On the Atom-Bond Connectivity Index of Two-Trees

Siyong YU¹, Haixing ZHAO²∗, Yaping MAO², Yuzhi XIAO¹
1. School of Computer, Qinghai Normal University, Qinghai 810008, P. R. China;
2. Department of Mathematics, Qinghai Normal University, Qinghai 810008, P. R. China

Abstract The atom-bond connectivity (ABC) index of a graph G, introduced by Estrada, Torres, Rodriguez 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, \( ABC(G) \leq (2n - 4)\frac{n}{4} + \frac{\sqrt{2n-4}}{2} \). We also determine the two-trees with the maximum and the second maximum ABC index.

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

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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.,

\[
ABC(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_id_j}}.
\]

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...
tree has the maximal $ABC$ value among all trees with $n \geq 2$ vertices. Bollobás and Erdős [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 $K_k \lor (K_1 \cup K_{n-k-1})$ 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 $\pi$, 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.

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 $n \geq 4$ 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 $g_{\text{max}}(2, d_2) = g_{\text{max}}(d_1, 2) = \frac{\sqrt{2}}{2}$.

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

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

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

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

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

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 $x$. 

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Proof Observe that
\[ f'(x) = \frac{1}{2\sqrt{x+1}} \left( \frac{\sqrt{2}(x-1)}{x+1} - \frac{2x^2 - 2x - 1}{x\sqrt{x-1}} \right). \]
Let \( a = \sqrt{\frac{x+1}{x}} \) and \( b = \frac{x^2-2x-1}{x\sqrt{x-1}} \). Then \( a^2 - b^2 = \frac{-6x^4 + 16x^2 - 5x - 1}{x^2(x+1)(2x-1)} \) for \( x \geq 3 \). Since \( -6x^4 + 16x^2 - 5x - 1 < x^3(-6x+16) < 0 \), it follows that \( a^2 - b^2 < 0 \). Since \( a + b > 0 \), it follows that \( a - b < 0 \) and hence \( \frac{\sqrt{x+1}}{x} > \frac{x^2 - 2x - 1}{x\sqrt{2x-1}} < 0 \). 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
\[ \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}} = \sqrt{\frac{1}{x+1} + \frac{1}{y+1} - \frac{2}{(x+1)(y+1)}} \geq \sqrt{\frac{y}{y+1} - \frac{2}{(y+1)^2}}. \]

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

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

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

Lemma 2.6 Let \( x \) and \( y \) be two integers with \( x \geq 3, y \geq 2 \). Then the function
\[ f(x,y) = \sqrt{\frac{1}{x-1} + \frac{1}{y} - \frac{2}{(x-1)y}} \]
is monotonic increasing for \( y \).

Proof For fixing \( x \), it follows that \( \frac{\partial f}{\partial y} = -\frac{x^2}{2\sqrt{y^3} \sqrt{3x+y-2}} - \frac{x-3}{2\sqrt{y^3} \sqrt{3x+y-2}} \frac{x-5}{2\sqrt{y^3} \sqrt{3x+y-2}} = \frac{1}{2\sqrt{y^3}} \left( \sqrt{3x+y-2} - \frac{3x+y-2}{2\sqrt{y^3}} \right) \). ***
Note that \( \frac{x^2 - 4}{\sqrt{x - 1} \sqrt{x + y - 3}} \). By computation, we have

\[
0 < (x^2 - x - 4)y + 2(x - 2)(x - 3) = (x - 2)^2(x + y - 3) - (x - 3)^2x(x + y - 2),
\]

which leads to

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

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

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

is monotonic decreasing for \( x \).

**Proof** Note that

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

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

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

is monotonic decreasing for \( y \).

