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Extremal Bounds of the Atom-Bond Connectivity Index in Trees with a Fixed Roman Domination Number

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Abstract

Let $\mathbb{G} = (\mathbb{X}, \mathbb{Y})$ be a simple, connected graph, where $\mathbb{X}$ denotes the set of vertices and $\mathbb{Y}$ represents the set of edges. The atom-bond connectivity (ABC) index, introduced by Estrada et al. [10], is a topological descriptor used in mathematical chemistry. It is given by,

$$ABC(\mathbb{G}) = \sum_{xy \in \mathbb{Y}} \sqrt{\frac{\zeta_x + \zeta_y - 2}{\zeta_x \zeta_y}},$$

where ζ_x and ζ_y are the degrees of the vertices x and y, respectively. This study investigates the behavior of the ABC index in tree graphs, deriving both upper and lower bounds in terms of the graph's order and its Roman domination number (RDN). Moreover, we identify the specific tree structures that attain these extremal values, providing insights into how the RDN influences the ABC index.

Keywords: ABC index; Roman domination number; tree; chemical graph theory; extremal bounds.

1 Introduction

In theoretical chemistry, mathematical chemistry is the study of chemistry without reference to quantum mechanics, aimed at explaining and predicting the properties of molecules. Graph theory is used to represent chemical events in the important topic of chemical graph theory within mathematical chemistry. The chemical sciences have advanced significantly as a result of this strategy.

A molecular graph is a fundamental graph where the edges represent bonds between atoms, and the vertices represent the atoms themselves. Hydrogen atoms are often omitted from these representations. As defined by IUPAC, a topological index is a numerical value that characterizes the structural properties of a chemical compound. This value is used to establish correlations between different physical and chemical attributes [13], biological activity, and chemical reactivity [16], and the chemical structure [17].

The Randić connectivity index is one of the most well-known topological indices, supported by a solid mathematical foundation and widely applied in pharmacology and chemistry. In 1998, Estrada et al. [10] introduced the $ABC(\mathbb{G})$ index as a notable alternative to the Randić index. According to Furtula [11], the ABC index ranks among the leading degree-based molecular descriptors,

$$ABC(\mathbb{G}) = \sum_{xy \in \mathbb{Y}} \sqrt{\frac{\zeta_x + \zeta_y - 2}{\zeta_x \zeta_y}}, \tag{1}$$

where $\mathbb{Y}$ represents the set of edges in the graph $\mathbb{G}$, and ζ_x and ζ_y are the degrees of the vertices x and y connected by the edge xy. The index has been widely used to predict molecular stability, boiling points, and other properties, and has proven to be a valuable tool in QSAR/QSPR studies and drug design. Chen and Das [6] confirmed the conjecture that the Turán graph maximizes the ABC index among graphs with a given chromatic number, resolving a problem posed by Zhang et al. [26]. Zheng et al. [28] established bounds for the general ABC index for connected graphs with fixed maximum degree, characterizing the extremal graphs for specific parameter ranges. Numerous studies have been conducted on this topological indicator, and research on it is still ongoing [20].

Al Khabyah et al. [2] conducted a comprehensive investigation of degree-based topological indices, including the general Randić, arithmetic, and Albertson indices, for borophene structures composed of boron atom networks. In a related contribution, Ain et al. [1] explored super line graph operations and determined the generalized Randić index for graphs of diameter three, ensuring the preservation of pendant vertices within the graph structure. Meanwhile, Hayat et al. [14] analyzed structural networks such as silicate and honeycomb lattices by evaluating degree-based indices, notably the ABC and geometric-arithmetic indices, to explore their structural characteristics.

In a subsequent study, Hayat et al. [15] assessed distance-based topological descriptors for polycyclic aromatic hydrocarbons, demonstrating that the ABC and GA indices provide superior predictive performance for thermal properties compared to conventional indices. Gowtham and Husin [12] explored reverse topological indices for bistar graphs $B(n;m)$ and corona products, linking graph structure with molecular properties in cheminformatics. Kuriachan and Parthiban [18] introduced power domination entropy via power domination polynomials.

Prior research Das et al. [8] has investigated the relations between different topological indices and the ABC index. Among other notable studies, Das and Trinajstić [9] looked at the relationship between the geometric-arithmetic and ABC index. Xu [25] established correlations between the Harmonic index and several other indices, including the ABC index, Randić index, and the first Zagreb index, based on the order, size, and number of pendant vertices in the graph. Further research was done on the connection between the ABC index and the distance-based variation of the ABC index by Das et al. [8]. Additionally, they determined which extremal trees reach these limits. In order to determine the structures of extremal graphs, Zhang et al. [27] investigated the extremal limits of the atom bond sum connectivity index for trees with certain matching and dominance values.

In order to find graphs with the highest and least values of these indices, Wang et al. [22] looked into extremal multiplicative Zagreb indices in graphs with provided vertices and cut edges. Most recently, Bermudo et al. [5] provided a maximum value for the geometric-arithmetic index of the tree, based on their order and total domination number. More recently, Ali et al. [4, 3] provided a maximum value for the $HZ_1(\mathbb{T})$ and $HZ_2(\mathbb{T})$, based on their order and RDN. Li et al. [19] explored extremal values of the atom-bond sum-connectivity index for graphs with fixed parameters like chromatic and clique numbers. Wang et al. [23] identified unicyclic graphs maximizing the atom-bond sum-connectivity index for a fixed diameter and described the associated extremal structures and research on the bounds of various topological indices with given parameters is still ongoing, as noted in [21].

