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On the Atom-Bond Connectivity Index of Two-Trees

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Abstract The atom-bond connectivity (ABC) index of a graph G, introduced by Estrada, Torres, Rodríguez and Gutman in 1998, is defined as the sum of the weights $\sqrt{\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}}$ of all edges v_iv_j of G, where d_i denotes the degree of the vertex v_i in G. In this paper, we give an upper bound of the ABC index of a two-tree G with n vertices, that is, $ABC(G)\le(2n-4)\frac{\sqrt{2}}{2}+\frac{\sqrt{2n-4}}{n-1}$. We also determine the two-trees with the maximum and the second maximum ABC index.

Keywords graph; two-trees; atom-bond connectivity; index

MR(2010) Subject Classification 05C35; 05C50

1. Introduction

Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [1]. On the topological indices, there are many publications [2–10]. One of the most important topological indices is the Randić index, which is aimed at use in the modeling of the branching of the carbon-atom skeleton of alkanes, introduced by Randić [11]. But a great variety of physico-chemical properties rest on factor rather than branching. In order to take this into consideration, Estrada et al. proposed a new index, known as the atom-bond connectivity (ABC) index [12] of graph G, which is defined as the sum of $\sqrt{\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}}$ of all edges v_iv_j of G, where $E(G)$ denotes the edge set and d_i denotes the degree of the vertex v_i of G, i.e.,

$$ABC(G)=\sum\nolimits_{v_iv_j\in E(G)}\sqrt{\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}}.$$

The ABC index keeps the spirit of the Randić index and it provides a good model for the stability of branched alkanes as well as the strain of cycloalkanes [12,13]. In 2009, Furtula et al. [14] studied the mathematical properties of ABC index of trees and proved that the star

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tree has the maximal ABC value among all trees with n ($n \geq 2$) vertices. Bollobás and Erdös [15] found that the Randić index of a graph decreases when an edge with maximal weight is deleted. For the ABC index of graphs, Chen and Guo [16] proved that the ABC index of a graph decreases when any edge is deleted.

The ABC index has an important result, for example, Chen et al. [17] showed that among all n-vertex graphs with vertex connectivity k, the graph $K_k \vee (K_1 \cup K_{n-k-1})$ is the unique graph with maximum ABC index. Gutman and Furtula [18] showed that the structure of trees with a single high-degree vertex and smallest ABC is determined. Gan et al. [19] characterized the trees with given degree sequences, extremal w.r.t. the ABC index. Lin et al. [20] proved that for any degree sequence π, there exists a BFS-graph with minimal ABC index in $C(\pi)$ and the result is applicable to obtain the minimal value or lower bounds of ABC index of connected graphs. For more results on the ABC index, we refer to [21–30].

The two-tree is defined as follows.

Step 1. When $t = 0$, let $G_0 = K_2$, where K_2 (an edge) is a two-tree with 2 vertices.

Step 2. Let G_t be a two-tree generated at the t-th step. Then, G_{t+1} generated at the $(t+1)$ step is the graph obtained from G_t by adding a new vertex adjacent to the two end vertices of one edge. Clearly, G_{t+1} has $t+3$ vertices.

The two-tree has a very important structure in complex networks. It is known that the small-world Farey graph [31], fractal scale-free networks [32], the pseudofractal scale-free web [33] and the generalized Farey graph [34] are some special classes of two-tree networks.

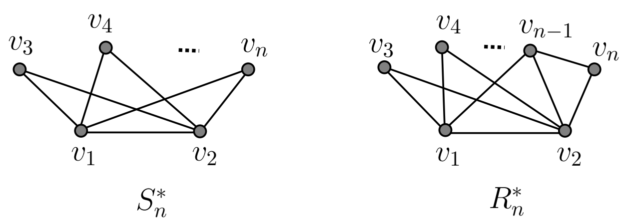

Figure 1 The graphs S_n^* and R_n^*

Let S_n^* denote the graph obtained from the complete bipartite graph $K_{2,n-2}$ by adding one edge in the part with two vertices (see Figure 1). Let R_n^* denote the graph obtained from the graph S_{n-1}^* by adding a new vertex and two new edges adjacent to the new vertex such that one edge is incident to a vertex of degree 2 in S_{n-1}^* and the other is incident to a vertex of degree $n-2$ in S_{n-1}^* (see Figure 1).

In this paper, we investigate the ABC index of two-trees and obtain the following results.