**Proof** Note that

\[
f'(y) = \frac{2 - y}{y^2 \sqrt{2y - 2}} - \frac{2y + 1 - 2y^2}{2y^2 (x + 1)^{\frac{3}{2}} \sqrt{2y - 2}} \leq \frac{2 - y}{y^2 \sqrt{2y - 2}} - \frac{2y + 1 - 2y^2}{2y^2 (y + 1)^{\frac{3}{2}} \sqrt{2y - 2}}
\]

\[
\leq \frac{2 - y}{y^2 \sqrt{2y - 2}} + \frac{2y^2 - 2y}{2y^2 (y + 1)^{\frac{3}{2}} \sqrt{2y - 2}} = \frac{1}{y^2 \sqrt{2y - 2}} \left( \frac{y^2 - y}{(y + 1)^{\frac{3}{2}}} - \frac{y - 2}{\sqrt{y}} \right).
\]

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

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

\[
f(x) = \sqrt{\frac{1}{x} + \frac{1}{x + 1} - \frac{2}{x(x + 1)}} - \sqrt{\frac{1}{x + 1} + \frac{1}{x} - \frac{2}{(x + 1)(x + 2)}}
\]
Lemma 2.10 \textit{Let} \(x, y\) \textit{be two integers with} \(y \geq x \geq 3\). \textit{Then}

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

\textbf{Proof} \textit{Set} \(M = \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}}\) \textit{and} \(N = \sqrt{\frac{1}{x+1} + \frac{1}{y+1} - \frac{2}{(x+1)(y+1)}}\). \textit{Suppose} \(y = x\). \textit{From Lemma 2.8, we have} \(M - N > 0\) \textit{for} \(y \geq 6\). \textit{When} \(y = 3, 4, 5\), \textit{one can easily check that} \(M > N\).

\textit{Suppose} \(y > x\). \textit{Note that}

\[
M - N = \sqrt{\frac{1}{y} \left( \frac{x+y-2}{x} - \frac{2y-1}{y+1} \right)} - \frac{1}{y+1} \left( \frac{x+y}{x} - \frac{2y+1}{y+2} \right).
\]

\textit{Let} \(y = x + k\) \((k \geq 1)\). \textit{From Lemma 2.2, we have} \(\frac{1}{y} \left( \frac{x+y-2}{x} - \frac{2y-1}{y+1} \right) > 0\) \textit{and} \(\sqrt{\frac{1}{y} \left( \frac{x+y-2}{x} - \frac{2y+1}{y+2} \right)} > 0\). \textit{Since} \(\sqrt{\frac{x+y-2}{x}} > \sqrt[3]{\frac{1}{y+1}}\), \textit{it suffices to show that} \(\frac{x+y-2}{x} \geq \frac{x+y}{x+1}\) \textit{and} \(\sqrt{\frac{2y+1}{y+2}} > \sqrt[3]{\frac{2y-1}{y+1}}\).

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

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

\textit{From above arguments, we know that} \(M > N\). \(\square\)

Lemma 2.11 \textit{Let} \(x, y\) \textit{be two integers with} \(y \geq x \geq 3\). \textit{Then}

\[
\sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}} = \sqrt{\frac{1}{x+1} + \frac{1}{y+1} - \frac{2}{(x+1)(y+1)}}
\]

is monotonic decreasing for \(x\).
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 \( N' = \sqrt{\frac{1}{y-1} + \frac{1}{y} - \frac{2}{(y-1)y}} - \sqrt{\frac{1}{y+1} + \frac{1}{y} - \frac{2}{y(y+1)}} \).

Note that

\[
M' - N' = \frac{1}{y} \left( \sqrt{\frac{x+y-2}{x}} - \sqrt{\frac{2y-3}{y-1}} \right) - \frac{1}{y+1} \left( \sqrt{\frac{x+y}{x+1}} - \sqrt{\frac{2y-1}{y}} \right).
\]

