Hindawi
Mathematical Problems in Engineering
Volume 2020, Article ID 2081241, 6 pages
https://doi.org/10.1155/2020/2081241

Research Article

Several Asymptotic Bounds on the Balaban Indices of Trees

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Received 16 August 2020; Revised 30 September 2020; Accepted 21 October 2020; Published 6 November 2020

Academic Editor: Jia-Bao Liu

The Balaban index (also called the J index) of a connected graph G is a distance-based topological index, which has been successfully used in various QSAR and QSPR modeling. Although the index was introduced 30 years ago, there are few results on the asymptotic relations. In this paper, several asymptotic bounds on the Balaban indices of trees with diameters 3 and 4 are shown, respectively.

1. Introduction

All graphs considered in this paper are simple and undirected. Let G be a graph with its edge set $E(G)$ and vertex set $V(G)$. We set $|V(G)| = n$ and $|E(G)| = m$. The star of order n is denoted by S_n. The distance between vertices u and v in G is denoted by $d_G(u, v)$, and the sum of the distance between vertex u and each vertex of G is denoted by $\sigma_G(u)$, that is, $\sigma_G(u) = \sum_{w\in V(G)} d_G(u, w)$.

The Balaban index [1] of a connected graph G (or the J index for short) is defined as

$$J(G) = \frac{m}{\mu + 1} \sum_{uv\in E(G)} \frac{1}{\sqrt{\sigma_G(u)\sigma_G(v)}}, \tag{1}$$

where μ is the cyclomatic number and $\mu = m - n + 1$.

The Balaban index (also called the J index) of a connected graph G is a distance-based topological index, which has been successfully used in various QSAR and QSPR modeling [2, 3]. Many applications in chemistry can be found in [4–6]. By comparing with the Wiener index regarding alkanes in [7], it was found that the Balaban index reduces the degeneracy of the latter index and provides much higher discriminating ability. So, the Balaban index is also called the sharpened Wiener index. Some results on the maximal and minimal Balaban index [8–10] have been presented. In [11–14], the asymptotic behaviors of the Balaban indices for various infinite families of graphs are observed.

Until now, there are few results on the asymptotic relations on the Balaban index. In this paper, several asymptotic bounds on the Balaban indices of trees with diameters 3 and 4 are shown, respectively. The two kinds of trees are depicted as follows.

If a tree is with diameter 3, then this tree can be obtained by attaching some pendent edges to the two end-vertices of one edge. Then, this tree is denoted by $T_n(3, a, b)$, see Figure 1, which has n vertices, diameter 3, and satisfies that there are a pendent edges attached at one end-vertex of one edge and b pendent edges attached at the other end-vertex of the edge, where $a \geq 1$, $b \geq 1$, and $a + b = n - 2$. The set of this kind of trees is denoted by $\mathcal{T}_n(3, a, b)$.

The tree with order n and diameter 4 denoted by $T_n^l(4, a_1, a_2, \ldots, a)_l$, see Figure 2, is obtained from a star S_{l+1} by attaching $a_1, a_2, \ldots, a_l$ pendent edges to the l pendent vertices of the star, respectively, where $a_i \geq 0, 1 \leq i \leq l$. The set of this kind of trees is denoted by $\mathcal{T}_n^l(4, a_1, a_2, \ldots, a_l)$.

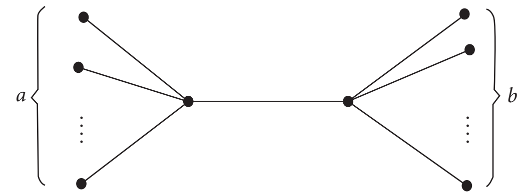

FIGURE 1: The graph $T_n(3, a, b)$.