Theorem 1.1 *Let G be a two-tree with n ($n \geq 4$) vertices. Then*

$$ABC(G) \leq (2n-4)\frac{\sqrt{2}}{2} + \frac{\sqrt{2n-4}}{n-1}$$

with the equality holding if and only if $G \cong S_n^*$.

Theorem 1.2 *Let G be a two-tree with n $(n \geq 5)$ vertices and $G \neq S_n^*$. Then*

$$ABC(G) \leq ABC(R_n^*) = (n-3)\sqrt{2} + \sqrt{\frac{2n-5}{(n-1)(n-2)}} + \sqrt{\frac{n}{3(n-1)}} + \sqrt{\frac{n-1}{3(n-2)}}.$$

2. Preliminary

In this section, we prove some lemmas, which is a preparation of our main results.

Observation 2.1 *Let $g(d_1, d_2) = \sqrt{\frac{1}{d_1} + \frac{1}{d_2} - \frac{2}{d_1 d_2}}$. Then $g(2, d_2) = g(d_1, 2) = \frac{\sqrt{2}}{2}$.*

Lemma 2.2 *Let d_1, d_2 be two integers with $d_1, d_2 \geq 2$. Then the function $g(d_1, d_2) = \sqrt{\frac{1}{d_1} + \frac{1}{d_2} - \frac{2}{d_1 d_2}}$ is monotonic decreasing for d_i $(i = 1, 2)$ and $g_{\max}(2, d_2) = g_{\max}(d_1, 2) = \frac{\sqrt{2}}{2}$.*

Proof Note that $\frac{\partial g}{\partial d_1} = \frac{2-d_2}{2d_1\sqrt{d_1 d_2 (d_1+d_2-2)}}$. Since $d_1, d_2 \geq 2$, it follows that $\frac{\partial g}{\partial d_1} \leq 0$ and hence $g(d_1, d_2)$ is monotonic decreasing for d_1. Therefore, $g_{\max}(2, d_2) = g_{\max}(d_1, 2) = \frac{\sqrt{2}}{2}$. □

Lemma 2.3 *Let x be an integer with $x \geq 3$. Then the function*

$$f(x) = \sqrt{\frac{1}{x} + \frac{1}{x} - \frac{2}{x^2}} - \sqrt{\frac{1}{x+1} + \frac{1}{x+1} - \frac{2}{(x+1)^2}}$$

is monotonic decreasing for x.

Proof Observe that

$$f(x) = \sqrt{\frac{2}{x} - \frac{2}{x^2}} - \sqrt{\frac{2}{x+1} - \frac{2}{(x+1)^2}}$$

and

$$f'(x) = \frac{2-x}{x^2\sqrt{2x-2}} - \frac{1-x}{\sqrt{2x}(x+1)^2} = \frac{x-1}{\sqrt{2x}(x+1)^2} - \frac{x-2}{x^2\sqrt{2x-2}}.$$

Therefore, we have

$$\Big(\frac{x-1}{\sqrt{2x}(x+1)^2}\Big)^2 - \Big(\frac{x-2}{x^2\sqrt{2x-2}}\Big)^2 = \frac{2x(-3x^5+9x^4+3x^3-9x^2-12x-4)}{4x^5(x-1)(x+1)^4}.$$

Since the maximum root of $-3x^5+9x^4+3x^3-9x^2-12x-4$ is less than 3, it follows that $-3x^5+9x^4+3x^3-9x^2-12x-4 < 0$ for $x \geq 3$, which implies

$$\frac{x-1}{\sqrt{2x}(x+1)^2} - \frac{x-2}{x^2\sqrt{2x-2}} < 0.$$

Hence $f'(x) < 0$ for $x \geq 3$, as desired. □

Lemma 2.4 *Let x be an integer with $x \geq 3$. Then the function*

$$f(x) = \sqrt{\frac{1}{x} + \frac{1}{x+1} - \frac{2}{x(x+1)}} - \sqrt{\frac{1}{x+1} + \frac{1}{x+1} - \frac{2}{(x+1)(x+1)}}$$

is monotonic decreasing for x.