Since \( y \geq x + 1 \), we have

\[
\sqrt{\frac{x+y-2}{x}} > \sqrt{\frac{2y-3}{y-1}} > 0 \quad \text{and} \quad \sqrt{\frac{x+y}{x+1}} > \sqrt{\frac{2y-1}{y}} > 0,
\]

where the equality holds if and only if \( y = x + 1 \). Since \( \frac{1}{y} > \frac{1}{y+1} \), it suffices to show that

\[
\sqrt{\frac{x+y-2}{x}} \geq \sqrt{\frac{x+y-2}{x}} \quad \text{and} \quad \sqrt{\frac{2y-3}{y-1}} > \sqrt{\frac{2y-1}{y}}.
\]

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, \( ABC(T_4) = 2\sqrt{2} + \frac{2}{3} \sqrt{3} = (2n - 4) \frac{2x}{3} + \frac{\sqrt{3n-3}}{n-1} \), 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

\[
ABC(T_n) \leq ABC(T_n - w) + \sqrt{2} - \left( \sqrt{\frac{1}{x-1} + \frac{1}{y-1} - \frac{2}{(x-1)(y-1)}} - \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}} \right)
\]

\[
\leq ABC(S_{n-1}^*) + \sqrt{2} - \left( \sqrt{\frac{1}{x-1} + \frac{1}{y-1} - \frac{2}{(x-1)(y-1)}} - \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}} \right).
\]

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
\[
M'' - N'' = \sqrt{\frac{1}{x-1} + \frac{1}{y-1} - \frac{2}{(x-1)(y-1)}} - \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}} \\
\geq \sqrt{\frac{1}{x-1} + \frac{1}{y-1} - \frac{2}{(x-1)(y-1)}} - \sqrt{\frac{1}{n-2} + \frac{1}{n-2} - \frac{2}{(n-2)^2}} \\
\geq \sqrt{\frac{1}{x-1} + \frac{1}{y-1} - \frac{2}{(x-1)(y-1)}} - \sqrt{\frac{1}{n-1} + \frac{1}{n-1} - \frac{2}{(n-1)^2}} \\
= (\sqrt{\frac{1}{y-1} + \frac{1}{y-1} - \frac{2}{(y-1)^2}} - \sqrt{\frac{1}{y} + \frac{1}{y} - \frac{2}{y^2}}) \quad \text{(by Lemma 2.3)}
\]
\geq 0 \quad \text{(by Lemma 2.5)}.

Hence
\[ABC(T_n)\]
\[\leq ABC(S_{n-1}^*) + \sqrt{2} - (\sqrt{\frac{1}{x-1} + \frac{1}{y-1} - \frac{2}{(x-1)(y-1)}} - \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}})\]
\[\leq ABC(S_{n-1}^*) + \sqrt{2} - (\sqrt{\frac{1}{n-2} + \frac{1}{n-2} - \frac{2}{(n-2)^2}} - \sqrt{\frac{1}{n-1} + \frac{1}{n-1} - \frac{2}{(n-1)^2}})\]
\[= ABC(S_n^*),\]
where the equality holds if and only if \(T_n - w = S_{n-1}^*\) and \(x = y = n - 1\), which completes the proof. \(\square\)