In this study, we take a look at a simple, undirected connected graph $\mathbb{G}$, which has a set of vertices $\mathbb{X}$ and an edge set $\mathbb{Y}$. An edge in graph $\mathbb{G}$ connecting two vertices, x and y, is represented by the symbol xy. The open neighborhood of any vertex $y \in \mathbb{X}$ is defined as $N(y) = \{x \in \mathbb{X} \mid xy \in \mathbb{Y}\}$, whereas $N[y] = N(y) \cup \{y\}$ indicates the closed neighbor. The size of an open neighborhood, $|N(x)|$, around a vertex x, denoted by ζ_x, is called its degree. A vertex x is called a leaf if $\zeta_x = 1$. The longest path between any two leaves in a tree is defined as its diameter. A diameter path in a tree $\mathbb{T}$ is denoted by $P_{d+1} = \{x_1, x_2, \ldots, x_{d+1}\}$, where the path between vertices $x_1, x_2, \ldots, x_{d+1}$ reaches this maximum length.

For a given vertex $y \in \mathbb{X}$, the graph $\mathbb{G} - \{y\}$ is obtained by removing y, which results in a new vertex set $\mathbb{X} - y$ and an edge set $\mathbb{Y} - \{yx \mid x \in N(y)\}$. Similarly, for an edge $e \in \mathbb{Y}$, the graph $\mathbb{G} - \{e\}$ retains the original vertex set $\mathbb{X}$ but removes the edge e, resulting in the edge set $\mathbb{Y} - \{e\}$.

For l vertices $x_1, \ldots, x_l$ or edges $e_1, \ldots, e_l$, we define the graph $\mathbb{G} - \{x_1, \ldots, x_l\}$ as $(\mathbb{G} - \{x_1, \ldots, x_{l-1}\}) - \{x_l\}$, and similarly, $\mathbb{G} - \{e_1, \ldots, e_l\}$ as $(\mathbb{G} - \{e_1, \ldots, e_{l-1}\}) - \{e_l\}$. The path graph with order n is denoted by P_n, and the star graph with n vertices is denoted by S_n. We direct the reader to [24] for definitions of any other notation and terminology not covered here.

The RDN of a graph $\mathbb{G}$ is the minimum weight of a Roman dominating function on $\mathbb{G}$. An RDN is a function $\aleph : \mathbb{X}(\mathbb{G}) \to \{0, 1, 2\}$ such that every vertex $y \in \mathbb{X}(\mathbb{G})$ with $\aleph(y) = 0$ is adjacent to at least one vertex $x \in \mathbb{X}(\mathbb{G})$ where $\aleph(x) = 2$. The weight of $\aleph$ is the sum $\aleph(\mathbb{X}) = \sum_{y \in \mathbb{X}(\mathbb{G})} \aleph(y)$ [7]. Essentially, the RDN ensures that any unguarded vertex (with $\aleph(y) = 0$) is adjacent to a heavily guarded vertex (with $\aleph(x) = 2$), and it is denoted by Γ_R.

This study bridges the gap in understanding the extremal values of the ABC index concerning the order and RDN of trees. The findings have significant implications for computational chemistry, particularly in predicting molecular properties such as stability, reactivity, and toxicity. By integrating the Roman domination number, this work enhances the predictive accuracy of QSAR and QSPR models, which rely on topological indices like the ABC index for molecular property estimation. Furthermore, identifying extremal tree structures that achieve these bounds provides a systematic, non-experimental approach to analyzing molecular behavior. Ultimately, this research advances both the theoretical aspects of chemical graph theory and its practical applications in molecular modeling and drug discovery.

2 Preliminary Results

In this section, we introduce a number of lemmas that will be utilized to demonstrate the primary theorem. Using the Mathematics program, all single and double variables function-related inequalities in these lemmas and the main theorem's proof have been confirmed.

Lemma 2.1. *Suppose,* $m(a) = (a-1)\sqrt{\frac{a-1}{a}} - (a-2)\sqrt{\frac{a-2}{a-1}}$ *with* $a \geq 3$. *Then,* $m(a)$ *is a positive function.*

Proof. Suppose that, $f(a) = (a-1)\sqrt{\frac{a-1}{a}}$ and $f(a) \geq 0$ for $a \geq 1$. The derivative is

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

The expression for $f'(a)$ is positive for $a \geq 2$. Since $f'(a) > 0$ in this range, the function is increasing. Thus, $f(a)$ is increasing for $a \geq 2$. Therefore, $m(a) = f(a) - f(a-1) \geq 0$. □

Lemma 2.2. *Suppose,* $q(a) = \sqrt{\frac{a+b-2}{ab}} - \sqrt{\frac{a+b-3}{(a-1)b}}$ *with* b, *and* $a \geq 3$. *Then,* $q(a)$ *is non-positive function for any* $b \geq 2$.

