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Balaban Index of Cubic Graphs

Martin Knor[a], **Riste Škrekovski**[b,c,d], **Aleksandra Tepeh**[d,e]

[a] *Slovak University of Technology in Bratislava, Faculty of Civil Engineering, Department of Mathematics, Radlinského 11, 813 68, Bratislava, Slovakia,*
knor@math.sk

[b] *Faculty of Information Studies, 8000 Novo Mesto, Slovenia,*
[c] *FAMNIT, University of Primorska, 6000 Koper, Slovenia,*
[d] *Faculty of Mathematics and Physics, University of Ljubljana, 1000 Ljubljana,*
skrekovski@gmail.com

[e] *Faculty of Electrical Engineering and Computer Science, University of Maribor, Smetanova ulica 17, 2000 Maribor, Slovenia,*
aleksandra.tepeh@gmail.com

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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 this paper, we give an upper bound for the Balaban index of r-regular graphs on n vertices. Then we concentrate on cubic graphs. We give a better upper bound for fullerene graphs and we show that the Balaban index tends to zero as the number of vertices increases. This means that Balaban index does not distinguish well the fullerene graphs when they are sufficiently large. We conclude the paper with a conjecture on the lower bound of Balaban index for cubic graphs.

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 edge sets of a graph G, respectively. We set $n = |V(G)|$ and $m = |E(G)|$. For vertices, $u, v \in V(G)$, by $\mathrm{dist}_G(u, v)$ we denote the distance from u to v in G. Balaban index $J(G)$ of G is defined as

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

where the sum is taken over all edges $e = uv$ of G and for $x \in V(G)$, we have $w(x) = \sum_{y \in V(G)} \mathrm{dist}_G(x, y)$.

Balaban index is a topological index introduced by Alexandru T. Balaban near to 30 years ago [7, 8]. This topological index was used successfully in QSAR/QSPR modeling [21, 31]. Several recent uses can be found in [18, 26, 28]. In [10] two different approaches were presented for the calculation of Balaban index by taking into account the chemical nature of elements. In [11], Balaban index is compared with Wiener index regarding the alkanes, and it was obtained that Balaban index reduces the degeneracy of the later index and provides much higher discriminating ability. Therefore Balaban index is also called "sharpened Wiener index". See [12] for another reference that involves these two indicies and infinite polymers.

However, mathematical properties of Balaban index are still not studied extensively. There are few theoretical results known. Zhou and Trinajstić [32] give tight lower and upper bounds for general graphs, and Sun [30] and Deng [19] give the bounds in the case of trees. Among all trees with n vertices, the star S_n and the path P_n have the maximal and the minimal Balaban index, respectively. Also trees with the second minimal and maximal Balaban index, respectively, were characterized, see [19].

Several authors have studied bounds on the Balaban index over given classes of graphs. In Balaban, Ionescu-Pallas, Balaban [16], the behavior of J for various infinite families of graphs is discussed. In many of these cases, J tends to a constant finite value. J has the asymptotic value π for an infinitely long n-alkane (a path). In Ghorbani [25], Balaban index of vertex transitive graphs is studied. For the study of this index over fullerene graphs see [17, 24, 27].

The largest Balaban index among all n-vertex unicyclic graphs and n-vertex bicyclic graphs was considered in Deng and Chang [20] and Dong and You [22]. The Balaban index of a class of dendrimers is computed in Ashrafi, Shabani, Diudea [3, 4]. Our research was motivated by the following problem from Dong and Guo [22]:

Problem 1. *Among n-vertex graphs, find those with the minimum Balaban index.*

Using the AutoGraphiX software, Aouchiche, Caporossi, Hansen [2] showed that, among all connected graphs on n vertices the path on n vertices is not a graph for which the lower bound is attained, as erroneously stated in [23].

Among graphs on n vertices, Balaban index attains its maximum for the complete graph K_n, where

$$J(K_n) = \frac{\binom{n}{2}}{\binom{n}{2} - n + 2} \binom{n}{2} \frac{1}{n-1} = \frac{n^3 - n^2}{2(n^2 - 3n + 4)},$$

which is slightly more than $\frac{n}{2}$. Its minimum value among n-vertex graphs is not known. However, if we consider n-vertex trees, then the Balaban index attains its minimum for the path on n vertices P_n, see [19, 30], and $\lim_{n\to\infty} J(P_n) = \pi$, see [16]. One may expect that, if G is an n-vertex r-regular graph, then $J(P_n) \leq J(G) \leq J(K_n)$. In the next section we show that this is not the case. We prove that if G is an n-vertex r-regular graph (i.e. a graph where each vertex has r neighbors), then $J(G)$ tends to 0 as n tends to ∞. In other words, zero is also an accumulation point for Balaban index.

