Research Article

Upper Bounds of AZI and ABC Index for Transformed Families of Graphs

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1.Introduction

Nowadays, graph theory has potential applications in different fields of science. It is especially used for theoretical study of chemical compounds in chemistry. This area of study named as chemical graph theory deals with the problems related to the properties in chemistry. In the middle of last century, theoretical study of chemical compounds attracted the researchers due to its effective applications such as prediction of physiochemical properties of substances in cheminformatics, pharmaceutical sciences, materials science, engineering, and so forth [1]. Cheminformatics is comparatively the latest area of information technology which comprises chemistry, mathematics, and other informational sciences that concentrate on gathering, storing, treating, and examining chemical data. There are many theoretical molecular descriptors in literature used to predict properties of chemical compounds. Among these molecular descriptors, topological indices have an impact in chemistry due to the prediction of physiochemical properties of underlying substance. Its role in "quantitative-structure property relationship" (QSPR) or "quantitative-structure activity relationship" (QSAR) investigation models is also remarkable [2, 3].

In 1947, Wiener for the first time introduced the use of topological index during his work on paraffin's boiling points [4] and provided that it has best correlation with the boiling points of alkanes. The discovery of the Wiener index provided emerging research platform to the research community. In the later years, researchers of different communities proposed many other topological indices and used them for approximation of the chemical properties of their own interest.

In the race for better prediction, Randić [5] in 1975 introduced degree-based topological index named Randić connectivity index which was the best predictive invariant in
those days. The Randić index was reported as the first degree-based index in QSPR study because Zagreb indices by Gutman and Trinajstić [6] were used for totally different purpose before Randić index. In 1998, parallel to the work of Bollobás and Erdős [7, Estrada et al. [8] defined atom bond connectivity (ABC) index as

\[
\text{ABC}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{\text{deg}_u + \text{deg}_v - 2}{\text{deg}_u \times \text{deg}_v},
\]

which has a good correlation with the heat of formation of alkanes. Star graph among trees and complete graph in general for fixed number of vertices have maximal value for ABC index [9]. For more details, one can see [10, 11]. Furtula et al. [12] made a generalization of ABC index as

\[
\text{ABC}_\lambda(\Gamma) = \sum_{uv \in E(\Gamma)} \left( \frac{\text{deg}_u + \text{deg}_v - 2}{\text{deg}_u \times \text{deg}_v} \right)^{-\lambda},
\]

by replacing 1/2 with $-\lambda$. The augmented Zagreb index AZI is $\text{ABC}_1, \lambda = 3$ as,

\[
\text{AZI}(\Gamma) = \sum_{uv \in E(\Gamma)} \left( \frac{\text{deg}_u \times \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3.
\]

Its correlation potential reported is even better than that of other indices in [13–15].

Mathematical study of ABC index and AZI [16–35] encouraged us to answer the fundamental question regarding characterization of transformed families of graphs with maximum and minimum values for ABC index and AZI. Gupta et al. determined bounds for symmetric division degree index in [36]. In this work, we studied ABC index and AZI for transformed graphs $\Gamma_n^{k,l}$ and $A_n(\Gamma_n^{k,l})$ under the fact of transformation $A_n, 0 \leq a \leq l - 2$. We characterize extremal graphs of these transformed families of graphs for AZI and ABC and established their bounds for $\Gamma_n^{k,l}$ and $A_n(\Gamma_n^{k,l})$. When a path is attached with the fully connected vertex (vertex with degree greater than one) of the graph, then it has an impact over the increase and decrease of the index under study. Throughout this work, consider graph $\Gamma_n^{k,l}$ [37]. It comprises $n$-vertex simple connected graph $\Gamma$ along with $k$ pendant paths of length $l \geq 2$ attached with $\nu \in \Gamma$ having degree $2 \leq d_\nu \leq \Delta_{\Gamma}$. Let $\text{deg}_u = \delta_\nu \leq \text{deg}_v \leq \text{deg}_{\nu_i} \leq \ldots \leq \Delta_{\Gamma} + 1$ be the degree sequence of $\Gamma_n^{k,l}$. $\Gamma_n^{k,l}$ is shown in Figure 1.

1.1. Graph Transformations. Let $H(\Gamma) \in E(\Gamma)$, $\Gamma' = \Gamma - H$ be the new graph generated by removing set edges of $H(\Gamma)$, and $\Gamma'' = \Gamma - V_1(\Gamma)$ be the new graph generated by deleting set of vertices $V_1(\Gamma) \subset V(\Gamma)$. We define following transformations.

Let $A_n, 0 \leq a \leq l - 2$ be the transformation defined over pendant paths attached with the graph [38]. $A_n$ has solid effect over increase and decrease of AZI and ABC.

