MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **78** (2017) 163-168

ISSN 0340 - 6253

A Note on Accumulation Points of Balaban Index

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(Received August 5, 2016)

Abstract

It is known that there are many classes of graphs whose Balaban index converges to a real number. Here we show that for an arbitrary positive number r there exists a sequence of graphs whose Balaban index converges to r. Moreover, we construct the corresponding sequence of graphs.

1 Introduction and results

Let G be a graph. By $V(G)$ and $E(G)$ we denote its vertex and edge sets, respectively. Further, $n = |V(G)|$ and $m = |E(G)|$. Let $u \in V(G)$. By $w(u)$ we denote the the sum of distances from u to all the vertices of G. That is, $w(u) = \sum_{v \in V(G)} d(u,v)$. Balaban index of G, $J(G)$, is defined as

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

where the sum is taken over all edges of G. This index was introduced by Balaban in [1,2] and it was used successfully in QSAR/QSPR modeling [5,14], see also [4,9]. Recent papers on mathematical properties of this index include [7, 8, 11] and the survey paper [13].

As regards the bounds for Balaban index, for the maximum value we have $J(G) \leq c \cdot n$ for $c \doteq 1/\sqrt{2}$, and the extremal graph is the complete graph on n vertices K_n if $n \leq 7$, and a star on n vertices if $n \geq 8$, see [6, 12]. For the minimum value we have $J(G) \geq 8/n + o(n^{-1})$ and there are graphs for which $J(G) \sim c/n$ where $c \doteq 10.15$, see [10]. Hence, there are classes of graphs G_n and H_n such that $\lim_{n\to\infty} J(G_n) = \infty$ (take the star on n vertices for G_n) and $\lim_{n\to\infty} J(H_n) = 0$ (take special dumbbell graphs for H_n, see [10]).

Let P_n be a path on n vertices. Already in [3] it was shown that $\lim_{n\to\infty} J(P_n) = \pi$, which is a result that attracts an attention. In fact, in [3] the accumulation points for many classes of graphs were determined, and there appeared a problem to determine which real numbers can be accumulation points for Balaban index of a class of graphs. More precisely, several mathematicians asked the following (personal communication):

Problem 1 *Is it true that for every positive real number r there exists a sequence of graphs $\{G^r_{n_i}\}_{i=1}^{\infty}$, where $|V(G^r_{n_i})| = n_i$ and $\{n_i\}_{i=1}^{\infty}$ is increasing, such that*

$$\lim_{n_i\to\infty} J(G^r_{n_i}) = r\,?$$

In this paper we answer Problem 1 affirmatively. In fact, we do more. We construct the sequence of corresponding graphs $\{G^r_{n_i}\}_{i=1}^{\infty}$.

Let $Q_{a,b}$ be a graph obtained from a clique K_a and a path P_{b+1} by identifying one vertex of the clique with an endvertex of the path (see Figure 1 for $Q_{6,3}$). Then $|V(Q_{a,b})| = a+b$.

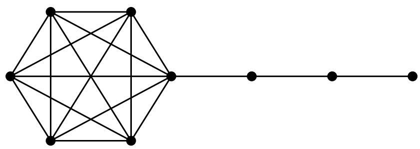

Figure 1. The graph $Q_{6,3}$.

We will prove the following statement:

Theorem 2 *Let $r \in \mathbb{R}$, $r > 0$, and let $\{b_a\}_{a=1}^{\infty}$ be a sequence of integers such that $\lim_{a\to\infty} b_a/a = 1/\sqrt{r}$. Then*

$$\lim_{a\to\infty} J(Q_{a,b_a}) = r\,.$$

To fulfill the assumptions in Theorem 2 it suffices to choose $b_a = \lfloor a/\sqrt{r} \rfloor$ for every $a \in \mathbb{N}$. Consequently, every positive number is an accumulation point for Balaban index of a class of graphs. However, the problem stil remains open for specific classes of graphs, such as the chemical ones:

