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Research Article

Some Bounds on a-Analogue Atom-Bond Connectivity Related Indices

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Abstract. For any non-real number a, the significance of the a-analogue Atom-Bond Connectivity indices lies within the actuality of their particular cases for well-chosen values for the variant a. In this paper, we obtained some bounds based on the vertex-degree along with the variant a value, inequalities in other degree-based indices, and characterizations of these novel a-analogue ABC indices.

Keywords. ABC indices, a-analogue ABC indices

Mathematics Subject Classification (2020). 05C05, 05C07, 05C09, 26D15

1. Introduction

The graphs $G = (V,E)$ chosen in this paper are simple with the vertex set $V(G)$ and the edge set $E(G)$. The numbers p and q denote the cardinality of $V(G)$ and $E(G)$, respectively. The each edge $e_h = v_i v_j \in E(G)$, v_i and v_j are incident vertices of e_h belongs to $V(G)$. Two vertices are said to be adjacent if it has a common edge between them, a neighborhood of v_i is the set of vertices adjacent to v_i. The cardinal number called the degree of the v_i, is represented as $d_G(v_i) = x_i$, the minimum value of x_i is $\delta(G)$, and maximum values of x_i is $\Delta(G)$. The number of edges adjacent to the edge $e_h = v_i v_j$ is said to be a degree of the edge e_h that is $d_G(e_h) = x_i + x_j - 2$. For more graph theoretic definitions, we refer to Harary [14], and Kulli [15].

In 1998, Estrada *et al.* [10] introduced the *ABC* index of a graph G and defined as

$$ABC(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{x_i + x_j - 2}{x_i x_j}}.$$

This descriptor is a useful predictive index for studying the temperature of alkane formation.

The general *ABC* index (Zheng [19]), is defined as

$$ABC^{\alpha}(G) = \sum_{v_i v_j \in E(G)} \left(\frac{x_i + x_j - 2}{x_i x_j}\right)^{\alpha}.$$

For more information about *ABC*-related indices and terminologies, we refer to Ahmadi *et al.* [1], Alsaadi *et al.* [2], Chaluvaraju and Shaikh [4], Das [5], Das *et al.* [6, 7], Estrada [9], Gutman and Furtula [13], Lin *et al.* [16], Palacios [17], Sarveshkumar *et al.* [18], and Zhou and Trinajstić [20].

We are motivated by Zheng [19] and defined the a-Analogue *ABC* index and coindex as

$$ABC_a(G) = \sum_{v_i v_j \in E(G)} \left(\frac{x_i^a + x_j^a - 2}{x_i^a x_j^a}\right)^{\frac{1}{2}}, \tag{1.1}$$

$$\overline{ABC}_a(G) = \sum_{v_i v_j \notin E(G)} \left(\frac{x_i^a + x_j^a - 2}{x_i^a x_j^a}\right)^{\frac{1}{2}}, \tag{1.2}$$

where $a \geq 1$, if $a < 1$, then we get contradiction for the equations (1.1) and (1.2), i.e., if $a < 1$, for each member of $e_h = x_i x_j \in E(G)$, $1 \leq x_i \leq x_j$, $\implies 0 \leq x_j^a \leq x_i^a \leq 1$.

If there exists a vertex $v_i \in V(G)$ such that $x_i > 1$, for any $a < 1$, then $x_i^a < 1$ and $x_i + x_j - 2 < 0$ which contradicts that square root of a negative value does not exist in the real number system. Therefore, $a \geq 0$ is necessary condition.

This paper aims to develop some inequalities based on the variant a using the limit value of the function, i.e., as a approaches some undefined values like ∞ and finally finds some bounds based on the values of x_i, we refer to Carothers [3], Dimitrov [8], Folland [11], and Gutman [12] for more information.

2. Main Results

Theorem 2.1. *Let $f(x_i, x_j, a)$ be a function with 3 variables and is defined as*

$$f(x_i, x_j, a) = \left(\frac{x_i^a + x_j^a - 2}{x_i^a x_j^a}\right)^{\frac{1}{2}}, \tag{2.1}$$

where $x_i, x_j \in \{1, 2, 3, \dots, p-1\}$, $a \geq 1$. Then the value of $f(x_i, x_j, a)$ is 1 and 0.