Proof. We can say that, $\sqrt{\frac{a+b-2}{ab}} \leq \sqrt{\frac{a+b-3}{(a-1)b}}$ for $a \geq 3$ and $b \geq 2$. So,

$$\sqrt{\frac{a+b-2}{ab}} - \sqrt{\frac{a+b-3}{(a-1)b}} \leq 0.$$

Therefore, $q(a)$ is a non-positive function for any $a \geq 3$ and $b \geq 2$. □

Lemma 2.3. *Suppose,*

$$\Xi(a,b) = (a-1)\sqrt{\frac{a-1}{a}} + \sqrt{\frac{a+b-2}{ab}} - (a-2)\sqrt{\frac{a-2}{a-1}} - \sqrt{\frac{a+b-3}{(a-1)b}} > \frac{\sqrt{5}}{2\sqrt{2}},$$

with $a \geq 3$, *and* $b \geq 2$.

Proof. We begin by decomposing the function $\Xi(a,b)$ into two parts,

$$f_1(a) = (a-1)\sqrt{\frac{a-1}{a}} - (a-2)\sqrt{\frac{a-2}{a-1}}, \quad \text{and}$$

$$f_2(a,b) = \sqrt{\frac{a+b-2}{ab}} - \sqrt{\frac{a+b-3}{(a-1)b}}.$$

By Lemma 2.1, $f_1(a)$ is positive function and it satisfies $f_1(a) \geq 0.9258$ ($f_1(3) = 0.9258$). By Lemma 2.2, $f_2(a,b)$ is negative function and it satisfies $f_2(a,b) \geq -0.1296$. Since,

$$\Xi(a,b) = f_1(a,b) + f_2(a,b),$$

we conclude $\Xi(a,b) \geq 0.7962 > \frac{\sqrt{5}}{2\sqrt{2}}$. Thus, it follows that $\Xi(a,b) > \frac{\sqrt{5}}{2\sqrt{2}}$. This completes the proof. □

Lemma 2.4. *Suppose that,* $p(a) = \sqrt{a-b}\sqrt{a-b-1} - \sqrt{a-b+1}\sqrt{a-b}$ *with* $a \geq 3$ *and* $b \leq \left\lceil \frac{2a}{3} \right\rceil$ *is a negative function, and* $-\sqrt{2} \leq p(a) < -1$.

Proof. Suppose that, $k(a) = \sqrt{a-b}\sqrt{a-b-1}$ and $k'(a) = \frac{2a-2b-1}{2\sqrt{a-b-1}\sqrt{a-b}}$, so $k(a)$ is a increasing and positive function for $a \geq 3$ and $b \leq \left\lceil \frac{2a}{3} \right\rceil$. Therefore, the function $p(a) = k(a) - k(a+1)$ is a negative function. We verified that given function hold the inequalities $-\sqrt{2} \leq p(a) < -1$. □

Lemma 2.5. *Let* $m(a) = \sqrt{a-b-1}\sqrt{a-b-2} - \sqrt{a-b+1}\sqrt{a-b}$ *with* $a \geq 4$ *and* $b \leq \left\lceil \frac{2a}{3} \right\rceil$ *is a negative function, and* $-\sqrt{6} \leq m(a) < -2$.

Proof. Derivative of $\alpha(a) = \sqrt{a-b-1}\sqrt{a-b-2}$ is $\alpha^{'}(a) = \frac{2a-2b-3}{2\sqrt{a-b-2}\sqrt{a-b-1}} > 0$. Therefore, $\alpha(a)$ is a increasing and positive function for $a \geq 4$ and $b \leq \left\lceil \frac{2a}{3} \right\rceil$. Hence, give function $m(a) = \alpha(a) - \alpha(a+2)$ is a negative function. We verified that given function hold the inequalities $-\sqrt{6} \leq m(a) < -2$. □

Theorem 2.1. [7] *For the path graph* P_n*, RDN is* $\Gamma_R(P_n) = \left\lceil \frac{2n}{3} \right\rceil$.

3 Main Results

This section presents the extremal values of the ABC index of trees in terms of their Roman domination number and order. We define two functions, $\mathbb{f}_{\min}(n, \Gamma_R)$ and $\mathbb{f}_{\max}(n, \Gamma_R)$, which represent the lower and upper bounds of the ABC index for trees, respectively, based on the order n and Γ_R. The proofs of these bounds are provided in Theorems 3.1 and 3.2. Additionally, Theorems 3.3 and 3.4 identify specific graphs that achieve these exact values:

$$\mathbb{f}_{\min}(n, \Gamma_R) = \frac{1}{\sqrt{2}}(n-1) + \left\lceil \frac{2n}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right) + \Gamma_R \left(\frac{1}{\sqrt{2}} - \frac{3}{4} \right),$$

$$\mathbb{f}_{\max}(n, \Gamma_R) = \sqrt{n - \Gamma_R + 1}\sqrt{n - \Gamma_R} - (\Gamma_R - 2)\left(\frac{1}{2} - \frac{3}{\sqrt{5}} \right).$$

The following lemma assists in establishing the minimum value of the ABC index in terms of the order and its RDN.