**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 \(T_5 \neq S_4^*\) or \(T_5 = R_5^*\). Since \(T_n \neq S_n^*\), we have \(T_n = R_n^*\). One can see that \(ABC(T_n) = 2\sqrt{2} + \frac{\sqrt{10}}{2} = (n-3)\sqrt{2} + \sqrt{\frac{2n-5}{(n-1)(n-2)}} + \sqrt{\frac{n}{2(n-1)}} + \sqrt{\frac{n-1}{3(n-2)}}\), 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
\[ABC(T_n)\]
\[\leq ABC(T_n - w) + \sqrt{2} - (\sqrt{\frac{1}{x-1} + \frac{1}{a} - \frac{2}{a(x-1)}} - \sqrt{\frac{1}{x} + \frac{1}{a} - \frac{2}{xa}})\]
\[
\left(\sqrt{\frac{1}{y - 1} + \frac{1}{a} - \frac{2}{a(y - 1)}} - \sqrt{\frac{1}{y} + \frac{1}{a} - \frac{2}{ya}}\right) - \\
\left(\sqrt{\frac{1}{x - 1} + \frac{1}{y - 1} - \frac{2}{(y - 1)(x - 1)}} - \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}}\right) \\
\leq ABC(R_{n-1}^*) + \sqrt{2} - \left(\sqrt{\frac{1}{n - 3} + \frac{1}{3} - \frac{2}{3(n - 3)}} - \sqrt{\frac{1}{n - 2} + \frac{1}{3} - \frac{2}{3(n - 2)}}\right) - \\
\left(\sqrt{\frac{1}{n - 2} + \frac{1}{3} - \frac{2}{3(n - 2)}} - \sqrt{\frac{1}{n - 1} + \frac{1}{3} - \frac{2}{3(n - 1)}}\right) - \\
\left(\sqrt{\frac{1}{n - 2} + \frac{1}{3} - \frac{2}{3(n - 2)}} - \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}}\right)\text{ (by Lemma 2.6)} \\
\leq ABC(R_{n-1}^*) + \sqrt{2} - \left(\sqrt{\frac{1}{n - 3} + \frac{1}{3} - \frac{2}{3(n - 3)}} - \sqrt{\frac{1}{n - 2} + \frac{1}{3} - \frac{2}{3(n - 2)}}\right) - \\
\left(\sqrt{\frac{1}{n - 2} + \frac{1}{3} - \frac{2}{3(n - 2)}} - \sqrt{\frac{1}{n - 1} + \frac{1}{3} - \frac{2}{3(n - 1)}}\right) - \\
\left(\sqrt{\frac{1}{n - 2} + \frac{1}{3} - \frac{2}{3(n - 2)}} - \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}}\right)\text{ (by Lemma 2.7)}.
\]

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

For \(x \leq y \leq n - 2\), by Lemmas 2.9 and 2.10 we have
\[
\left(\sqrt{\frac{1}{n - 3} + \frac{1}{n - 2} - \frac{2}{(n - 2)(n - 3)}} - \sqrt{\frac{1}{n - 1} + \frac{1}{n - 2} - \frac{2}{(n - 1)(n - 2)}}\right) > \\
\left(\sqrt{\frac{1}{n - 1} + \frac{1}{n - 2} - \frac{2}{(n - 1)(n - 2)}} - \sqrt{\frac{1}{n - 1} + \frac{1}{n - 2} - \frac{2}{(n - 1)(n - 2)}}\right) > 0.
\]

For \(y = n - 1\) and \(y \geq x + 1\), by Lemmas 2.9 and 2.11 we have
\[
\left(\sqrt{\frac{1}{n - 3} + \frac{1}{n - 2} - \frac{2}{(n - 2)(n - 3)}} - \sqrt{\frac{1}{n - 1} + \frac{1}{n - 2} - \frac{2}{(n - 1)(n - 2)}}\right) \geq \\
\left(\sqrt{\frac{1}{n - 1} + \frac{1}{n - 2} - \frac{2}{(n - 1)(n - 2)}} - \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}}\right) \geq 0.
\]
where the equality holds if and only if \( y = n - 1 \) and \( x = n - 2 \). Therefore,

\[
ABC(T_n) \\
\leq ABC(R^*_{n-1}) + \sqrt{2} - \left( \sqrt{\frac{1}{3} + \frac{1}{n-3} - \frac{2}{3(n-3)}} - \sqrt{\frac{1}{3} + \frac{1}{n-2} - \frac{2}{3(n-2)}} \right) \\
\left( \frac{1}{n-3} + \frac{1}{n-2} - \frac{2}{(n-2)(n-3)} - \frac{1}{n-1} + \frac{1}{n-2} - \frac{2}{(n-1)(n-2)} \right) \\
= ABC(R^*_n),
\]

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.

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 \( n \ (n \geq 6) \) vertices, \( ABC(G) \geq 2\sqrt{2} + \frac{2\sqrt{15}}{3} + (2n-11)\frac{\sqrt{6}}{4} \). The graph attaining this bound is shown in Figure 2.

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References