Proof. Let $f(x_i, x_j, a)$ be a function with 3 variables $x_i, x_j \in \{1, 2, 3, \dots, p-1\}$ and $a \geq 1$. We present a few cases to discuss the maximum value and the minimum value of $f(x_i, x_j, a)$ by fixing some variables present in it.

Case 1: If $x_i = x_j = 1$, then degree of each edge is equal to 0. Equation (2.1) attained its minimum value, that is, $f(1,1,a) = 0$, for $a \geq 1$.

Case 2: If $x_i = 1$ and $x_j \neq 1$, then by equation (2.1), we have

$$f(1,x_j,a) = \left(\frac{x_j^a - 1}{x_j^a}\right)^{\frac{1}{2}}. \tag{2.2}$$

Equation (2.2) is an increasing function, and it attains the minimum value as $x_j \to 2$, that is,

$$\lim_{x_j \to 2} f(1,x_j,a) = \lim_{x_j \to 2} \left(\frac{x_j^a - 1}{x_j^a}\right)^{\frac{1}{2}} = \left(\frac{2^a - 1}{2^a}\right)^{\frac{1}{2}},$$

it reaches the minimum value at $x_j = 2$ for all $a \geq 1$.

The maximum value of equation (2.2) attained as $x_j \to (p-1)$, i.e.,

$$\lim_{x_j \to (p-1)} f(1,x_j,a) = \lim_{x_j \to (p-1)} \left(\frac{x_j^a - 1}{x_j^a}\right)^{\frac{1}{2}} = \left(\frac{(p-1)^a - 1}{(p-1)^a}\right)^{\frac{1}{2}},$$

it reaches the maximum value at $x_j = p-1$ for all $a \geq 1$.

We have another variant $a \geq 1$, which plays an important role on the function $f(1,x_j,a)$ to attains its maximum value, that is

$$\lim_{a \to \infty} f(1,x_j,a) = \lim_{a \to \infty} \left(\frac{x_j^a - 1}{x_j^a}\right)^{\frac{1}{2}} \approx 1, \tag{2.3}$$

if $x_i < x_j$, then $\lim_{a \to \infty} f(1,x_i,a) < \lim_{a \to \infty} f(1,x_j,a)$, that is as $x_j \to (p-1)$, $\lim_{a \to \infty} f(1,x_j,a) \approxeq 1$.

Case 3: If $x_i \neq 1$ and $x_j \neq 1$, then the functional $f(x_i,x_j,a)$ value always lies between 0 and 1. If $x_i = x_j$, then equation (2.1) becomes

$$f(x_i,x_i,a) = \left(\frac{2x_i^a - 2}{x_i^{2a}}\right)^{\frac{1}{2}} = \left(\frac{2\left(1 - \frac{1}{x_i^a}\right)}{x_i^a}\right)^{\frac{1}{2}}, \tag{2.4}$$

the functional value will decrease as the value of x_i approaches its supremum, i.e.,

$$\lim_{(x_i,a) \to (p-1,\infty)} f(x_i,x_i,a) = \lim_{a \to \infty} \left(\frac{2\left(1 - \frac{1}{(p-1)_i^a}\right)}{(p-1)_i^a}\right)^{\frac{1}{2}} \approx 0. \qquad \square$$

The variant a plays the most important role, as it tends to ∞ the functional value of $f(x_i,x_j,a)$ approaches to 0 or 1. The value a must be a finite to characterize the invariants of the graphs.

Further, for $x_i < x_j$, then

$$f(x_j,x_j,a) < f(x_i,x_j,a) < f(x_i,x_i,a), \quad \text{for all } e_h \in E(G). \tag{2.5}$$

By Theorem 2.1, we have the following observation.