Lemma 3.1. *Suppose that, $\mathbb{T}$ is a tree graph and Γ_R is an RDN, a vertex $x \in V(\mathbb{T})$ such that $\zeta(x) = \xi \geq 3$, $N(x) = \{y_1, y_2, \ldots, y_\xi\}$, $\zeta(y_\xi) = j \geq 2$, $\zeta(y_a) = 1$ for every $a \in \{1, 2, 3, \ldots, \xi - 1\}$. If we take $T' = T - \{y_1\}$, we have;*

Proof. Since $\mathbb{T}' = \mathbb{T} - \{y_1\}$, we have

$$\begin{aligned} ABC(\mathbb{T}) &= ABC(\mathbb{T}') + (\xi-1)\sqrt{\frac{\xi-1}{\xi}} - (\xi-2)\sqrt{\frac{\xi-2}{\xi-1}} + \sqrt{\frac{\xi+j-2}{\xi j}} - \sqrt{\frac{\xi+j-3}{(\xi-1)j}} \\ &\geq \frac{1}{\sqrt{2}}(n-1) - \frac{1}{\sqrt{2}} + \left\lceil \frac{2(n-1)}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) + \Gamma_R\left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right) + (\xi-1)\sqrt{\frac{\xi-1}{\xi}} \\ &\quad + \sqrt{\frac{\xi+j-2}{\xi j}} - (\xi-2)\sqrt{\frac{\xi-2}{\xi-1}} - \sqrt{\frac{\xi+j-3}{(\xi-1)j}} \\ &\geq \mathbb{f}_{\min}(n, \Gamma_R) + (\xi-1)\sqrt{\frac{\xi-1}{\xi}} + \sqrt{\frac{\xi+j-2}{\xi j}} - (\xi-2)\sqrt{\frac{\xi-2}{\xi-1}} - \sqrt{\frac{\xi+j-3}{(\xi-1)j}} \\ &\quad - \frac{1}{\sqrt{2}} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right). \end{aligned}$$

Suppose that, $\alpha(\xi, j) = (\xi-1)\sqrt{\frac{\xi-1}{\xi}} + \sqrt{\frac{\xi+j-2}{\xi j}} - (\xi-2)\sqrt{\frac{\xi-2}{\xi-1}} - \sqrt{\frac{\xi+j-3}{(\xi-1)j}}$. Using Lemma 2.3, we say $\alpha(\xi, j) > \frac{\sqrt{5}}{2\sqrt{2}}$. So,

$$ABC(\mathbb{T}) \geq \mathbb{f}_{\max}(n, \Gamma_R) + \frac{\sqrt{5}}{2\sqrt{2}} - \frac{1}{\sqrt{2}} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) > \mathbb{f}_{\max}(n, \Gamma_R).$$

□

Theorem 3.1. *Suppose that $\mathbb{T}$ is a tree graph and let Γ_R denote its RDN. Then, the ABC index of $\mathbb{T}$ satisfies the inequality $ABC(\mathbb{T}) \geq \mathbb{f}_{\min}(n, \Gamma_R)$.*

Proof. Let us demonstrate the outcome using induction regarding the vertex count. T is either a star S_4 or a path P_4. As we have already observed,

$$ABC(P_4) = \mathbb{f}_{\min}(4, 3), \qquad \text{and} \qquad ABC(S_4) = 2.44 > \mathbb{f}_{\min}(4, 3) = 2.1213.$$

We examine a $\mathbb{T}$ with order n and Γ_R. We consider that the inequality holds for every $\mathbb{T}$ with $n-1$ vertices. Now, we prove that for when $\mathbb{T}$ has n vertices. We discuss some cases.

Case 1: We consider that, $x - y - z$ is a path in $\mathbb{T}$. If x is a leaf, $\zeta(y) = \xi \geq 3$ and $\zeta(z) = j \geq 2$, then, we apply Lemma 3.1 and get the result.

Case 2: Let $P_{d+1} = \{x_1, x_2, \ldots, x_{d+1}\}$ is a diametral path of the tree graph. Now, let degree of x_2 is 2.

Case 2.1: Suppose that,

$$\begin{aligned} &d(x_3) = \xi \geq 4, && N(x_3) = \{x_2, x_4, w_1, \ldots, w_{\xi-2}\}, \\ &d(w_\alpha) = \Upsilon_\alpha \leq 2, && \alpha = \{2, \ldots, \xi-2\}, \\ &d(w_1) = 1, \quad \text{and} && d(x_4) = k, \quad \text{where} \quad 3 \leq k \leq \xi. \end{aligned}$$

If $\mathbb{T} = \mathbb{T}_1 - \{x_1, x_2, w_1\}$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_1) + 1$, we get:

$$\begin{aligned}
ABC(\mathbb{T}) &= ABC(\mathbb{T}_1) + \sum_{\alpha=1}^{\xi-3}\left(\frac{1}{\sqrt{\Upsilon_\alpha}}\right)\left(\sqrt{\frac{\xi+\Upsilon_\alpha-2}{\xi}} - \sqrt{\frac{\xi+\Upsilon_\alpha-4}{\xi-2}}\right) \\
&\quad + \frac{1}{\sqrt{k}}\left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-4}{\xi-2}}\right) + \sqrt{\frac{\xi-1}{\xi}} + \sqrt{2} \\
&\geq \frac{1}{\sqrt{2}}(n-1) - \frac{3}{\sqrt{2}} + \left\lceil\frac{2(n-3)}{3}\right\rceil\left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) + \Gamma_R\left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right) \\
&\quad - \left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right) + \sum_{\alpha=1}^{\xi-3}\left(\frac{1}{\sqrt{\Upsilon_\alpha}}\right)\left(\sqrt{\frac{\xi+\Upsilon_\alpha-2}{\xi}} - \sqrt{\frac{\xi+\Upsilon_\alpha-3}{\xi-1}}\right) \\
&\quad + \frac{1}{\sqrt{k}}\left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-3}{\xi-1}}\right) + \sqrt{\frac{\xi-1}{\xi}} + \sqrt{2} \\
&\geq \mathfrak{f}_{\min}(n,\Gamma_R) + \sum_{\alpha=1}^{\xi-3}\left(\frac{1}{\sqrt{\Upsilon_\alpha}}\right)\left(\sqrt{\frac{\xi+\Upsilon_\alpha-2}{\xi}} - \sqrt{\frac{\xi+\Upsilon_\alpha-4}{\xi-2}}\right) \\
&\quad + \frac{1}{\sqrt{k}}\left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-4}{\xi-2}}\right) + \sqrt{\frac{\xi-1}{\xi}} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) \\
&\quad - \frac{3}{\sqrt{2}} + \sqrt{2} \\
&\geq \mathfrak{f}_{\min}(n,\Gamma_R) + \left(\frac{\xi-3}{\sqrt{3}}\right)\left(\sqrt{\frac{\xi+1}{\xi}} - \sqrt{\frac{\xi-1}{\xi-2}}\right) \\
&\quad + \frac{1}{\sqrt{k}}\left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-4}{\xi-2}}\right) + \sqrt{\frac{\xi-1}{\xi}} - \frac{3}{4}.
\end{aligned}$$