Proof Observe that

$$f'(x) = \frac{1}{2\sqrt{x}(x+1)^{\frac{3}{2}}}(\frac{\sqrt{2}(x-1)}{(x+1)^{\frac{1}{2}}} - \frac{2x^2-2x-1}{x\sqrt{2x-1}}).$$

Let $a = \frac{\sqrt{2}(x-1)}{(x+1)^{\frac{1}{2}}}$ and $b = \frac{2x^2-2x-1}{x\sqrt{2x-1}}$. Then $a^2 - b^2 = \frac{-6x^4+16x^3-6x^2-5x-1}{x^2(x+1)(2x-1)}$ for $x \geq 3$. Since $-6x^4+16x^3-6x^2-5x-1 < x^3(-6x+16) < 0$, it follows that $a^2 - b^2 < 0$. Since $a+b > 0$, it follows that $a - b < 0$ and hence $\frac{\sqrt{2}(x-1)}{(x+1)^{\frac{1}{2}}} - \frac{2x^2-2x-1}{x\sqrt{2x-1}} < 0$. So $f'(x) < 0$ and the result holds. □

Lemma 2.5 *Let x and y be two integers with $y \geq x \geq 2$. Then*

$$\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}} - \sqrt{\frac{1}{x+1}+\frac{1}{y+1}-\frac{2}{(x+1)(y+1)}} \geq \sqrt{\frac{2}{y}-\frac{2}{y^2}} - \sqrt{\frac{2}{y+1}-\frac{2}{(y+1)^2}}.$$

Proof Notice that

$$\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}} - \sqrt{\frac{1}{x+1}+\frac{1}{y+1}-\frac{2}{(x+1)(y+1)}} - (\sqrt{\frac{1}{y}+\frac{1}{y}-\frac{2}{y^2}} - \sqrt{\frac{1}{y+1}+\frac{1}{y+1}-\frac{2}{(y+1)^2}})$$
$$= \sqrt{\frac{1}{y}}(\sqrt{\frac{x+y-2}{x}} - \sqrt{\frac{y+y-2}{y}}) + \sqrt{\frac{1}{y+1}}(\sqrt{\frac{y+y}{y+1}} - \sqrt{\frac{x+y}{x+1}}).$$

Set $L(x,y) = \sqrt{\frac{1}{y}}(\sqrt{\frac{x+y-2}{x}} - \sqrt{\frac{y+y-2}{y}}) + \sqrt{\frac{1}{y+1}}(\sqrt{\frac{y+y}{y+1}} - \sqrt{\frac{x+y}{x+1}})$. When $x = y$, one can easily check that $L(x,y) = 0$. We now suppose $y > x$. From Lemma 2.2, we have $\sqrt{\frac{1}{y}}(\sqrt{\frac{x+y-2}{x}} - \sqrt{\frac{y+y-2}{y}}) > 0$ and $\sqrt{\frac{1}{y+1}}(\sqrt{\frac{y+y}{y+1}} - \sqrt{\frac{x+y}{x+1}}) < 0$. Since $\sqrt{\frac{1}{y}} > \sqrt{\frac{1}{y+1}}$, it suffices to show that $\sqrt{\frac{x+y-2}{x}} \geq \sqrt{\frac{x+y}{x+1}}$ and $\sqrt{\frac{y+y-2}{y}} < \sqrt{\frac{y+y}{y+1}}$.

Consider the latter case. Observe that $\frac{y+y-2}{y} - \frac{y+y}{y+1} = \frac{-2}{y(y+1)} < 0$, which implies that $\sqrt{\frac{y+y-2}{y}} < \sqrt{\frac{y+y}{y+1}}$.

Consider the former case. Note that $\frac{x+y-2}{x} - \frac{x+y}{x+1} = \frac{y-x-2}{x(x+1)}$. Suppose that $y = x+k$ and $k \geq 1$. If $k \geq 2$, then $\frac{k-2}{x(x+1)} \geq 0$, so $\frac{x+y-2}{x} - \frac{x+y}{x+1} = \frac{k-2}{x(x+1)} \geq 0$, which implies that $\sqrt{\frac{x+y-2}{x}} - \sqrt{\frac{x+y}{x+1}} \geq 0$ $(k \geq 2)$. From the above arguments, we have $L(x,y) \geq 0$ for $k \geq 2$. If $k = 1$, then $L(x,y) = \sqrt{\frac{2x-1}{x(x+1)}} - \sqrt{\frac{2x+1}{(x+1)(x+2)}} - (\sqrt{\frac{2x}{(x+1)(x+1)}} - \sqrt{\frac{2x+2}{(x+2)(x+2)}})$. By Lemma 2.4, we can get $L(x,y) > 0$. So, we have

$$\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}} - \sqrt{\frac{1}{x+1}+\frac{1}{y+1}-\frac{2}{(x+1)(y+1)}} \geq \sqrt{\frac{2}{y}-\frac{2}{y^2}} - \sqrt{\frac{2}{y+1}-\frac{2}{(y+1)^2}}. \quad \square$$

Lemma 2.6 *Let x and y be two integers with $x \geq 3, y \geq 2$. Then the function*

$$f(x,y) = \sqrt{\frac{1}{x-1}+\frac{1}{y}-\frac{2}{(x-1)y}} - \sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}$$

is monotonic increasing for y.

