt{(3n-8)(2n-6)}} + \frac{1}{\sqrt{(2n-6)(n+2)}} + \frac{n-5}{\sqrt{(n+2)2n}}\right).$$

Since there is no $D_{n-4,4}$ for $n \leq 7$, we have $T_5 = H_{n-3,2,2}$ if $6 \leq n \leq 7$. The case $n = 8$ was checked by a computer and it was found that $T_5 = H_{2,5,2}$. (In fact, it suffices to check the graphs $H_{a,b,c}$, and the star convexity rules out all of them except $H_{2,5,2}$ and $H_{5,2,2}$, for which $J(H_{2,5,2}) > J(H_{5,2,2})$ by path-sliding.) Hence, it suffices to consider $n \geq 9$.

For $n \geq 18$, the following holds

$$J(H_{n-3,2,2}) > J(D_{n-4,4}), \tag{7}$$

which implies that $T_5 = H_{n-3,2,2}$ for $n \geq 18$. Again including a rigorous proof of (7) would be too complicated. We only show that the difference $J(H_{n-3,2,2}) - J(D_{n-4,4})$ tends to a positive constant. By (4) and (5) we have

$$\begin{aligned}\lim_{n\to\infty}\left(J(H_{n-3,2,2}) - J(D_{n-4,4})\right) &= \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} - \frac{3}{\sqrt{6}} - \frac{1}{\sqrt{2}} \\ &= \frac{1+\sqrt{6}-2\sqrt{2}}{\sqrt{12}} \doteq 0.179285 > 0.\end{aligned}$$

The difference $J(H_{n-3,2,2}) - J(D_{n-4,4})$ is increasing with n, and we obtain the first four decimals 0.1792 of the above limit when n is of order $37 \cdot 10^3$.

For $9 \leq n \leq 17$ it holds $J(D_{n-4,4}) > J(H_{n-3,2,2})$, and so $T_5 = D_{n-4,4}$ in these cases.

Now we concentrate on T_6.

Lemma 15. *Let ν be an invariant with SLC-property. If $\{T_i^\nu;\, 1 \leq i \leq 5\} = \{S_n, D_{n-2,2}, D_{n-3,3}, H_{2,n-3,2}, H_{n-3,2,2}\}$, then $T_6^\nu = D_{n-4,4}$.*

Proof. Analogously as in Lemma 13, T_6^ν may be of diameter 3, 4 or 5. By star-convexity $D_{n-4,4}$ is the only candidate among trees of diameter 3. Further, $H_{3,n-4,2}$ and $H_{3,n-5,3}$ are the only candidates among caterpillars of diameter 4, but in Lemma 11 we have already found that $\nu(D_{n-4,4}) > \nu(H_{3,n-4,2})$ and $\nu(D_{n-4,4}) > \nu(H_{3,n-5,3})$.

If T_6^ν has diameter 4 and is not a caterpillar, then the central vertex of T_6^ν is adjacent with three distinct vertices of degree at least 2, and every edge-lifting of T_6^ν must result in $H_{2,n-3,2}$ or $H_{n-3,2,2}$. Consequently, every edge-lifting of T_6^ν must result in $H_{2,n-3,2}$ and T_6^ν is R_n. Since in Lemma 13 we derived $\nu(D_{n-4,4}) > \nu(R_n)$, also R_n is out of consideration.

Finally, if T_6^ν is a tree of diameter 5, it must be a caterpillar since every edge-lifting of T_6^ν results in a caterpillar of diameter 4. If T_6^ν has a unique vertex of degree at least 3 then it is $H_{2,n-4,2,2}$. However, an edge-lifting of $H_{2,n-4,2,2}$ results in $H_{3,n-4,2}$. Since $\nu(D_{n-4,4}) > \nu(H_{3,n-4,2})$, we have $\nu(D_{n-4,4}) > \nu(H_{2,n-4,2,2})$. On the other hand, if T_6^ν has at least two vertices of degree at least 3 then there is an edge-lifting of T_6^ν which results in a caterpillar of diameter 4 with at least two vertices of degree at least 3. Since such a caterpillar is not in $\{T_i^\nu;\, 1 \le i \le 5\}$, also this tree is out of consideration. Therefore, $T_6^\nu = D_{n-4,4}$.