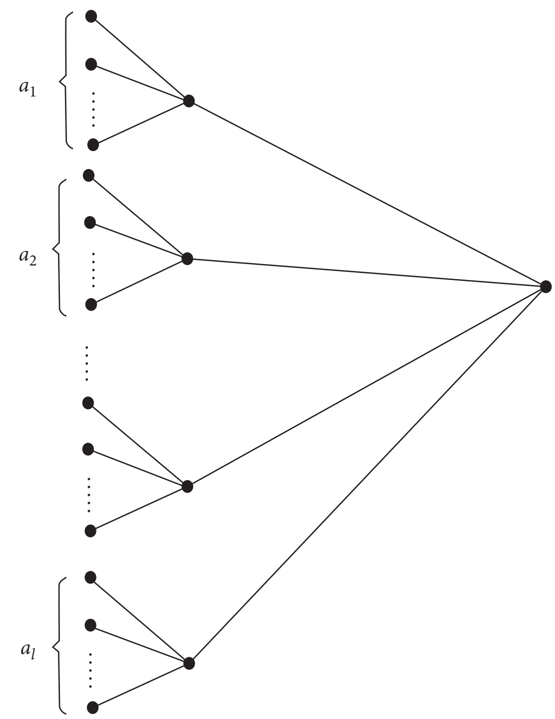

FIGURE 2: The graph $T_n^l(4, a_1, a_2, \ldots, a_l)$.

2. The Balaban Indices of Trees with Diameter 3

In this section, the asymptotic bounds on the Balaban indices of trees with diameter 3 will be given.

Theorem 1. *For any tree $T_n(3, a, b) \in \mathcal{T}_n(3, a, b)$, we have*

$$O\left(\frac{2n}{\sqrt{15}}\right) \leq J\left(T_n(3, a, b)\right) \leq O\left(\frac{n}{\sqrt{2}}\right). \tag{2}$$

Proof. Suppose $a \leq b$. Then, by $a + b = n - 2$, we have $a \leq ((n-2)/2)$. By direct calculation, the Balaban index of $T_n(3, a, b) = T_n((3, a, n-a-2))$ is as follows:

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

Through computation, the derivative of $J(T_n(3, a, n-a-2))$ related to a is

$$\frac{\partial J\left(T_n(3,a,n-a-2)\right)}{\partial a}=\frac{n-1}{2}\cdot\left[\frac{a(5n-2a-8)}{((3n-a-5)(2n-a-3))^{3/2}}+\frac{2}{\sqrt{(3n-a-5)(2n-a-3)}}+\frac{2+2a-n}{((2n-a-3)(n+a-1))^{3/2}}\right.$$
$$\left.-\frac{2}{\sqrt{(n+a-1)(2n+a-3)}}+\frac{(2+a-n)(3n+2a-4)}{((2n+a-3)(n+a-1))^{3/2}}\right]. \tag{4}$$

Next, the sign of $(\partial J(T_n(3,a,n-a-2)))/\partial a$ will be determined. For the above equation, we see that the first two terms are positive, and the last three terms are nonpositive. Then, we use the sum of the first two terms to divide the sum of the absolute values of the last three terms. So, we get that

$$\frac{\left(a(5n-2a-8)/((3n-a-5)(2n-a-3))^{3/2}\right)+(2/(\sqrt{(3n-a-5)(2n-a-3)}))}{n-2a-2/((2n-a-3)(n+a-1))^{3/2}+2/\sqrt{(n+a-1)(2n+a-3)}+(n-a-2)(3n+2a-4)/((2n+a-3)(n+a-1))^{3/2}}$$
$$=\frac{12n^2-38n+a(8-5n)+30}{((3n-a-5)(2n-a-3))^{3/2}\left(\left((n-2a-2)/((n+a-1)(2n-a-3))^{3/2}\right)+(2/\sqrt{(n+a-1)(2n+a-3)})+\left((n-a-2)(3n+2a-4)/((2n+a-3)(n+a-1))^{3/2}\right)\right)}. \tag{5}$$

Denote the above fraction by $f(n,a)$. Observing this quotient, its value is equal to 1 if $n=2k+2$ and $a=k$ for $k=2,3,\ldots,[n-2/2]$. In this case, it means that $T_n(3,a,n-a-2)$ attains the minimum value. Otherwise, its value is less than 1 as n tends to infinity, that is,

$$\lim_{n\longrightarrow\infty} f(n,a)=\frac{4}{7\sqrt{3}}<1. \tag{6}$$

Thus, the derivative of $J(T_n(3,a,n-a-2))$ related to a is negative as n is big enough. In this case, $J(T_n(3,a,n-a-2))$ increases along with parameter a decreasing. Since $1\le a\le\lfloor(n-2)/2\rfloor$, we see that

$$\begin{aligned}J\left(T_n(3,a,n-a-2)\right)&\le J\left(T_n(3,1,n-3)\right),\\ J\left(T_n(3,a,n-a-2)\right)&\ge J\left(T_n(3,\lfloor(n-2)/2\rfloor,\lceil(n-2)/2\rceil)\right).\end{aligned} \tag{7}$$