Proof For fixing x, it follows that $\frac{\partial f}{\partial y} = \frac{x-2}{2\sqrt{y^3}\cdot\sqrt{x}\cdot\sqrt{x+y-2}} - \frac{x-3}{2\sqrt{y^3}\cdot\sqrt{x-1}\cdot\sqrt{x+y-3}} = \frac{1}{2\sqrt{y^3}}(\frac{x-2}{\sqrt{x}\cdot\sqrt{x+y-2}} -$

$\frac{x-3}{\sqrt{x-1}\cdot\sqrt{x+y-3}}$). By computation, we have

$$\begin{aligned}0 <&(x^2-x-4)y+2(x-2)(x-3)\\ =&(x-2)^2(x-1)(x+y-3)-(x-3)^2x(x+y-2),\end{aligned}$$

which leads to

$$\frac{x-2}{\sqrt{x}\cdot\sqrt{x+y-2}} > \frac{x-3}{\sqrt{x-1}\cdot\sqrt{x+y-3}}.$$

That is, $\frac{\partial f}{\partial y} > 0$, which implies that the lemma is true. □

Lemma 2.7 *Let x, y be two integers with $x \geq 3, y \geq 2$. Then*

$$f(x,y) = \sqrt{\frac{1}{x-1}+\frac{1}{y}-\frac{2}{(x-1)y}} - \sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}$$

is monotonic decreasing for x.

Proof Note that

$$\frac{\partial f}{\partial x} = \frac{y-2}{2x\sqrt{xy(x+y-2)}} - \frac{y-2}{2(x-1)\sqrt{(x-1)y(x+y-3)}}.$$

Since

$$(x-1)\sqrt{(x-1)y(x+y-3)} < x\sqrt{xy(x+y-2)},$$

we have

$$\frac{y-2}{x\sqrt{xy(x+y-2)}} < \frac{y-2}{(x-1)\sqrt{(x-1)y(x+y-3)}}.$$

Hence $\frac{\partial f}{\partial x} < 0$, as desired. □

Lemma 2.8 *Let y be an integer with $y \geq 6$. Then the function*

$$f(y) = \sqrt{\frac{1}{y}+\frac{1}{y}-\frac{2}{y^2}} - \sqrt{\frac{1}{y}+\frac{1}{y+1}-\frac{2}{y(y+1)}}$$

is monotonic decreasing for y.

Proof Note that

$$\begin{aligned}f'(y) =&\frac{2-y}{y^2\sqrt{2y-2}} - \frac{2y+1-2y^2}{2y^{\frac{3}{2}}(x+1)^{\frac{3}{2}}\sqrt{2y-1}} \leq \frac{2-y}{y^2\sqrt{2y-2}} - \frac{2y+1-2y^2}{2y^{\frac{3}{2}}(y+1)^{\frac{3}{2}}\sqrt{2y-2}}\\ \leq&\frac{2-y}{y^2\sqrt{2y-2}} + \frac{2y^2-2y}{2y^{\frac{3}{2}}(y+1)^{\frac{3}{2}}\sqrt{2y-2}} = \frac{1}{y^{\frac{3}{2}}\sqrt{2y-2}}\Big(\frac{y^2-y}{(y+1)^{\frac{3}{2}}} - \frac{y-2}{\sqrt{y}}\Big).\end{aligned}$$

Let $a = \frac{y^2-y}{(y+1)^{\frac{3}{2}}}$ and $b = \frac{y-2}{\sqrt{y}}$. Then $a^2-b^2 = \frac{-y^4+6y^3-y^2-8y-4}{y(y+1)^3}$. For $y \geq 6$, $-y^4+6y^3-y^2-8y-4 < y^3(-y+6) \leq 0$, so we have $a^2-b^2 = \frac{-y^4+6y^3-y^2-8y-4}{y(y+1)^3} < 0$, which implies that $f'(y) < 0$, as desired. □