Proposition 16. *The following holds:*

$$T_6 = \begin{cases} P_6, & \textit{if } n = 6 \\ H_{3,3,2}, & \textit{if } n = 7 \\ D_{5,5}, & \textit{if } n = 10 \\ H_{n-3,2,2}, & \textit{if } n \in \{8,9\} \textit{ or } 11 \le n \le 17 \\ D_{n-4,4}, & \textit{if } n \ge 18. \end{cases}$$

Proof. Since for $n \ge 18$ we have $\{T_i;\, 1 \le i \le 5\} = \{S_n, D_{n-2,2}, D_{n-3,3}, H_{2,n-3,2}, H_{n-3,2,2}\}$ and the Balaban index has SLC-property, $T_6 = D_{n-4,4}$ if $n \ge 18$, by Lemma 15. The other cases were solved by a computer. (Analogously as for the case $n = 8$ in the proof of Proposition 14, for each n it suffices to check the Balaban index of a few graphs.)

In what follows we assume that $n \ge 7$, as otherwise T_7 does not exist.

Lemma 17. *Let ν be an invariant with SLC-property. If $\{T_i^\nu;\, 1 \le i \le 6\} = \{S_n, D_{n-2,2}, D_{n-3,3}, D_{n-4,4}, H_{2,n-3,2}, H_{n-3,2,2},\}$, then*

$$T_7^\nu \in \{D_{n-5,5}, H_{3,n-4,2}, H_{n-4,3,2}, H_{n-4,2,3}\}.$$

Proof. Analogously as in Lemmas 13 and 15, T_7^ν may be of diameter 3, 4 or 5. Moreover, in the very same way as in Lemma 15 one can derive that there is no candidate among trees of diameter 5, and the only candidate among trees of diameter 4 which is not a caterpillar is R_n. Further, $D_{n-5,5}$ is the only candidate among trees of diameter 3, so it remains to consider caterpillars $H_{a,b,c}$ of diameter 4. However, if two from a,b,c are at least 5, then $\nu(H_{a,b,c}) < \nu(D_{n-5,5})$ due to edge-lifting. Analogously, if $a \ge 5$ and $b + c \ge 6$, then $\nu(H_{a,b,c}) < \nu(D_{n-5,5})$ due to edge-lifting. Therefore, we have 9 candidates, namely $D_{n-5,5}$, $H_{3,n-4,2}$, $H_{4,n-5,2}$, $H_{3,n-5,3}$, $H_{4,n-6,3}$, $H_{4,n-7,4}$, $H_{n-4,3,2}$, $H_{n-4,2,3}$ and R_n.

In Lemma 13 we have already shown that $\nu(H_{3,n-4,2}) > \nu(R_n)$, so R_n is out of consideration. The function $\nu(H_{x,n-5,6-x})$ is strictly convex due to star-convexity, and so $\nu(D_{n-5,5}) > \nu(H_{4,n-5,2})$ and $\nu(D_{n-5,5}) > \nu(H_{3,n-5,3})$. Analogously, $\nu(D_{n-5,5}) > \nu(D_{n-6,6}) > \nu(H_{4,n-6,3})$ and $\nu(D_{n-5,5}) > \nu(D_{n-7,7}) > \nu(H_{4,n-7,4})$. Hence, $T_7^\nu \in \{D_{n-5,5}, H_{3,n-4,2}, H_{n-4,3,2}, H_{n-4,2,3}\}$.

Proposition 18. *The following holds:*

$$T_7 = \begin{cases} R_7, & \textit{if } n = 7 \\ H_{7,2,2}, & \textit{if } n = 10 \\ D_{6,5}, & \textit{if } n = 11 \\ H_{3,n-4,2}, & \textit{if } n \in \{8,9\} \textit{ or } n \ge 12. \end{cases}$$

Proof. Since for $n \geq 8$ and $n \neq 10$ we have $\{T_i;\, 1 \leq i \leq 6\} = \{S_n, D_{n-2,2}, D_{n-3,3}, D_{n-4,4}, H_{2,n-3,2}, H_{n-3,2,2}\}$ and the Balaban index has SLC-property, $T_7 \in \{D_{n-5,5}, H_{3,n-4,2}, H_{n-4,3,2}, H_{n-4,2,3}\}$ if $n \geq 8$ and $n \neq 10$, by Lemma 17. In these cases it suffices to compare $J(H_{3,n-4,2})$, $J(H_{n-4,2,3})$, $J(H_{n-4,3,2})$ and $J(D_{n-5,5})$.