By calculation, we get

$$\begin{aligned}J\left(T_n(3,1,n-3)\right)&=O\left(\frac{n}{\sqrt{2}}\right),\\ J\left(\left(T_n(3,\lfloor(n-2)/2\rfloor,\lceil(n-2)/2\rceil)\right)=O\left(\frac{2n}{\sqrt{15}}\right)\right).\end{aligned} \tag{8}$$

Hence, we obtain

$$O\left(\frac{2n}{\sqrt{15}}\right)\le J\left(T_n(3,a,b)\right)\le O\left(\frac{n}{\sqrt{2}}\right). \tag{9}$$

□

3. The Balaban Indices of Trees with Diameter 4

In this section, we present some asymptotic bounds for the Balaban indices of trees with diameter 4.

Theorem 2. *For any tree $T_n^l(4,a_1,a_2,\ldots,a_l)\in\mathcal{T}_n^l(4,a_1,a_2,\ldots,a_l)$, we have*

$$J\left(4,a_1,a_2,\ldots,a_l\right)\le O\left(\frac{n}{\sqrt{2}}\right). \tag{10}$$

Proof. The Balaban index of a tree $T_n^l(4,a_1,a_2,\ldots,a_l)$ is as follows:

$$J\left(T_n^l(4,a_1,a_2,\ldots,a_l)\right)=(n-1)\cdot\left[\sum_{i=1}^{l}\frac{a_i}{\sqrt{(4n-2a_i-l-6)(3n-2a_i-l-4)}}+\sum_{i=1}^{l}\frac{1}{\sqrt{(2n-l-2)(3n-2a_i-l-4)}}\right]. \tag{11}$$

Suppose $1\le a_1\le a_2$, and let $a_1=a$ and $c=n-a-a_2$. Then,

$$J\left(T_n^l(4,a_1,a_2,\ldots,a_l)\right) = (n-1)\cdot\left[\begin{array}{c} \frac{a}{\sqrt{(4n-2a-l-6)(3n-2a-l-4)}} \\ +\frac{n-a-c}{\sqrt{(2n+2a+2c-l-6)(n+2a+2c-l-4)}} \\ +\sum_{i=3}^{l}\frac{a_i}{\sqrt{(4n-2a_i-l-6)(3n-2a_i-l-4)}} \\ +\frac{1}{\sqrt{(2n-l-2)(3n-2a-l-4)}}+\frac{1}{\sqrt{(2n-l-2)(n+2a+2c-l-4)}} \\ +\sum_{i=3}^{l}\frac{1}{\sqrt{(2n-l-2)(3n-2a_i-l-4)}} \end{array}\right]. \tag{12}$$

And we get the derivative of $J(T_n^l(4,a,a_2,\ldots,a_l))$ related to a as follows:

$$\frac{\partial J\left(T_n^l(4,a,a_2,\cdots,a_l)\right)}{\partial a} = (n-1)\cdot\left[\begin{array}{c} \frac{-2-l+2n}{((-2-l+2n)(-4-2a-l+3n))^{3/2}} \\ +\frac{1}{((-4-2a-l+3n)(-6-2a-l+4n))^{1/2}} \\ -\frac{-2-l+2n}{((-2-l+2n)(-4-l+n+2a+2c))^{3/2}} \\ -\frac{1}{((-4-l+n+2a+2c)(-6-l+2n+2a+2c))^{1/2}} \\ +\frac{a(-20-8a-4l+14n)}{2((-4-2a-l+3n)(-6-2a-l+4n))^{3/2}} \\ -\frac{(-a-c+n)(-20-4l+6n+8a+8c)}{2((-4-l+n+2a+2c)(-6-l+2n+2a+2c))^{3/2}} \end{array}\right]. \tag{13}$$

The sum of positive terms above is denoted by $S^+(n,a,l)$, i.e.,

$$S^+(n,a,l) = (n-1)\cdot\left[\begin{array}{c} \frac{-2-l+2n}{((-2-l+2n)(-4-2a-l+3n))^{3/2}} \\ +\frac{1}{((-4-2a-l+3n)(-6-2a-l+4n))^{1/2}} \\ +\frac{a(-20-8a-4l+14n)}{2((-4-2a-l+3n)(-6-2a-l+4n))^{3/2}} \end{array}\right]. \tag{14}$$