Lemma 2.9 *Let x be an integer with $x \geq 2$. Then the function*

$$f(x) = \sqrt{\frac{1}{x}+\frac{1}{x+1}-\frac{2}{x(x+1)}} - \sqrt{\frac{1}{x+1}+\frac{1}{x+2}-\frac{2}{(x+1)(x+2)}}$$

is monotonic decreasing for x*.*

Proof Notice that

$$f'(x)=\frac{1}{2}\Big(\frac{2x^2+2x-1}{(x+1)(x+2)\sqrt{(x+1)(x+2)(2x+1)}}-\frac{2x^2-2x-1}{x(x+1)\sqrt{x(x+1)(2x-1)}}\Big).$$

Set $a=\frac{2x^2+2x-1}{(x+1)(x+2)\sqrt{(x+1)(x+2)(2x+1)}}$ and $b=\frac{2x^2-2x-1}{x(x+1)\sqrt{x(x+1)(2x-1)}}$. Then

$$a^2-b^2=\frac{-24x^7-24x^6+112x^5+144x^4-70x^3-142x^2-60x-8}{(x+1)^3(x+2)^3(2x+1)(2x-1)x^3}.$$

Observe that $-24x^7-24x^6+112x^5+144x^4-70x^3-142x^2-60x-8<8x^4(-3x^3-3x^2+14x+18)$. Since $-3x^3-3x^2+14x+18=x(-3x^2-3x+14)+18<0$, it follows that $a^2-b^2<0$. For $x\geq 3$, from above $-24x^7-24x^6+112x^5+144x^4-70x^3-142x^2-60x-8<0$. Then $a^2-b^2<0$ and hence $a-b<0$. Therefore, $f'(x)<0$ for $x\geq 3$. The result follows. □

Lemma 2.10 *Let* x,y *be two integers with* $y\geq x\geq 3$*. Then*

$$\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}-\sqrt{\frac{1}{x+1}+\frac{1}{y+1}-\frac{2}{(x+1)(y+1)}}$$
$$>\sqrt{\frac{1}{y}+\frac{1}{y+1}-\frac{2}{y(y+1)}}-\sqrt{\frac{1}{y+1}+\frac{1}{y+2}-\frac{2}{(y+1)(y+2)}}.$$

Proof Set $M=\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}-\sqrt{\frac{1}{x+1}+\frac{1}{y+1}-\frac{2}{(x+1)(y+1)}}$ and $N=\sqrt{\frac{1}{y}+\frac{1}{y+1}-\frac{2}{y(y+1)}}-\sqrt{\frac{1}{y+1}+\frac{1}{y+2}-\frac{2}{(y+1)(y+2)}}$.

Suppose $y=x$. From Lemma 2.8, we have $M-N>0$ for $y\geq 6$. When $y=3,4,5$, one can easily check that $M-N>0$.

Suppose $y>x$. Note that

$$M-N=\sqrt{\frac{1}{y}}\Big(\sqrt{\frac{x+y-2}{x}}-\sqrt{\frac{2y-1}{y+1}}\Big)-\sqrt{\frac{1}{y+1}}\Big(\sqrt{\frac{x+y}{x+1}}-\sqrt{\frac{2y+1}{y+2}}\Big).$$

Let $y=x+k$ $(k\geq 1)$. From Lemma 2.2, we have $\sqrt{\frac{1}{y}}(\sqrt{\frac{x+y-2}{x}}-\sqrt{\frac{2y-1}{y+1}})>0$ and $\sqrt{\frac{1}{y+1}}(\sqrt{\frac{x+y}{x+1}}-\sqrt{\frac{2y+1}{y+2}})>0$. Since $\sqrt{\frac{1}{y}}>\sqrt{\frac{1}{y+1}}$, it suffices to show that $\sqrt{\frac{x+y-2}{x}}\geq\sqrt{\frac{x+y}{x+1}}$ and $\sqrt{\frac{2y+1}{y+2}}>\sqrt{\frac{2y-1}{y+1}}$.

Consider the latter case. Observe that $\frac{2y-1}{y+1}-\frac{2y+1}{y+2}=\frac{-3}{(y+1)(y+2)}<0$, that is, $\sqrt{\frac{2y-1}{y+1}}-\sqrt{\frac{2y+1}{y+2}}<0$, as desired.