Suppose that,

$$\begin{aligned}
\alpha(\xi,k) = \left(\frac{\xi-3}{\sqrt{3}}\right)\left(\sqrt{\frac{\xi+1}{\xi}} - \sqrt{\frac{\xi-1}{\xi-2}}\right) + \frac{1}{\sqrt{k}}\left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-4}{\xi-2}}\right) \\
+ \sqrt{\frac{\xi-1}{\xi}} - \frac{3}{4}.
\end{aligned}$$

$\alpha(\xi,k) > 0$ for $\xi \geq 4$ and $3 \leq k \leq \xi$. So,

$$ABC(\mathbb{T}) \geq \mathfrak{f}_{\min}(n,\Gamma_R) + \alpha(m,k) > \mathfrak{f}_{\min}(n,\Gamma_R).$$

Case 2.2: Assume $\zeta(x_3) = 3$, $N(x_3) = \{x_2, x_4, y_1\}$, y_1 is the leaf of the $\mathbb{T}$ and $\zeta(x_4) = k$.

Case 2.2.1: Suppose that, $1 \leq k \leq 4$.

If we take $\mathbb{T}_2 = \mathbb{T} - \{x_1, x_2\}$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_2) + 1$, we get:

$$\begin{aligned}
ABC(\mathbb{T}) &= ABC(\mathbb{T}_2) + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{2}{3}} \\
&\geq \frac{1}{\sqrt{2}}(n-1) - \frac{2}{\sqrt{2}} + \left\lceil \frac{2(n-2)}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right) \\
&\quad + (\Gamma_R - 1)\left(\frac{1}{\sqrt{2}} - \frac{3}{4} \right) + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{2}{3}} \\
&\geq \mathbb{f}_{\min}(n, \Gamma_R) + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{2}{3}} - \sqrt{2} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right).
\end{aligned}$$

Suppose that, $\beta(k) = \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{2}{3}} - \sqrt{2} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right)$. $\beta(k) > 0$ for $1 \leq k \leq 4$. Therefore, $ABC(\mathbb{T}) \geq \mathbb{f}_{\min}(n, \Gamma_R) + \beta(k) > \mathbb{f}_{\min}(n, \Gamma_R)$.

Case 2.2.2: Suppose that, $k \geq 5$, $\zeta(x_5) = u$, $N(x_4) = \{x_3, x_5, y_1, \ldots, y_{k-2}\}$, $\zeta(y_1) = 1$ and $\zeta(y_a) = b_a \leq 5$ where $a = \{2, 3, \ldots, k-2\}$. If we take $\mathbb{T}_3 = \mathbb{T} - \{x_1, x_2, x_3, x_4, y_1\}$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_3) + 3$, we get:

$$\begin{aligned}
ABC(\mathbb{T}) &= ABC(\mathbb{T}_3) + \sum_{a=1}^{u-2} \sqrt{\frac{k+b_a-2}{kb_a}} - \sum_{a=1}^{u-3} \sqrt{\frac{k+b_a-3}{(k-1)\,b_a}} + \sqrt{\frac{k-1}{k}} \\
&\quad + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{k+u-2}{ku}} - \sqrt{\frac{k+u-3}{(k-1)u}} + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} \\
&\geq \frac{1}{\sqrt{2}}(n-1) - \frac{5}{\sqrt{2}} + \left\lceil \frac{2(n-5)}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right) + (\Gamma_R - 3)\left(\frac{1}{\sqrt{2}} - \frac{3}{4} \right) \\
&\quad + \sum_{a=1}^{u-2} \sqrt{\frac{k+b_a-2}{kb_a}} - \sum_{a=1}^{u-3} \sqrt{\frac{k+b_a-3}{(k-1)\,b_a}} + \sqrt{\frac{k+u-2}{ku}} \\
&\quad - \sqrt{\frac{k+u-3}{(k-1)u}} + \sqrt{\frac{k-1}{k}} + \sqrt{\frac{k+1}{3k}} + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} \\
&\geq \mathbb{f}_{\min}(n, \Gamma_R) + \sum_{a=1}^{u-2} \sqrt{\frac{k+b_a-2}{kb_a}} - \sum_{a=1}^{u-3} \sqrt{\frac{k+b_a-3}{(k-1)\,b_a}} + \sqrt{\frac{k-1}{k}} \\
&\quad + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{k+u-2}{ku}} - \sqrt{\frac{k+u-3}{(k-1)u}} + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} - \frac{5}{\sqrt{2}} \\
&\geq \mathbb{f}_{\min}(n, \Gamma_R) + (k-2)\sqrt{\frac{k+3}{5k}} - (k-3)\sqrt{\frac{k+2}{5\,(k-1)}} + \sqrt{\frac{k-1}{k}} \\
&\quad + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{k+u-2}{ku}} - \sqrt{\frac{k+u-3}{(k-1)u}} + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} - \frac{5}{\sqrt{2}}.
\end{aligned}$$