2 Balaban index of regular graphs

In this section we concentrate on r-regular graphs with $r \geq 3$. In the following result we give an upper bound for $J(G)$ for such graphs.

Theorem 2. *Let G be an r-regular graph on n vertices with $r \geq 3$. Then*

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

Proof. Let $u \in V(G)$ and let n_i be the number of vertices at distance i from u. Thus,

$$w(u) = \sum_i i \cdot n_i \qquad \text{and} \qquad \sum_i n_i = n\,.$$

Since the graph is r-regular, we have $n_i \leq r \cdot (r-1)^{i-1}$. Let s and c be such that

$$n = 1 + r + r \cdot (r-1) + \cdots + r \cdot (r-1)^{s-1} + c \quad \text{and} \quad 0 \leq c < r \cdot (r-1)^s\,.$$

Then we can bound $w(u)$ from below in the following way:

$$w(u) = \sum_{i=0}^{s+1} i \cdot n_i \geq 1 \cdot r + 2 \cdot r(r-1) + \cdots + s \cdot r(r-1)^{s-1} + (s+1) \cdot c\,.$$

In other words, a lower bound on $w(u)$ is attained if the breadth-search tree, rooted at u, is an almost complete tree with all leaves at distance s and maybe $s+1$ from u, and every non-leaf vertex is of degree r. So, we have

$$1 + (r-1) + (r-1)^2 + \cdots + (r-1)^{s-1} = \frac{n-1-c}{r},$$

and hence

$$\frac{(r-1)^s - 1}{r-2} = \frac{n-1-c}{r},$$

which gives

$$s = \log_{r-1}\left(\frac{(r-2)n+2-c(r-2)}{r}\right). \tag{1}$$

From (1) and from $c < r \cdot (r-1)^s$ we get

$$\frac{(r-2)n+2}{r} = (r-1)^s + \frac{c(r-2)}{r} < (r-1)^s + (r-1)^s(r-2) = (r-1)^{s+1},$$

which means that $\log_{r-1}(\frac{(r-2)n+2}{r}) < s+1$. Since $\log_{r-1}(\frac{(r-2)n+2}{r}) \geq s$ by (1), we have $s = \lfloor \log_{r-1}(\frac{(r-2)n+2}{r}) \rfloor$. Consequently,

$$\begin{aligned} w(u) &\geq s \cdot r(r-1)^{s-1} = \left\lfloor \log_{r-1}\left(\frac{(r-2)n+2}{r}\right)\right\rfloor \cdot r \cdot (r-1)^{\lfloor \log_{r-1}(\frac{(r-2)n+2}{r})\rfloor - 1} \\ &\geq \left\lfloor \log_{r-1}\left(\frac{(r-2)n+2}{r}\right)\right\rfloor \cdot r \cdot \frac{(r-2)n+2}{r} \cdot \frac{1}{(r-1)^2} \\ &= \left\lfloor \log_{r-1}\left(\frac{(r-2)n+2}{r}\right)\right\rfloor \cdot \frac{(r-2)n+2}{(r-1)^2}. \end{aligned}$$

Thus,

$$\begin{aligned} J(G) &\leq \frac{m}{m-n+2} \cdot m \cdot \frac{1}{w(u)} \leq \frac{\frac{rn}{2}}{\frac{rn}{2}-n+2} \cdot \frac{rn}{2} \cdot \frac{1}{\left\lfloor \log_{r-1}\left(\frac{(r-2)n+2}{r}\right)\right\rfloor \cdot \frac{(r-2)n+2}{(r-1)^2}} \\ &< \frac{r^2(r-1)^2 n^2}{2((r-2)n+2)^2 \left\lfloor \log_{r-1}\left(\frac{(r-2)n+2}{r}\right)\right\rfloor} < \frac{r^2(r-1)^2}{2(r-2)^2 \left\lfloor \log_{r-1}\left(\frac{(r-2)n+2}{r}\right)\right\rfloor}. \end{aligned}$$

□

Now we may state the following interesting consequence.

Corollary 3. *For r-regular graphs G on n vertices, where $r \geq 3$, it holds*

$$\lim_{n\to\infty} J(G) = 0.$$

Proof. Let G be an r-regular graph on n vertices. By Theorem 2, we have

$$J(G) \leq \frac{r^2(r-1)^2}{2(r-2)^2 \left\lfloor \log_{r-1} \frac{(r-2)n+2}{r}\right\rfloor} < \frac{c_1}{\ln(n)+c_2},$$

where c_1 and c_2 are constants depending on r, but not on n. Hence,

$$\lim_{n\to\infty} J(G) \leq \lim_{n\to\infty} \frac{c_1}{\ln(n)+c_2} = 0.$$

□

In other words, Balaban index of regular graphs which are really big in the number of vertices, is close to 0. The number of such graphs is enormously large, and we conclude that the Balaban index does not distinguish them well.