Consider the former case. For $y\geq x+2$, $\frac{x+y-2}{x}-\frac{x+y}{x+1}=\frac{y-x-2}{x(x+1)}\geq 0$; for $y=x+1$, by Lemma 2.9 we have $M>N$.

From above arguments, we know that $M>N$. □

Lemma 2.11 *Let* x,y *be two integers with* $y>x\geq 3$*. Then*

$$\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}-\sqrt{\frac{1}{x+1}+\frac{1}{y+1}-\frac{2}{(x+1)(y+1)}}$$

$$\geq \sqrt{\frac{1}{y-1}+\frac{1}{y}-\frac{2}{(y-1)y}}-\sqrt{\frac{1}{y}+\frac{1}{y+1}-\frac{2}{y(y+1)}},$$

where the equality holds if and only if $y=x+1$.

Proof Set $M'=\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}-\sqrt{\frac{1}{x+1}+\frac{1}{y+1}-\frac{2}{(x+1)(y+1)}}$ and $N'=\sqrt{\frac{1}{y-1}+\frac{1}{y}-\frac{2}{(y-1)y}}-\sqrt{\frac{1}{y}+\frac{1}{y+1}-\frac{2}{y(y+1)}}$.

Note that

$$M'-N'=\sqrt{\frac{1}{y}}\Big(\sqrt{\frac{x+y-2}{x}}-\sqrt{\frac{2y-3}{y-1}}\Big)-\sqrt{\frac{1}{y+1}}\Big(\sqrt{\frac{x+y}{x+1}}-\sqrt{\frac{2y-1}{y}}\Big).$$

Since $y\geq x+1$, we have $\sqrt{\frac{x+y-2}{x}}-\sqrt{\frac{2y-3}{y-1}}\geq 0$ and $\sqrt{\frac{x+y}{x+1}}-\sqrt{\frac{2y-1}{y}}\geq 0$, where the equality holds if and only if $y=x+1$. Since $\sqrt{\frac{1}{y}}>\sqrt{\frac{1}{y+1}}$, it suffices to show that $\sqrt{\frac{x+y-2}{x}}\geq\sqrt{\frac{x+y}{x+1}}$ and $\sqrt{\frac{2y-1}{y}}>\sqrt{\frac{2y-3}{y-1}}$.

A similar argument of Lemma 2.10, the lemma is true. $\Box$

3. Proofs of main results

We are now in a position to prove our main results.

Proof of Theorem 1.1 We prove this theorem by induction on n. Let T_n be a two-tree with n vertices.

For $n=4$, the two-tree T_n is a unique graph obtained from the complete graph of order 4 by deleting one edge. Clearly, $ABC(T_n)=2\sqrt{2}+\frac{2}{3}\sqrt{3}=(2n-4)\frac{\sqrt{2}}{2}+\frac{\sqrt{2n-4}}{n-1}$, as desired.

Suppose that the result holds for all integers smaller than n. Pick up one vertex of degree 2 from the graph T_n, say w. Observe that T_n-w is a two-tree of order $n-1$. By induction hypothesis, $ABC(T_n-w)\leq ABC(S^*_{n-1})$ with the equality holding if and only if $T_n-w\cong S^*_{n-1}$. Now we prove that $ABC(T_n)\leq ABC(S^*_n)$.

Let u and v be two vertices adjacent to the vertex w in T_n. Let $d_{T_n}(u)=x$ and $d_{T_n}(v)=y$, where $d_{T_n}(u)$ denotes the degree of the vertex u in T_n. Clearly, $3\leq x\leq n-1$ and $3\leq y\leq n-1$. Without loss of generality, let $y\geq x\geq 3$. Notice that

$$\begin{aligned}ABC(T_n)&\leq ABC(T_n-w)+\sqrt{2}-\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(x-1)(y-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big)\\&\leq ABC(S^*_{n-1})+\sqrt{2}-\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(x-1)(y-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big).\end{aligned}$$

Set

$$M''=\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(x-1)(y-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}$$

and

$$N''=\sqrt{\frac{1}{n-2}+\frac{1}{n-2}-\frac{2}{(n-2)^2}}-\sqrt{\frac{1}{n-1}+\frac{1}{n-1}-\frac{2}{(n-1)^2}}.$$