By Lemma 6,

$$J(D_{n-5,5}) = (n-1)\left(\frac{4}{\sqrt{(3n-9)(2n-7)}} + \frac{1}{\sqrt{(2n-7)(n+3)}} + \frac{n-6}{\sqrt{(n+3)(2n+1)}}\right).$$

In $H_{3,n-4,2}$ there are six orbits of vertices with values of w equal to $3n-4$, $2n-2$, $3n-6$, $2n-4$, $n+2$ and $2n$. Therefore

$$J(H_{3,n-4,2}) = (n-1)\left(\frac{1}{\sqrt{(3n-4)(2n-2)}} + \frac{1}{\sqrt{(2n-2)(n+2)}} + \frac{2}{\sqrt{(3n-6)(2n-4)}} + \frac{1}{\sqrt{(2n-4)(n+2)}} + \frac{n-6}{\sqrt{(n+2)2n}}\right).$$

In $H_{n-4,3,2}$ there are also six orbits of vertices with values of w equal to $4n-11$, $3n-9$, $2n-5$, $3n-7$, $n+3$ and $2n+1$. Therefore

$$J(H_{n-4,3,2}) = (n-1)\left(\frac{1}{\sqrt{(4n-11)(3n-9)}} + \frac{1}{\sqrt{(3n-9)(2n-5)}} + \frac{1}{\sqrt{(2n-5)(3n-7)}} + \frac{1}{\sqrt{(2n-5)(n+3)}} + \frac{n-5}{\sqrt{(n+3)(2n+1)}}\right).$$

Finally, in $H_{n-4,2,3}$ there are five orbits of vertices with values of w equal to $4n-12$, $3n-10$, $2n-4$, $n+4$ and $2n+2$. Therefore

$$J(H_{n-4,2,3}) = (n-1)\left(\frac{2}{\sqrt{(4n-12)(3n-10)}} + \frac{1}{\sqrt{(3n-10)(2n-4)}} + \frac{1}{\sqrt{(2n-4)(n+4)}} + \frac{n-5}{\sqrt{(n+4)(2n+2)}}\right).$$

For $n \geq 8$, the following holds

$$J(H_{3,n-4,2}) > J(H_{n-4,3,2}) > J(H_{n-4,2,3}). \tag{8}$$

Again giving a rigorous proof of (8) would be tedious. We only show that each of the differences $J(H_{3,n-4,2}) - J(H_{n-4,3,2})$ and $J(H_{n-4,3,2}) - J(H_{n-4,2,3})$ tends to the same positive constant. By (4) and (5) we have

$$\lim_{n\to\infty}\left(J(H_{3,n-4,2}) - J(H_{n-4,3,2})\right) = \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{12}} - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} + \frac{3}{4\sqrt{2}} = \frac{4-2\sqrt{2}+3\sqrt{3}}{4\sqrt{6}} \doteq 0.649903 > 0$$

and

$$\lim_{n\to\infty}\left(J(H_{n-4,3,2}) - J(H_{n-4,2,3})\right) = \frac{1}{\sqrt{12}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} - \frac{2}{\sqrt{12}} - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} + \frac{3}{4\sqrt{2}} = \frac{4-2\sqrt{2}+3\sqrt{3}}{4\sqrt{6}} \doteq 0.649903 > 0.$$

Let us remark that both differences $J(H_{3,n-4,2}) - J(H_{n-4,3,2})$ and $J(H_{n-4,3,2}) - J(H_{n-4,2,3})$ are increasing with n, and we obtain the first four decimals 0.6499 of the above limit when n is of order $8 \cdot 10^4$.