Suppose that,

$$\alpha(k) = (k-2)\sqrt{\frac{k+3}{5k}} - (k-3)\sqrt{\frac{k+2}{5\,(k-1)}} + \sqrt{\frac{k-1}{k}} + \sqrt{\frac{k+1}{3k}}.$$

It has been verified that $\alpha(k) > 1.57$. Let $\beta(k, u) = \sqrt{\frac{k+u-2}{ku}} - \sqrt{\frac{k+u-3}{(k-1)u}}$.

By using Lemma 2.2, we have $\beta(k,u) > -0.013$. Therefore,

$$ABC(\mathbb{T}) \geq \mathfrak{f}_{\min}(n,\Gamma_R) + \alpha(k) + \beta(k,u) + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} - \frac{5}{\sqrt{2}} > \mathfrak{f}_{\min}(n,\Gamma_R).$$

Case 2.3: Assume that $\zeta(x_3) = 2$, $\zeta(x_4) = l \geq 2$, and $N(x_4) = \{x_3, x_5, y_1, \ldots, y_{l-2}\}$, where $\zeta(y_i) = a_i \leq 5$ for $i \in \{1,2,\ldots,l-2\}$ and $\zeta(x_5) = t \leq l$.
If we take $\mathbb{T}_4 = \mathbb{T} - \{x_1,x_2,x_3,y_1\}$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_4) + 2$, we get:

$$\begin{aligned}
ABC(\mathbb{T}) &= ABC(\mathbb{T}_4) + \sum_{i=1}^{l-3} \frac{1}{\sqrt{a_i}} \left(\sqrt{\frac{l+a_i-2}{l}} - \sqrt{\frac{l+a_i-3}{l-1}} \right) + \sqrt{\frac{l-1}{l}} \\
&\quad + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right) + \frac{3}{\sqrt{2}} \\
&\geq \frac{1}{\sqrt{2}}(n-1) - \frac{4}{\sqrt{2}} + \left\lceil \frac{2(n-4)}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right) + (\Gamma_R - 2) \left(\frac{1}{\sqrt{2}} - \frac{3}{4} \right) \\
&\quad + \sum_{i=1}^{l-3} \frac{1}{\sqrt{a_i}} \left(\sqrt{\frac{l+a_i-2}{l}} - \sqrt{\frac{l+a_i-3}{l-1}} \right) + \sqrt{\frac{l-1}{l}} \\
&\quad + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right) + \frac{3}{\sqrt{2}} \\
&\geq \mathfrak{f}_{\min}(n,\Gamma_R) + \sum_{i=1}^{l-3} \frac{1}{\sqrt{a_i}} \left(\sqrt{\frac{l+a_i-2}{l}} - \sqrt{\frac{l+a_i-3}{l-1}} \right) + \sqrt{\frac{l-1}{l}} \\
&\quad + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right) - \frac{1}{\sqrt{2}} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right) \\
&> \mathfrak{f}_{\min}(n,\Gamma_R) + \frac{l-3}{\sqrt{5}} \left(\sqrt{\frac{l+3}{l}} - \sqrt{\frac{l+2}{l-1}} \right) + \sqrt{1 - \frac{1}{l}} \\
&\quad + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right) - \frac{3}{4}.
\end{aligned}$$

Let, $\alpha(l) = \frac{l-3}{\sqrt{5}} \left(\sqrt{\frac{l+3}{l}} - \sqrt{\frac{l+2}{l-1}} \right) + \sqrt{1-\frac{1}{l}}$. Since $\alpha(l)$ is an increasing function for every $l \geq 3$, we define

$$\beta(l,k) = \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right).$$

By Lemma 2.2, $\beta(l,k)$ is a decreasing function. Therefore, the inequality holds,

$$ABC(\mathbb{T}) \geq \mathfrak{f}_{\min}(n,\Gamma_R) + \alpha(l) + \beta(l,k) - \frac{3}{4} > \mathfrak{f}_{\min}(n,\Gamma_R).$$

□

Theorem 3.2. *If $\mathbb{T}$ be a tree graph and let Γ_R denote its RDN. Then, the ABC index of $\mathbb{T}$ satisfies the inequality, $ABC(\mathbb{T}) \leq \mathfrak{f}_{\max}(n,\Gamma_R)$.*

Proof. Let us demonstrate the outcome using induction regarding the vertex count. $\mathbb{T}$ is either a star S_4 or a path P_4. As we have already observed,

$$ABC(P_4) = 2.121 < \mathbb{f}_{\max}(4,3), \quad \text{and} \quad ABC(S_4) = \mathbb{f}_{\max}(4,3) = 2.44.$$

We examine a $\mathbb{T}$ with order n and $RDN\ \Gamma_R$. We consider that the inequality holds for every $\mathbb{T}$ with $n-1$ vertices. Now, we prove that for when $\mathbb{T}$ has n vertices. We discuss some cases.