Then

$$\begin{aligned}
M''-N'' =&\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(x-1)(y-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}-\\
&\sqrt{\frac{1}{n-2}+\frac{1}{n-2}-\frac{2}{(n-2)^2}}+\sqrt{\frac{1}{n-1}+\frac{1}{n-1}-\frac{2}{(n-1)^2}}\\
\geq&\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(x-1)(y-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}-\\
&\Big(\sqrt{\frac{1}{y-1}+\frac{1}{y-1}-\frac{2}{(y-1)^2}}-\sqrt{\frac{1}{y}+\frac{1}{y}-\frac{2}{y^2}}\Big) \quad \text{(by Lemma 2.3)}\\
\geq&0 \quad \text{(by Lemma 2.5)}.
\end{aligned}$$

Hence

$$\begin{aligned}
&ABC(T_n)\\
&\leq ABC(S^*_{n-1})+\sqrt{2}-\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(x-1)(y-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big)\\
&\leq ABC(S^*_{n-1})+\sqrt{2}-\Big(\sqrt{\frac{1}{n-2}+\frac{1}{n-2}-\frac{2}{(n-2)^2}}-\sqrt{\frac{1}{n-1}+\frac{1}{n-1}-\frac{2}{(n-1)^2}}\Big)\\
&=ABC(S^*_n),
\end{aligned}$$

where the equality holds if and only if $T_n - w = S^*_{n-1}$ and $x = y = n-1$, which completes the proof. □

Proof of Theorem 1.2 We prove this theorem by induction on n. Let T_n be a two-tree with n vertices and $T_n \neq S^*_n$.

For $n = 5$, one can see that $T_n = S^*_n$ or $T_n = R^*_n$. Since $T_n \neq S^*_n$, we have $T_n = R^*_n$. One can see that $ABC(T_n) = 2\sqrt{2}+\frac{2}{3}+\frac{\sqrt{15}}{3} = (n-3)\sqrt{2}+\sqrt{\frac{2n-5}{(n-1)(n-2)}}+\sqrt{\frac{n}{3(n-1)}}+\sqrt{\frac{n-1}{3(n-2)}}$, as desired.

Suppose that the result holds for any integer smaller than n. Choose one vertex w of degree 2 from the graph T_n such that $T_n - w \neq S^*_{n-1}$. By induction hypothesis, $ABC(T_n - w) \leq ABC(R^*_{n-1})$. Our aim is to prove that $ABC(T_n) \leq ABC(R^*_n)$.

Let u and v be two vertices adjacent to the vertex w in T_n. Then there must exist a vertex p with $d_{T_n-w}(p) \geq 3$ (otherwise, $T_n - w \cong S^*_{n-1}$). Let $d_{T_n}(u) = x$, $d_{T_n}(v) = y$ and $d_{T_n}(p) = a$. Then $3 \leq x, y, a \leq n-1$. Let $\max\{x, y, a\} = y$. Then $y \leq n-1$ and $\max\{x, a\} \leq n-2$ (Otherwise $T_n = S^*_n$).

By Lemma 2.2, we have that

$$\begin{aligned}
&ABC(T_n)\\
&\leq ABC(T_n-w)+\sqrt{2}-\Big(\sqrt{\frac{1}{x-1}+\frac{1}{a}-\frac{2}{a(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{a}-\frac{2}{xa}}\Big)-
\end{aligned}$$

$$\Big(\sqrt{\frac{1}{y-1}+\frac{1}{a}-\frac{2}{a(y-1)}}-\sqrt{\frac{1}{y}+\frac{1}{a}-\frac{2}{ya}}\Big)-$$
$$\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(y-1)(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big)$$
$$\le ABC(R_{n-1}^{*})+\sqrt{2}-\Bigg(\sqrt{\frac{1}{x-1}+\frac{1}{3}-\frac{2}{3(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{3}-\frac{2}{3x}}\Big)-$$
$$\Big(\sqrt{\frac{1}{y-1}+\frac{1}{3}-\frac{2}{3(y-1)}}-\sqrt{\frac{1}{y}+\frac{1}{3}-\frac{2}{3y}}\Big)-$$
$$\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(y-1)(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big)\ \text{(by Lemma 2.6)}$$
$$\le ABC(R_{n-1}^{*})+\sqrt{2}-\Big(\sqrt{\frac{1}{n-3}+\frac{1}{3}-\frac{2}{3(n-3)}}-\sqrt{\frac{1}{n-2}+\frac{1}{3}-\frac{2}{3(n-2)}}\Big)-$$
$$\Big(\sqrt{\frac{1}{n-2}+\frac{1}{3}-\frac{2}{3(n-2)}}-\sqrt{\frac{1}{n-1}+\frac{1}{3}-\frac{2}{3(n-1)}}\Big)-$$
$$\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(y-1)(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big)\ \text{(by Lemma 2.7).}$$

We now give a lower bound of $\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(y-1)(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}$.