Analogously, for $n \geq 12$ we have

$$J(H_{3,n-4,2}) > J(D_{n-5,5}). \tag{9}$$

Again we only find the limit

$$\begin{aligned}\lim_{n\to\infty}\left(J(H_{3,n-4,2}) - J(D_{n-5,5})\right) &= \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{2}} - \frac{4}{\sqrt{6}} - \frac{1}{\sqrt{2}} + \frac{3}{4\sqrt{2}} \\ &= \frac{7\sqrt{3}-4}{4\sqrt{6}} \doteq 0.829188 > 0.\end{aligned}$$

The difference $J(H_{3,n-4,2}) - J(D_{n-5,5})$ is increasing with n, and we obtain the first four decimals 0.8291 of the above limit when n is of order $8 \cdot 10^4$.

Consequently, $T_7 = H_{3,n-4,2}$ if $n \geq 12$. We have $T_7 = H_{3,n-4,2}$ also if $n \in \{8,9\}$ since in these cases $D_{n-5,5}$ does not exists. For $n = 11$ the inequality (9) does not hold so in this case $T_7 = D_{n-5,5}$, and the cases $n \in \{7,10\}$ were found by a computer.

We remark that it is possible to continue in this manner, but the situation is more and more complicated. It would be helpful to obtain a further structural statement, not to increase the number of graphs one has to compare.

Our results are summarized in Table 1. We remark that for all $n \leq 17$ we found the seven trees with the maximum Balaban index also using the computer program Sage. We first generate all trees on n vertices using the computer program Nauty, and then determine the corresponding extremes in Sage. This is doable only for small values of n (not much bigger than 20) on our computer resources.

Table 1 First seven trees with maximal values of 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="11">S_n</td><td></td><td rowspan="2"></td><td rowspan="4"></td><td rowspan="4"></td><td rowspan="4"></td><td rowspan="5"></td></tr>
<tr><td>4</td><td rowspan="10">$D_{n-2,2}$</td></tr>
<tr><td>5</td><td>P_5</td></tr>
<tr><td>6</td><td rowspan="8">$D_{n-3,3}$</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="5">$H_{2,n-3,2}$</td><td rowspan="4">$D_{n-4,4}$</td></tr>
<tr><td>10</td><td>$D_{5,5}$</td><td>$H_{n-3,2,2}$</td></tr>
<tr><td>11</td><td rowspan="2">$H_{n-3,2,2}$</td><td>$D_{6,5}$</td></tr>
<tr><td>$12-17$</td><td rowspan="2">$H_{3,n-4,2}$</td></tr>
<tr><td>$18-\infty$</td><td>$H_{n-3,2,2}$</td><td>$D_{n-4,4}$</td></tr>
</table>

Observe that

$$J(S_n) = (n-1)\left(\frac{n-1}{\sqrt{(n-1)(2n-3)}}\right).$$

By (4) and (5) we have

$$\begin{aligned}\lim_{n\to\infty}\left(J(S_n) - J(H_{3,n-4,2})\right) &= \frac{5}{\sqrt{2}} - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{2}} + \frac{9}{4\sqrt{2}} \\ &= \frac{21\sqrt{3}-12}{4\sqrt{6}} \doteq 2.487565.\end{aligned}$$

Hence, although $J(S_n) \sim \frac{n}{\sqrt{2}}$, the difference $J(T_1) - J(T_7)$ is tending to a constant. The same can be noted for the difference $J(T_1) - J(D_{n-k,k})$. Namely, using (4), (5) and Lemma 6 we derive

$$\lim_{n\to\infty} \big(J(S_n) - J(D_{n-k,k})\big) = (k-1)\frac{7\sqrt{3}-4}{4\sqrt{6}}.$$

Since the star-convexity implies $J(T_k) \geq J(D_{n-k,k})$, we obtain that $J(T_1) - J(T_k)$ is at most $J(S_n) - J(D_{n-k,k})$, which tends to a constant. Thus we have the following.

Corollary 19. *For every k, $J(T_1) - J(T_k)$ is bounded by a constant depending on k but not on n.*

In fact, we believe that the difference $J(T_1) - J(T_k)$ is not just bounded by a constant, but it tends to a real number. Hence, we have the following conjecture.

Conjecture 20. *For every k, $\lim_{n\to\infty} \big(J(T_1) - J(T_k)\big)$ is a constant.*

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