Problem 3 *Is it true that for every positive real number r there exists a sequence of graphs $\{G^r_{n_i}\}_{i=1}^{\infty}$, where $|V(G^r_{n_i})| = n_i$, $\{n_i\}_{i=1}^{\infty}$ is increasing and G^r_n has maximum degree at most 4, such that*

$$\lim_{n_i \to \infty} J(G^r_{n_i}) = r\,?$$

2 Proof of the main result

Observe that the function $f(x) = \frac{2}{x^2+(1-x)^2}$ has a Riemann integral on $[0,1]$, which implies that

$$\int_0^1 \frac{2 \cdot dx}{x^2 + (1-x)^2} = \lim_{b \to \infty} \sum_{i=0}^{b} \frac{1}{b} \cdot \frac{2}{(\frac{i}{b})^2 + (\frac{b-i}{b})^2}$$

or in other notation

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

Now multiplying both sides by $\frac{1}{b}$ we get

$$\sum_{i=0}^{b} \frac{2}{i^2 + (b-i)^2} \sim \frac{\pi}{b}. \tag{1}$$

We use (1) in the proof of Theorem 2.

Proof of Theorem 2. For the sake of simplicity, let $b = b_a$. We denote by $v_0, v_1, \ldots, v_b$ the vertices of path P_{b+1}, where v_0 was identified with a vertex of K_a to obtain $Q_{a,b}$. First we determine the sums of distances $w(x)$ for vertices of $Q_{a,b}$. Let $u \in V(Q_{a,b}) \setminus \{v_0, v_1, \ldots, v_b\}$. Then

$$w(u) = (a-2) + 1 + 2 + \cdots + (b+1) = a - 1 + \frac{b^2 + 3b}{2}. \tag{2}$$

On the other hand, for v_i, $0 \le i \le b$, we have

$$w(v_i) = (i+1)(a-1) + (1+2+\cdots+i) + (1+2+\cdots+(b-i)) = ai + a - i - 1 + \frac{i^2+i}{2} + \frac{(b-i)^2 + (b-i)}{2}.$$
(3)

By the assumption we have $\lim_{a\to\infty} b_a/a = 1/\sqrt{r}$, which implies $b_a \in \Theta(a)$, and since $a+b=n$, we get $a, b \in \Theta(n)$. Consequently, from (2) and (3) we have

$$w(u) \sim \frac{b^2}{2} \qquad \text{and} \qquad w(v_i) \sim ai + \frac{i^2}{2} + \frac{(b-i)^2}{2} \geq \frac{i^2}{2} + \frac{(b-i)^2}{2}, \tag{4}$$

where $u \in V(Q_{a,b}) \setminus \{v_0, v_1, \ldots, v_b\}$.

There are $\binom{a}{2} \sim \frac{a^2}{2}$ edges in the complete graph in $Q_{a,b}$, and they contribute to the sum $\sum_{xy\in E(Q_{a,b})} \frac{1}{\sqrt{w(u)\cdot w(v)}}$ asymptotically by $\frac{a^2}{2}\cdot\frac{2}{b^2} = \frac{a^2}{b^2}$ (observe that $w(v_0) \sim w(u)$).

Now we determine the contribution of edges of P_{b+1}. Denote $w^*(v_i) = \frac{i^2}{2} + \frac{(b-i)^2}{2}$. By (4), for a (and $b = b_a$) big enough we have

$$\sum_{i=0}^{b-1} \frac{1}{\sqrt{w(v_i)\cdot w(v_{i+1})}} \leq \sum_{i=0}^{b-1} \frac{1}{\sqrt{w^*(v_i)\cdot w^*(v_{i+1})}}. \tag{5}$$

Claim 1. *The following holds*

$$\sum_{i=0}^{b-1} \frac{1}{\sqrt{w^*(v_i)\cdot w^*(v_{i+1})}} \sim \frac{\pi}{b}. \tag{6}$$