For $x\le y\le n-2$, by Lemmas 2.9 and 2.10 we have

$$\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(y-1)(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big)-$$
$$\Big(\sqrt{\frac{1}{n-3}+\frac{1}{n-2}-\frac{2}{(n-2)(n-3)}}-\sqrt{\frac{1}{n-1}+\frac{1}{n-2}-\frac{2}{(n-1)(n-2)}}\Big)$$
$$>\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(y-1)(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big)-$$
$$\Big(\sqrt{\frac{1}{y-1}+\frac{1}{y}-\frac{2}{y(y-1)}}-\sqrt{\frac{1}{y}+\frac{1}{y+1}-\frac{2}{y(y+1)}}\Big)>0.$$

For $y=n-1$ and $y\ge x+1$, by Lemmas 2.9 and 2.11 we have

$$\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(y-1)(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big)-$$
$$\Big(\sqrt{\frac{1}{n-3}+\frac{1}{n-2}-\frac{2}{(n-2)(n-3)}}-\sqrt{\frac{1}{n-1}+\frac{1}{n-2}-\frac{2}{(n-1)(n-2)}}\Big)$$
$$\ge\Big(\sqrt{\frac{1}{x-1}+\frac{1}{y-1}-\frac{2}{(y-1)(x-1)}}-\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{xy}}\Big)-$$
$$\Big(\sqrt{\frac{1}{y-2}+\frac{1}{y-1}-\frac{2}{(y-2)(y-1)}}-\sqrt{\frac{1}{y-1}+\frac{1}{y}-\frac{2}{y(y-1)}}\Big)\ge 0,$$

where the equality holds if and only if $y = n-1$ and $x = n-2$. Therefore,

$$\begin{aligned}
&ABC(T_n)\\
&\le ABC(R^*_{n-1}) + \sqrt{2} - \Big(\sqrt{\frac{1}{3} + \frac{1}{n-3} - \frac{2}{3(n-3)}} - \sqrt{\frac{1}{3} + \frac{1}{n-2} - \frac{2}{3(n-2)}}\Big) - \\
&\Big(\sqrt{\frac{1}{3} + \frac{1}{n-2} - \frac{2}{3(n-2)}} - \sqrt{\frac{1}{3} + \frac{1}{n-1} - \frac{2}{3(n-1)}}\Big) - \\
&\Big(\sqrt{\frac{1}{n-3} + \frac{1}{n-2} - \frac{2}{(n-2)(n-3)}} - \sqrt{\frac{1}{n-1} + \frac{1}{n-2} - \frac{2}{(n-1)(n-2)}}\Big)\\
&= ABC(R^*_n),
\end{aligned}$$

where the equality holds if and only if $T_n - w = R^*_{n-1}$, $a = 3$, $x = n-2$ and $y = n-1$, which completes the proof. □

4. Concluding Remark

In this paper, we investigated ABC index of a two-tree, which has a very important structure in complex networks.

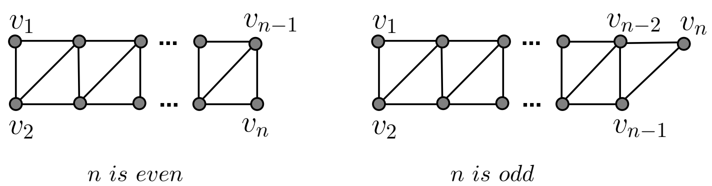

Figure 2 Graphs with $ABC(G) = 2\sqrt{2} + \frac{2\sqrt{15}}{3} + (2n-11)\frac{\sqrt{6}}{4}$

From Theorems 1.1 and 1.2, we determine the two-trees with the first two largest ABC index, but the two-trees with the minimum ABC index are still unknown, this seems to be a difficult problem. For the minimum ABC index, we conjecture the following result holds: For a two-tree G on n ($n \ge 6$) vertices, $ABC(G) \ge 2\sqrt{2} + \frac{2\sqrt{15}}{3} + (2n-11)\frac{\sqrt{6}}{4}$. The graph attaining this bound is shown in Figure 2.

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