Observation 2.1. *In general, for* $1 \leq x_1 \leq x_2 \leq \cdots \leq x_p \leq p-1$*:*

(i) *by equation* (2.2)*,* $f(1,x_1,a) \leq f(1,x_2,a) \leq \cdots \leq f(1,x_p,a)$*.*

(ii) *by equation* (2.4)*,* $f(x_1,x_1,a) \geq f(x_2,x_2,a) \geq \cdots \geq f(x_p,x_p,a)$*, if* $x_1 > 1$.

(iii) *by equation* (2.4) *and equation* (2.5),

$$\begin{aligned} f(x_1,x_1,a) &\geq f(x_1,x_2,a) \geq f(x_2,x_2,a) \geq f(x_2,x_3,a) \\ &\vdots \\ &\geq f(x_{p-1},x_{p-1},a) \geq f(x_{p-1},x_p,a) \geq f(x_p,x_p,a). \end{aligned}$$

Further, the equality is satisfied if and only if $x_1 = x_2 = \cdots = x_p$.

Theorem 2.2. *Let* G *be an acyclic graph with* p*-vertices and* q*-edges. Then*

$$0 \leq ABC_a(G) \leq q\left(\frac{q^a-1}{q^a}\right)^{\frac{1}{2}}.$$

Further, if there is a unique path between v_i *and* v_j *for all* $x_j, x_j \geq 1$, *then*

$$(q-2)\left(\frac{2(2^a-1)}{2^{2a}}\right)^{\frac{1}{2}} + \left(\frac{2^a-1}{2^{a-1}}\right)^{\frac{1}{2}} \leq ABC_a(G) \leq q\left(\frac{q^a-1}{q^a}\right)^{\frac{1}{2}}.$$

Proof. Let G be acyclic graph with p-vertices and q-edges.
If $x_i = x_j = 1$ for all $e_h = v_iv_j \in E(G)$, then using equation (2.1), $\left(\frac{x_i+x_j-2}{x_ix_j}\right)^{\frac{1}{2}} = 0$ for each $e_h \in E(G)$, here we get the minimum value and using equation (2.3), the maximum value of $\left(\frac{x_i+x_j-2}{x_ix_j}\right)^{\frac{1}{2}}$ attains for each $e_h \in E(G)$, $x_i = 1$, $x_j = q$, that is $\left(\frac{x_i+x_j-2}{x_ix_j}\right)^{\frac{1}{2}} = \left(\frac{q^a-1}{q^a}\right)^{\frac{1}{2}}$, so we conclude that for each edge $e_h \in E(G)$,

$$0 \leq \left(\frac{x_i+x_j-2}{x_ix_j}\right)^{\frac{1}{2}} \leq \left(\frac{q^a-1}{q^a}\right)^{\frac{1}{2}}. \tag{2.6}$$

Taking the sum of each $e_h \in E(G)$, we have

$$0 \leq ABC_a(G) \leq q\left(\frac{q^a-1}{q^a}\right)^{\frac{1}{2}}.$$

Further, unique path between v_i and v_j for all $x_j, x_j \geq 1$, then the minimum value will attain for the path with q edges and $ABC_a(G) = (q-2)\left(\frac{2(2^a-1)}{2^{2a}}\right)^{\frac{1}{2}} + \left(\frac{2^a-1}{2^{a-1}}\right)^{\frac{1}{2}}$. The maximum value attains if the degree of incident vertices of each edge is 1 and q and $ABC_a(G) = q\left(\frac{q^a-1}{q^a}\right)^{\frac{1}{2}}$.

$$(q-2)\left(\frac{2(2^a-1)}{2^{2a}}\right)^{\frac{1}{2}} + \left(\frac{2^a-1}{2^{a-1}}\right)^{\frac{1}{2}} \leq ABC_a(G) \leq q\left(\frac{q^a-1}{q^a}\right)^{\frac{1}{2}}.$$ □

By Theorem 2.2, we have

Corollary 2.1. *Let* G *be any tree with* p*-vertices and* q*-edges. Then*

$$(p-3)\left(\frac{2(2^a-1)}{2^{2a}}\right)^{\frac{1}{2}} + \left(\frac{2^a-1}{2^{a-1}}\right)^{\frac{1}{2}} \leq ABC_a(G) \leq (p-1)\left(\frac{(p-1)^a-1}{(p-1)^a}\right)^{\frac{1}{2}}.$$