Let v_iv_{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 $\frac{1}{w_i^+} \leq \frac{1}{\sqrt{w^*(v_i)\cdot w^*(v_{i+1})}} \leq \frac{1}{w_i^-}$. Therefore

$$\sum_{i=0}^{b-1} \frac{1}{w_i^+} \leq \sum_{i=0}^{b-1} \frac{1}{\sqrt{w^*(v_i)\cdot w^*(v_{i+1})}} \leq \sum_{i=0}^{b-1} \frac{1}{w_i^-}. \tag{7}$$

Since $g(x) = \frac{x^2}{2} + \frac{(b-x)^2}{2}$ is decreasing on $[0, \frac{b}{2}]$ and increasing on $[\frac{b}{2}, b]$, we have

$$\begin{aligned}\sum_{i=0}^{b-1} \frac{1}{w_i^+} &= \frac{1}{w^*(v_0)} + \frac{1}{w^*(v_1)} + \cdots + \frac{1}{w^*(v_{\lfloor\frac{b}{2}\rfloor-1})} + \frac{1}{w^*(v_{\lfloor\frac{b}{2}\rfloor+1})} + \frac{1}{w^*(v_{\lfloor\frac{b}{2}\rfloor+2})} + \cdots + \frac{1}{w^*(v_b)} \\ &\sim \sum_{i=0}^{b} \frac{2}{i^2+(b-i)^2} - \frac{2}{\lfloor\frac{b}{2}\rfloor^2 + (b-\lfloor\frac{b}{2}\rfloor)^2}\end{aligned}$$

and analogously we get

$$\sum_{i=0}^{b-1} \frac{1}{w_i^-} \sim \sum_{i=0}^{b} \frac{2}{i^2+(b-i)^2} - \frac{2}{0^2+b^2} + \frac{2}{\lfloor\frac{b}{2}\rfloor^2 + (b-\lfloor\frac{b}{2}\rfloor)^2} - \frac{2}{b^2+0^2}.$$

Notice that the four isolated terms in the above expressions are of order $O(b^{-2})$, and thus by (1), both sums $\sum_{i=0}^{b-1} \frac{1}{w_i^+}$ and $\sum_{i=0}^{b-1} \frac{1}{w_i^-}$ converge to $\frac{\pi}{b}$. Now, the claim follows by (7).

By Claim 1, $\sum_{xy\in E(Q_{a,b})} \frac{1}{\sqrt{w(x)\cdot w(y)}}$ has asymptotical lower and upper bounds a^2/b^2 and $a^2/b^2 + \pi/b$, respectively. Since $b_a \in \Theta(a)$ and $a, b \in \Theta(n)$, we have $a^2/b^2 \in \Theta(1)$ and

$\pi/b \in \Theta(n^{-1})$ which means that

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

Further, $n = a+b$ and $m = \binom{a}{2} + b = \frac{a^2-a}{2} + b \sim a^2/2$. Consequently, $m-n+2 \sim a^2/2$ as well. This implies that

$$J(Q_{a,b}) = \frac{m}{m-n+2} \sum_{xy \in E(Q_{a,b})} \frac{1}{\sqrt{w(x) \cdot w(y)}} \sim \frac{a^2/2}{a^2/2} \cdot \frac{a^2}{b^2} = \frac{a^2}{b^2}.$$

Since $\lim_{a\to\infty} b_a/a = 1/\sqrt{r}$, we have

$$\lim_{a\to\infty} J(Q_{a,b}) = r$$

as required. ■

Acknowledgements: The first author acknowledges partial support by Slovak research grants VEGA 1/0007/14, VEGA 1/0026/16 and APVV 0136–12. The research was partially supported by Slovenian research agency ARRS, program no. P1–0383 and project no. L1–4292, as well as the National Scholarschip Programme of the Slovac Republic SAIA.

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