3 Fullerene graphs

Here we consider chemical structures called fullerenes. Fullerenes [29] are polyhedral molecules made of carbon atoms arranged in pentagonal and hexagonal faces, and their corresponding graphs, *fullerene graphs*, are 3-connected, cubic planar graphs with only pentagonal and hexagonal faces.

By Corollary 3, if $\mathcal{G}$ is the class of fullerenes, then $\lim_{n\to\infty}\{J(G);\, G \in \mathcal{G} \text{ and } |V(G)| = n\} = 0$. We remark that the upper bound given in Theorem 2 is very rough. For instance, if G is the well-known Buckminster fullerene, then our bound with $r = 3$ gives $J(G) \le \frac{36}{2\lfloor \log_2 62/3 \rfloor} = 4.5$, while $J(G) = \frac{90}{32} \cdot 90 \cdot \frac{1}{278} = \frac{2025}{2224} = 0.91$ (by a mistake, in [25] this value is doubled).

In what follows, for fullerenes we give a better upper bound for the Balaban index. Notice that the bound in the next theorem tends to 0 for $n \to \infty$ much faster than $18/\lfloor \log_2 (n+2)/3 \rfloor$.

Theorem 4. *Let G be a fullerene graph on $n \ge 60$ vertices. Then*

$$J(G) \le \frac{25}{\sqrt{n}}\,.$$

Proof. We argue similarly as in the previous proof. Let G be a fullerene on n vertices and let $u \in V(G)$. Let n_i be the number of vertices at distance i from u. Then $n_0 = 1$ and $n_1 = 3$. Moreover in [1, Lemma 6], it is shown that $n_{i+1} \le n_i + 3$ for $i \ge 1$. This immediately gives the bound $n_i \le 3i$ for $i \ge 1$. We obtain a lower bound of $w(u)$ by assuming each $n_i = 3i$ for $i \ge 1$, as in this way we have fewer vertices at higher distance. So

$$w(u) = \sum_i i \cdot n_i \ge 1 \cdot 3 + 2 \cdot 6 + 3 \cdot 9 + \cdots + s \cdot 3s + (s+1)c,$$

for some c and s, where $0 \le c < 3s + 3$ and $1 + 3 + 6 + 9 + \cdots + 3s + c = n$. Hence,

$$3(1 + 2 + 3 + \cdots + s + (s+1)) \ge n,$$

and from here

$$s^2 + 3s + 2 \ge \frac{2n}{3}\,.$$

Since $n \geq 60$, we have $s \geq 5$, and hence $s^2 \geq 3s+2$, which gives $s \geq \sqrt{n/3}$. Since s is integer, we obtain

$$s \geq \left\lceil \sqrt{n/3} \right\rceil .$$

Consequently,

$$\begin{aligned} w(u) &\geq 1\cdot 3 + 2\cdot 6 + 3\cdot 9 + \cdots + 3\left\lceil \sqrt{n/3}\right\rceil^2 + c(\lceil \sqrt{n/3}\rceil + 1) \geq 3 \sum_{j=1}^{\lceil \sqrt{n/3}\rceil} j^2 \\ &> 3\frac{2\left(\sqrt{n/3}\right)^3 + 3\left(\sqrt{n/3}\right)^2 + \sqrt{n/3}}{6} > \frac{n}{3}\sqrt{\frac{n}{3}}. \end{aligned}$$

Thus,

$$\begin{aligned} J(G) &\leq \frac{m}{m-n+2}\cdot m \cdot \frac{1}{w(u)} \leq \frac{\frac{3}{2}n}{\frac{3}{2}n - n + 2}\cdot \frac{3}{2}n \cdot \frac{1}{\frac{n}{3}\sqrt{\frac{n}{3}}} \\ &\leq \frac{27\sqrt{3}}{2\sqrt{n}} < \frac{25}{\sqrt{n}}. \end{aligned}$$

□

4 Cubic graphs with small value of Balaban index

There are cubic graphs for which the Balaban index tends to 0 even faster than for the fullerene graphs. While for the fullerene graphs Balaban index is bounded by $25n^{-1/2}$, these cubic graphs have the Balaban index $32n^{-1}$ and even less.

Let n be divisible by 4, and let H_n be a graph obtained from the cycle of length $3 \cdot \frac{n}{4}$, in which every third vertex is doubled, see Figure 1 for H_{16}. Observe that H_n is obtained from $n/4$ copies of $K_4 - e$ (i.e., K_4 without one edge) which are joined by $n/4$ extra edges to form a connected cubic graph. Obviously, H_n has n vertices. We have the following statement.