Theorem 2.3. *Let* G *be a connected graph with* p*-vertices and* q*-edges. Then*

$$q\left(\frac{2\Delta^a-2}{\Delta^{2a}}\right)^{\frac{1}{2}} \leq ABC_a(G) \leq q\left(\frac{\delta^a+\Delta^a-2}{\delta^a\Delta^a}\right)^{\frac{1}{2}}.$$

Proof. Let G be a connected graph, using equation (2.5) and Observation 2.1, the minimum value attains if $x_i = x_j = \Delta$ and maximum value attains if $x_i = \delta$, $x_j = \Delta$ for all $e_h \in E(G)$. Taking the maximum and minimum values of each term corresponding to e_h and summing, we have

$$q\left(\frac{2\Delta^a - 2}{\Delta^{2a}}\right)^{\frac{1}{2}} \le ABC_a(G) \le q\left(\frac{\delta^a + \Delta^a - 2}{\delta^a \Delta^a}\right)^{\frac{1}{2}}. \qquad \square$$

3. Inequalities in Terms of General Zagreb Indices

Now, we obtain an inequality of $ABC_a(G)$ in terms of the first and second general Zagreb indices,

$$M_1^{a+1}(G) = \sum_{uv \in E(G)} [x_i^a + x_j^a], \tag{3.1}$$

$$M_2^a(G) = \sum_{uv \in E(G)} [x_i^a x_j^a], \tag{3.2}$$

where x_i denotes the degree of the vertex v_i and a is a non-zero real number.

Theorem 3.1. *Let G be a graph with p-vertices and q-edges. Then*

$$ABC_a(G) \le \frac{M_1^{a+1}(G) + M_2^{-a}(G)}{2} - q.$$

Proof. Let n_1, n_2 are any two positive real numbers, the inequality of arithmetic and geometric means is given by $\sqrt{n_1 n_2} \le \frac{n_1+n_2}{2}$.
Replacing n_1 by $x_i^a + x_j^a - 2$ and n_2 by $x_i^a x_j^a$, we have

$$\sqrt{\frac{x_i^a + x_j^a - 2}{x_i^a x_j^a}} \le \frac{x_i^a + x_j^a - 2 + \frac{1}{x_i^a x_j^a}}{2}$$

$$\Rightarrow \quad \sqrt{\frac{x_i^a + x_j^a - 2}{x_i^a x_j^a}} \le \frac{x_i^a + x_j^a}{2} - 1 + \frac{1}{2x_i^a x_j^a}. \tag{3.3}$$

The inequality (3.3) satisfies for each $e_h = x_i x_j \in E(G)$, taking the sum of those inequalities, we have

$$\sum_{v_i v_j \in E(G)} \sqrt{\frac{x_i^a + x_j^a - 2}{x_i^a x_j^a}} \le \sum_{v_i v_j \in E(G)} \left(\frac{x_i^a + x_j^a}{2} + \frac{1}{2x_i^a x_j^a}\right) - \sum_{h=1}^{q} 1.$$

Using equation (3.1) and equation (3.2), we have the required bounds,

$$ABC_a(G) \le \frac{M_1^{a+1}(G) + M_2^{-a}(G)}{2} - q. \qquad \square$$

Observation 3.1. *Let G be a connected graph with p-vertices and q-edges. Then*

$$ABC_a(G) \le ABC^{\frac{a}{2}}(G).$$

Further, the equality holds if $a = 1$.