1.1.1. Transformation $A_n$. Let $w_j \in V(\Gamma), \text{deg}_w_j \geq 2$, for $1 \leq j \leq k \leq n$ and paths pendant at $w_j$ of the form $\{w_j u_j, u_j^1 u_j^2, u_j^2 u_j^3, \ldots, u_j^{l-1} u_j^l\}$ comprise $\Gamma_n^{k,l}$. Then,

\[
A(\Gamma_n^{k,l}) = \Gamma_n^{k,l} - \sum_{j=1}^{k} \{u_j^1 u_j^2, u_j^2 u_j^3, \ldots, u_j^{l-1} u_j^l\} + \sum_{j=1}^{k} \{w_j u_j^1, u_j^1 u_j^2, u_j^2 u_j^3, \ldots, u_j^{l-1} u_j^l\}.
\]

The transformation $A$ is shown in Figure 2.

1.1.2. Transformation $A_n$. $A_n$ is the $a \geq 0$ time repetition of transformation $A$.

Let graph $\Gamma = \Gamma(V, E)$ with degree of vertex $u \in \Gamma, \delta_v \leq \text{deg}_u \leq \Delta_{\Gamma}$ and $\delta_v \leq \text{deg}_v \leq \Delta_{\Gamma} + 1$ be the degree of $v \in \Gamma_n^{k,l}$.

2. Upper Bounds for AZI $\text{AZI}(\Gamma_n^{k,l})$ and AZI $A_n(\Gamma_n^{k,l})$ Initially, we proved Proposition 1, which is helpful to prove the main results for AZI.

\[
f(\eta, \zeta) = f(\zeta, \eta) = \left(\frac{\eta \zeta}{\eta + \zeta - 2}\right)^3.
\]

Proposition 1. Let

\[
f(\eta, \zeta) = f(\zeta, \eta)
\]

Then, for $a \geq b$ and $\zeta \geq 2$, $f(a, \zeta) \geq f(b, \zeta)$.

Proof. Let

\[
f(\eta, \zeta) = f(\zeta, \eta) = \left(\frac{\eta \zeta}{\eta + \zeta - 2}\right)^3.
\]
Figure 1: Graph $\Gamma^{k,l}_n$.

\[
\begin{align*}
  f(a, \zeta) - f(b, \zeta) &= \left(\frac{a\zeta}{a + \zeta - 2}\right)^3 - \left(\frac{b\zeta}{b + \zeta - 2}\right)^3 \\
  &= \frac{(a^3\zeta^3(b + \zeta - 2)^3 - b^3\zeta^3(a + \zeta - 2)^3)}{(a + \zeta - 2)^3(b + \zeta - 2)^3} \\
  &= \frac{\zeta^3\left((a^3 - b^3)\zeta - 2\right)^3 + 3a^2b^2(a - b)(\eta - 2) + 3ab\left(a^2 - b^2\right)(\eta - 2)\zeta}{(a + \zeta - 2)^3(b + \zeta - 2)^3} \\
  &= \frac{\zeta^3\left((a - b)(a^2 + ab + b^2)(\zeta - 2)^3 + 3a^2b^2(a - b)(\zeta - 2) + 3ab(a + b)(a - b)(\zeta - 2)^3\right)}{(a + \zeta - 2)^3(b + \zeta - 2)^3} \\
  &= \frac{\zeta^3(a - b)((a^2 + ab + b^2)(\zeta - 2)^3 + 3a^2b^2(\zeta - 2) + 3ab(a + b)(\zeta - 2)^2)}{(a + \zeta - 2)^3(b + \zeta - 2)^3} \\
  &\geq 0. 
\end{align*}
\]

This implies

\[
f(a, \zeta) \geq f(b, \zeta). \tag{7} \]

Lemma 1 (see [15]). Let

\[
\Phi(u, v) = \Phi(v, u) = \left(\frac{uv}{u + v - 2}\right)^3. \tag{8}
\]

Then,

\[
\text{AZI}(\Gamma_n^{k,l}) \leq k \frac{\Delta_r}{2} \left[\left(\frac{(\Delta_r + 1)^3}{2\Delta_r}\right)^3 + \left(\frac{(\Delta_r + 1)}{2\Delta_r - 1}\right)^3\right] + \text{AZI}(\Gamma) - k \frac{\delta_1}{2} \left[\left(\frac{\delta_1(\delta_1 + 1)}{2\delta_1 - 1}\right)^3 + \left(\frac{\delta_1^2}{2\delta_1 - 2}\right)^3\right] + 8kl + p \left[8 - \left(\frac{\Delta_r + 1}{\Delta_r}\right)^3\right]. \tag{9}
\]

(1) $\Phi(1, v)$ is decreasing for $v \geq 2$.
(2) $\Phi(2, v) = 8$ for any real number $v$.
(3) For fixed $v \geq 3$, $\Phi(u, v)$ is increasing and $\Phi(u, v) > 8$ for $u > 2$.

In Theorem 1, we discuss the effect of pendent paths over AZI and determine its upper bound.

Theorem 1. Let graph $\Gamma^{k,l}_n$ comprise $n$-vertex graph $\Gamma$ having $m$ edges and $p \geq 0$ pendent vertices. Then,
Equality holds for a complete graph \( \Gamma \) of size \( n \) with pendent paths of length \( l \) at each vertex, i.e., \( k = n \).