And the sum of absolute values of negative terms above is denoted by $S^-(n,a,l)$, i.e.,

$$S^{-}(n,a,l)=(n-1)\cdot\left[\frac{-2-l+2n}{((-2-l+2n)(-4-l+n+2a+2c))^{3/2}}+\frac{1}{((-4-l+n+2a+2c)(-6-l+2n+2a+2c))^{1/2}}+\frac{(-a-c+n)(-20-4l+6n+8a+8c)}{2((-4-l+n+2a+2c)(-6-l+2n+2a+2c))^{3/2}}\right]. \quad (15)$$

Then, we use $S^{+}(n,a,l)$ to divide $S^{-}(n,a,l)$, and we get

$$\lim_{n\longrightarrow\infty}\frac{S^{-}(n,a,l)}{S^{+}(n,a,l)}=\frac{5}{2^{3/2}}>1. \quad (16)$$

So, the derivative of $J(T_n^l(4,a_1,a_2,\ldots,a_l))$ related to a_1 is less than 0 as n is big enough. It means that the corresponding Balaban index increases along with the number of pendent edges a_1 decreasing and the number of pendent edges a_2 increasing, i.e.,

$$J\left(T_n^l(4,a_1,a_2,\ldots,a_l)\right)\leq J\left(T_n^l(4,a_1-1,a_2+1,\ldots,a_l)\right). \quad (17)$$

Analogously, we obtain

$$\begin{aligned}J\left(T_n^l(4,a_1,a_2,\ldots,a_l)\right)&\leq J\left(T_n^l(4,1,a_1+a_2+a_3+\cdots a_l-1,0,\ldots,0)\right)\\&=J\left(T_n^l(4,1,n-l-2,0,\ldots,0)\right).\end{aligned} \quad (18)$$

For the above tree $T_n^l(4,1,n-l-2,0,\ldots,0)$, it can be seen that there are only two numbers, i.e., 1 and $n-l-2$, as the numbers of pendent edges, respectively, attach to two pendent vertices of a star S_{l+1}. Thus, it is easy to check that

$$J\left(T_n^l(4,1,n-l-2,0,\ldots,0)\right)=O\left(\frac{n}{\sqrt{2}}\right). \quad (19)$$

Hence,

$$J\left(T_n^l(4,a_1,a_2,\ldots,a_l)\right)\leq O\left(\frac{n}{\sqrt{2}}\right). \quad (20)$$

On the contrary, the asymptotically tight lower bound of such a tree is not easy to be given due to the determination of parameter l, but we find that, in $\mathcal{T}_n^l(4,a_1,a_2,\ldots,a_l)$, the tree attained the asymptotically tight lower bound which possesses a property satisfying $|a_i-a_j|\leq 1$ for $1\leq i\neq j\leq l$. In case of $l=2$, we obtain the following result. □

Theorem 3. *For any tree* $T_n^2(4,a_1,a_2)\in\mathcal{T}_n^2(4,a_1,a_2)$, *where* $1\leq a_1\leq a_2$, *we have*

$$J\left(T_n^2(4,a_1,a_2)\right)\geq O\left(\frac{n}{\sqrt{6}}\right). \quad (21)$$

Proof. From the proof of Theorem 2, we see that the derivative of $J(T_n^2(4,a_1,a_2))$ related to a_1 is less than 0 as n is big enough. Thus, if $a_1=\lfloor n-3/2\rfloor, a_2=\lceil n-3/2\rceil$, then

$$J\left(T_n^2(4,a_1,a_2)\right)\geq J\left(T_n^2\left(4,\left\lfloor\frac{n-3}{2}\right\rfloor,\left\lceil\frac{n-3}{2}\right\rceil\right)\right). \quad (22)$$

Note that

$$J\left(T_n^2\left(4,\left\lfloor\frac{n-3}{2}\right\rfloor,\left\lceil\frac{n-3}{2}\right\rceil\right)\right)=O\left(\frac{n}{\sqrt{6}}\right). \quad (23)$$

Thus,

$$J\left(T_n^2(4,a_1,a_2)\right)\geq O\left(\frac{n}{\sqrt{6}}\right). \quad (24)$$

□

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

This research was supported by the NSFQH (no. 2018-ZJ-925Q) and NSFC (no. 11701311).

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