4. Special Classes of Graphs

Theorem 4.1. *Let G be a regular graph with $x_i = r$ for each $v_i \in V(G)$, $p \ge 2$. Then*

(i) $ABC_a(G) = \frac{pr}{2}\left(\frac{2r^a-2}{r^{2a}}\right)^{\frac{1}{2}}$,

(ii) $\overline{ABC}_a(G) = \frac{p(p-r-1)}{2}\left(\frac{2r^a-2}{r^{2a}}\right)^{\frac{1}{2}}$,

(iii) $ABC_a(\overline{G}) = \frac{p(p-r-1)}{2}\left(\frac{2(p-r-1)^a-2}{(p-r-1)^{2a}}\right)^{\frac{1}{2}}$,

(iv) $\overline{ABC}_a(\overline{G}) = \frac{pr}{2}\left(\frac{2(p-r-1)^a-2}{(p-r-1)^{2a}}\right)^{\frac{1}{2}}$,

where $a \geq 1$.

Proof. Let G be a regular graph with $d_G(v_i) = r$ for all $1 \leq i \leq p$. The degree of each edge is $x_i^a + x_j^a - 2 = 2r^a - 2$, also $x_i^a x_j^a = r^{2a}$ for $a \geq 1$.
By equation (1.1), we have

$$ABC_a(G) = q\left(\frac{2r^a-2}{r^{2a}}\right)^{\frac{1}{2}},$$

also, we have for the complementary graph

$$\overline{ABC}_a(G) = \frac{p(p-r-1)}{2}\left(\frac{2r^a-2}{r^{2a}}\right)^{\frac{1}{2}}.$$ □

We can also prove the cases (iii) and (iv) in a similar way.

Corollary 4.1. *Let G be a graph with $p \geq 3$ vertices. By Theorem 4.1, we have*

(i) $ABC_a(C_p) = p(2^{1-a} - 2^{1-2a})^{\frac{1}{2}}$ *and* $\overline{ABC}_a(G) = \frac{p(p-3)}{2}(2^{1-a} - 2^{1-2a})^{\frac{1}{2}}$, *for any cycle C_p with* $p \geq 3$.

(ii) $ABC_a(G) = \frac{p(p-1)}{2}\left(\frac{2(p-1)^a-2}{(p-1)^{2a}}\right)^{\frac{1}{2}}$ *and* $\overline{ABC}_a(G) = 0$, *for complete graph K_p.*

Corollary 4.2. *Let $K_{m,n}$ be a complete bipartite graph with m and n cardinal vertex set partitions. Then*

(i) $ABC_a(K_{m,n}) = mn\left(\frac{m^a+n^a-2}{m^a n^a}\right)^{\frac{1}{2}}$,

(ii) $\overline{ABC}_a(K_{m,n}) = \left(\frac{p(p-1)}{2} - mn\right)\left(\frac{m^a+n^a-2}{m^a n^a}\right)^{\frac{1}{2}}$,

(iii) $ABC_a(\overline{K_{m,n}}) = \frac{m(m-1)}{2}\left(\frac{2(m-1)^a-2}{(m-1)^{2a}}\right)^{\frac{1}{2}} + \frac{n(-1)}{2}\left(\frac{2(n-1)^a-2}{(n-1)^{2a}}\right)^{\frac{1}{2}}$,

(iv) $\overline{ABC}_a(\overline{K_{m,n}}) = mn\left(\frac{(n-1)^a+(m-1)^a-2}{(n-1)^a(m-1)^a}\right)^{\frac{1}{2}}$,

where $a \geq 1$.

5. Conclusions

The novel *Atom-Bond Connectivity* related indices of a graph, the a-analogue *ABC* indices lie in their specific cases for relevantly chosen parameter a values. From the mathematical point of view, applications, and comparative advantages, many questions are suggested by this research, among them the following. The extremum value of the terms of $ABC_a(G)$ is based on the value of x_i and x_j of incident vertices of the edge $e_h = v_i v_j$.

(i) The value of $ABC_a(G)$ increases as the degree of adjacent vertices of an arbitrary edge approaches 1 and $p-1$.

(ii) The value of $ABC_a(G)$ decreases as the degree of the incident vertices approaches to $p-1$.

(iii) In the case of a non-cyclic graph, the maximum value of $ABC_a(G)$ attains if it has a subgraph with a degree of incident vertices of each edge is 1 and q.

(iv) For various values of the variant a results in the convex function since it has fractional power.

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Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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