Case 1: Consider a vertex x where $\zeta(x) = \xi \geq 3$, $N(x) = \{y_1, y_2, \ldots, y_\xi\}$, $\zeta(y_\xi) = j \geq 2$, $\zeta(y_a) = 1$ for every $a \in \{1,2,3,\ldots,\xi-1\}$. If we take $\mathbb{T}_1 = \mathbb{T} - y_1$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_1)$. We have

$$\begin{aligned} ABC(\mathbb{T}) = ABC(\mathbb{T}_1) &+ \frac{1}{\sqrt{\xi}}\left((\xi-1)^{\frac{3}{2}} + \sqrt{\frac{\xi+j-2}{j}}\right) \\ &- \frac{1}{\xi-1}\left((\xi-2)^{\frac{3}{2}} + \sqrt{\frac{\xi+j-3}{j}}\right) \\ &\leq \sqrt{n-\Gamma_R}\sqrt{n-\Gamma_R-1} - (\Gamma_R-2)\left(\frac{1}{2} - \frac{3}{\sqrt{5}}\right) \\ &\quad + \frac{1}{\sqrt{\xi}}\left((\xi-1)^{\frac{3}{2}} + \sqrt{\frac{\xi+j-2}{j}}\right) - \frac{1}{\sqrt{\xi-1}}\left((\xi-2)^{\frac{3}{2}} + \sqrt{\frac{\xi+j-3}{j}}\right) \\ &\leq \mathbb{f}_{\max}(n,\Gamma_R) + \sqrt{n-\Gamma_R}\sqrt{n-\Gamma_R-1} - \sqrt{n-\Gamma_R+1}\sqrt{n-\Gamma_R} \\ &\quad + \frac{1}{\sqrt{\xi}}\left((\xi-1)^{\frac{3}{2}} + \sqrt{\frac{\xi+j-2}{j}}\right) - \frac{1}{\sqrt{\xi-1}}\left((\xi-2)^{\frac{3}{2}} + \sqrt{\frac{\xi+j-3}{j}}\right). \end{aligned}$$

Assume that,

$$\alpha(n) = \sqrt{n-\Gamma_R}\sqrt{n-\Gamma_R-1} - \sqrt{n-\Gamma_R+1}\sqrt{n-\Gamma_R}, \quad \text{and}$$
$$\beta(\xi,j) = \frac{1}{\sqrt{\xi}}\left((\xi-1)^{\frac{3}{2}} + \sqrt{\frac{\xi+j-2}{j}}\right) - \frac{1}{\sqrt{\xi-1}}\left((\xi-2)^{\frac{3}{2}} + \sqrt{\frac{\xi+j-3}{j}}\right).$$

By using Lemma 2.4, we get $-\sqrt{2} \leq \alpha(n) < -1$ for $n \geq 3$ and $2 \leq \Gamma_R \leq \left\lceil \frac{2n}{3} \right\rceil$ and by Lemma 2.3, we get $\frac{\sqrt{5}}{2\sqrt{2}} \leq \beta(\xi,j) < 1$ for any $\xi \geq 3$ and $j \geq 2$. Therefore, $\eta(n,\xi,j) = \alpha(n) + \beta(\xi,j)$ is negative function. So,

$$ABC(\mathbb{T}) \leq \mathbb{f}_{\max}(n,\Gamma_R) + \eta(n,\xi,j) < \mathbb{f}_{\max}(n,\Gamma_R).$$

Case 2: Let, $P_{d+1} = \{x_1, x_2, \ldots, x_{d+1}\}$ is a diametral path of the tree. Let $\zeta(x_2) = 2$, $\zeta(x_3) = \xi$, $N(x_3) = \{x_2, x_4, y_1, \ldots, y_{\xi-2}\}$, $\zeta(y_i) = \Upsilon_i$, where $i \in \{1,2,\ldots,\xi-2\}$, and $\zeta(x_4) = k$.

If we take $\mathbb{T}_2 = \mathbb{T} - \{x_1, x_2\}$, then, $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_2) + 1$, we get:

$$\begin{aligned}
ABC(\mathbb{T}) &= ABC(\mathbb{T}_2) + \sum_{i=1}^{\xi-1} \frac{1}{\sqrt{\Upsilon_i}} + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-3}{\xi-1}} \right) \\
&\quad \left(\sqrt{\frac{\xi+\Upsilon_i-2}{\xi}} - \sqrt{\frac{\xi+\Upsilon_i-3}{\xi-1}} \right) + \sqrt{2} \\
&\leq \sqrt{n-\Gamma_R-1}\sqrt{n-\Gamma_R-2} - (\Gamma_R - 3)\left(\frac{1}{2} - \frac{3}{\sqrt{5}}\right) \\
&\quad + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-3}{\xi-1}} \right) \\
&\quad + \sum_{i=1}^{\xi-2} \frac{1}{\sqrt{\Upsilon_i}} \left(\sqrt{\frac{\xi+\Upsilon_i-2}{\xi}} - \sqrt{\frac{\xi+\Upsilon_i-3}{\xi-1}} \right) + \sqrt{2} \\
&\leq \mathfrak{f}_{\max}(n, \Gamma_R) + \sqrt{n-\Gamma_R-1}\sqrt{n-\Gamma_R-2} - \sqrt{n-\Gamma_R+1}\sqrt{n-\Gamma_R} \\
&\quad + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-3}{\xi-1}} \right) \\
&\quad + \sum_{i=1}^{\xi-2} \frac{1}{\sqrt{\Upsilon_i}} \left(\sqrt{\frac{\xi+\Upsilon_i-2}{\xi}} - \sqrt{\frac{\xi+\Upsilon_i-3}{\xi-1}} \right) + \sqrt{2} + \left(\frac{1}{2} - \frac{3}{\sqrt{5}}\right) \\
&\leq \mathfrak{f}_{\max}(n, \Gamma_R) + \sqrt{n-\Gamma_R-1}\sqrt{n-\Gamma_R-2} - \sqrt{n-\Gamma_R+1}\sqrt{n-\Gamma_R} \\
&\quad + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-3}{\xi-1}} \right) + \frac{\xi-2}{\sqrt{5}} \left(\sqrt{\frac{\xi+3}{\xi}} - \sqrt{\frac{\xi+2}{\xi-1}} \right) \\
&\quad + \sqrt{2} + \left(\frac{1}{2} - \frac{3}{\sqrt{5}}\right).
\end{aligned}$$

Assume that,

$$\begin{aligned}
\alpha(n) &= \sqrt{n-\Gamma_R-1}\sqrt{n-\Gamma_R-2} - \sqrt{n-\Gamma_R+1}\sqrt{n-\Gamma_R}, \\
\beta(\xi, k) &= \frac{1}{\sqrt{k}} \left(\sqrt{\frac{\xi+k-2}{\xi}} - \sqrt{\frac{\xi+k-3}{\xi-1}} \right), \quad \text{and} \\
\gamma(\xi) &= \frac{\xi-2}{\sqrt{5}} \left(\sqrt{\frac{\xi+3}{\xi}} - \sqrt{\frac{\xi+2}{\xi-1}} \right).
\end{aligned}$$

By using Lemma 2.5, we get $-\sqrt{6} \leq \alpha(n) < -2$. By Lemma 2.2, $\beta(\xi, k)$ is decreasing function, and $\gamma(\xi)$ is negative function for any $\xi \geq 3$. Hence,

$$ABC(\mathbb{T}) \leq \mathfrak{f}_{\max}(n, \Gamma_R) + \alpha(n) + \beta(\xi, k) + \gamma(\xi) + \sqrt{2} + \left(\frac{1}{2} - \frac{3}{\sqrt{5}}\right) < \mathfrak{f}_{\max}(n, \Gamma_R).$$

□

Theorem 3.3. *Suppose that, $\mathbb{T}$ be a tree with order n and Roman domination number Γ_R, then, we have $ABC(\mathbb{T}) = \mathfrak{f}_{\min}(n, \Gamma_R)$ if and only if $\mathbb{T} = P_n$.*

Proof. Using (1), we know that for the path graph P_n, the ABC index is $ABC(P_n) = \frac{1}{\sqrt{2}}(n-1)$. By Theorem 2.1, the RDN of the path graph P_n is, $\Gamma_R(P_n) = \left\lceil \frac{2n}{3} \right\rceil$. Substituting this into the formula for $\mathbb{f}_{\max}(n, \Gamma_R)$, we get

$$\mathbb{f}_{\max}(n, \Gamma_R) = \frac{1}{\sqrt{2}}(n-1) + \left\lceil \frac{2n}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right) + \Gamma_R(P_n) \left(\frac{1}{\sqrt{2}} - \frac{3}{4} \right) = \frac{1}{\sqrt{2}}(n-1) = ABC(P_n).$$

□

Theorem 3.4. *Suppose that,* $\mathbb{T}$ *a tree with order* n *and* Γ_R*, then we have* $ABC(\mathbb{T}) = \mathbb{f}_{\max}(n, \Gamma_R)$ *if and only if* $\mathbb{T} = S_n$*.*

Proof. By using (1), we know that for the star graph S_n, the ABC index in the term of order of S_n is given by $ABC(S_n) = \sqrt{n-1}\sqrt{n-2}$ and RDN of S_n is 2 ($\Gamma_R(S_n) = 2$). Hence, we substitute this into the formula for $\mathbb{f}_{\max}(n, \Gamma_R(S_n))$, giving

$$\mathbb{f}_{\max}(n, \Gamma_R(S_n)) = \sqrt{n-1}\sqrt{n-2} = ABC(S_n).$$

This is exactly equal to the ABC index of S_n, so we conclude that,

$$ABC(S_n) = \mathbb{f}_{\max}(n, \Gamma_R(S_n)).$$

□

4 Conclusion

In this study, we examined the ABC index of tree graphs, focusing on its dependence on the RDN and the tree's order. We established the lower and upper bounds of the ABC index, as detailed in Theorems 3.1 and 3.2, demonstrating that these bounds are determined by the tree's order and RDN. Specifically, Theorem 3.3 shows that P_n achieves the minimum ABC index, while Theorem 3.4 reveals that S_n trees attain the maximum index, illustrating the significant impact of the RDN on these extremal values. These results enhance the understanding of the relationship between tree parameters and topological indices, providing a basis for future research to explore these interactions in broader graph classes and uncover new connections between the ABC index and other graph invariants.

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