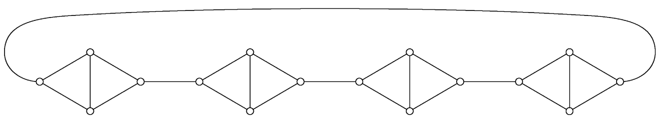

Figure 1: The graph H_{16}.

Proposition 5. *For positive n divisible by 4, it holds*

$$J(H_n) \leq \frac{32}{n} .$$

Proof. For simplicity, let $l = 3n/4$. Analogously as in the previous proofs, first we give a lower bound for $w(u)$, $u \in V(H_n)$. In order to do so, we find the total distance $\mathrm{cw}(u)$ from u to the vertices of the original cycle. If l is even, then

$$\mathrm{cw}(u) = 1 + 2 + \cdots + \frac{l}{2} + 1 + 2 + \cdots + \left(\frac{l}{2} - 1\right) = \binom{\frac{l}{2}+1}{2} + \binom{\frac{l}{2}}{2} = \frac{l^2}{4}.$$

Similarly, if l is odd, then

$$\mathrm{cw}(u) = 2\Big(1 + 2 + \cdots + \frac{l-1}{2}\Big) = 2\binom{\frac{l+1}{2}}{2} = \frac{l^2-1}{4}.$$

As there is at least one vertex in H_n not on the original cycle and different from u, and as the distance of this vertex to u is at least one, for both the above cases we get

$$w(u) \ge \mathrm{cw}(u) + 1 > \frac{l^2}{4} = \frac{9n^2}{64}.$$

Hence,

$$J(G) \le \frac{\frac{3}{2}n}{\frac{3}{2}n - n + 2} \cdot \frac{3n}{2} \cdot \frac{1}{\frac{9n^2}{64}} < \frac{32}{n}.$$

□

The last result means that if n approaches to ∞, then $J(H_n)$ approaches to 0 quite fast. However, among cubic graphs on n vertices H_n does not have the smallest value of Balaban index. We introduce a class of graphs L_n with $J(L_n) < J(H_n)$. Since it seems to be difficult to find a good upper bound for $J(L_n)$, below we present a table of values obtained by a computer program.

Let n be even and $n \ge 10$. If $4 \nmid n$, then L_n is obtained from $(n-10)/4$ copies of $K_4 - e$ joined to a path by edges connecting the vertices of degree 2, to which at the ends we attach two pendant blocks, each on 5 vertices, see Figure 2 for L_{18}. On the other hand if $4 \mid n$, then L_n is obtained from $(n-12)/4$ copies of $K_4 - e$, joined into a path by edges connecting the vertices of degree 2, to which ends we attach two pendant blocks, one on 5 vertices and the other on 7 vertices, see Figure 3 for L_{20}.

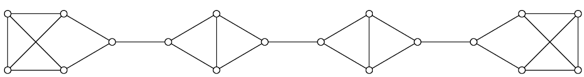

Figure 2: The graph L_{18}.

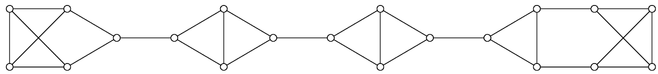

Figure 3: The graph L_{20}.

n	8	10	12	14	16	18	20	22	24	26	28	30
$32/n$	4	-	2.68	-	2	-	1.60	-	1.33	-	1.14	-
$J(H_n)$	1.92	-	1.50	-	1.19	-	1.00	-	0.85	-	0.75	-
$J(L_n)$	-	1.48	1.36	1.10	1.03	0.89	0.83	0.74	0.70	0.64	0.61	0.56

Table 1: Balaban index for H_n and L_n for small numbers of vertices.

In Table 1 we have $J(L_n)$ for small values of n, as well as $J(H_n)$ (if n is divisible by 4) and the bound $\frac{32}{n}$.

We conclude the paper with a conjecture about L_n.

Conjecture 6. *Among n-vertex cubic graphs, L_n has the smallest Balaban index.*

5 Concluding remarks

Beside the above conjecture one can study some more problems related to the results of this paper. As a diversity of the Balaban index J, further indices were developed omitting the fraction factor $m/(m-n+2)$ before the sum, and it would be interesting to *explore similar bounds as in this paper for indices* introduced in [13].

Shortly speaking, the main result of our paper is showing that 0 (beside π and other values mentioned in [16]) is also an accumulation point for Balaban index. From this point of view, it would be interesting problem to *find some more new accumulation points for this index.*

In this paper, we were restricted to simple cubic but general graphs. Note that from the point of view of chemistry one interesting class of cubic multigraphs are annulenes, and also some other particular cubic graphs are. So as further work one could *extend our study to multigraphs* as well as *restrict to some particular regular graphs.* See [5,6,9,14,15] for some (chemical) results of such classes of graphs.

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