**Proof.** Let \( \Gamma^{k,l}_n \) be the graph formed by \( k \) number of paths having length \( l \) pendent at distinct vertices \( u \in \Gamma \) such that \( 2 \leq \text{deg}_u \leq \delta_1 + 1 \). Then,

\[
\text{AZI}(\Gamma) = \sum_{uv \in E(\Gamma)} \left( \frac{\text{deg}_u \cdot \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3.
\]  

The construction of \( \Gamma^{k,l}_n \), \( l \geq 2 \), implies \( |E(\Gamma^{k,l}_n)| = m + kl \), and for

\[
(uv \in E(\Gamma^{k,l}_n), (\text{deg}_u + \text{deg}_v) \in \{3, 4, \text{deg}_u + 3, \text{deg}_v, \text{deg}_u + \text{deg}_v, \text{deg}_u + \text{deg}_v + 1\}).
\]  

The edge set of \( \Gamma^{k,l}_n \) is partitioned as

\[
A_1 = \{uv \in \Gamma^{k,l}_n : \text{deg}_u = 1, \text{deg}_v = 2\},
\]

\[
A_2 = \{uv \in \Gamma^{k,l}_n : \text{deg}_u = \text{deg}_v = 2\},
\]

\[
A_{\text{deg}_u \leq \delta_1} = \{uv \in \Gamma^{k,l}_n : \delta_1 \leq \text{deg}_u = \text{deg}_v \leq \Delta_1 + 1, \text{deg}_u = 2\},
\]

\[
A_{\text{deg}_u, \text{deg}_v} = \{uv \in \Gamma^{k,l}_n : \delta_1 \leq \text{deg}_u = \text{deg}_v, \text{deg}_u = \text{deg}_v \leq \Delta_1\},
\]

\[
A_{\text{deg}_u, \text{deg}_v + 1} = \{uv \in \Gamma^{k,l}_n : \delta_1 \leq \text{deg}_u = \text{deg}_v, \text{deg}_u = \text{deg}_v + 1 \leq \Delta_1 + 1\}.
\]

\[
\text{AZI}(\Gamma^{k,l}_n) = \sum_{uv \text{ are edges of pendent paths}} \left( \frac{\text{deg}_u \cdot \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3 + \sum_{uv \text{ are edges of } \Gamma} \left( \frac{\text{deg}_u \cdot \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3.
\]

\[
\text{AZI}(\Gamma^{k,l}_n) = \sum_{uv \in A_1} \left( \frac{\text{deg}_u \cdot \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3 + \sum_{uv \in A_2} \left( \frac{\text{deg}_u \cdot \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3 + \sum_{uv \in A_{\text{deg}_u \leq \delta_1}} \left( \frac{\text{deg}_u \cdot \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3 + \sum_{uv \in A_{\text{deg}_u, \text{deg}_v}} \left( \frac{\text{deg}_u \cdot \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3 + \sum_{uv \in A_{\text{deg}_u, \text{deg}_v + 1}} \left( \frac{\text{deg}_u \cdot \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3 + \sum_{uv \text{ are pendent edges of } \Gamma} \left( \frac{\text{deg}_u \cdot \text{deg}_v}{\text{deg}_u + \text{deg}_v - 2} \right)^3.
\]
The construction of $\text{AZI}(r_{n}^{k,l})$ implies that the cardinality of $A_{i}$ is $k$, i.e., $|A_{i}| = k$, $|A_{1}| = k(l - 2)$, $|A_{\text{deg} + 1}| = k$, $|A_{\text{deg} + 2}| = k$. For $\Delta_{r}$, minimum degree of vertices of $\Gamma$ and maximum degree $\Delta_{r}$, using Proposition 1 and Lemma 1, we have

$$\sum_{uv \text{ are pendant edges of } \Gamma} \left(\frac{\text{deg}_{u} \text{deg}_{v}}{\text{deg}_{u} + \text{deg}_{v} - 2}\right)^{3} \leq 8 \rho,$$

$$\sum_{uv \in A_{\text{deg} + \text{deg} + 1}} \left(\frac{\text{deg}_{u} \text{deg}_{v}}{\text{deg}_{u} + \text{deg}_{v} - 2}\right)^{3} \leq \frac{k \Delta_{r}}{2} \left[\left(\frac{\Delta_{r} + 1}{2 \Delta_{r}}\right)^{3} + \left(\frac{\Delta_{r} (\Delta_{r} + 1)}{2 \Delta_{r} - 1}\right)^{3}\right],$$

$$\sum_{uv \in A} \left(\frac{\text{deg}_{u} \text{deg}_{v}}{\text{deg}_{u} + \text{deg}_{v} - 2}\right)^{3} \leq \text{AZI} (\Gamma) - \rho \left(\frac{\Delta_{r} + 1}{\Delta_{r}}\right)^{3} - \frac{k \delta_{r}}{2} \left[\left(\frac{\delta_{r} (\delta_{r} + 1)}{2 \delta_{r} - 1}\right)^{3} + \left(\frac{\delta_{r}^{2}}{2 \delta_{r} - 2}\right)^{3}\right].$$

Now, from equation (12), we get

$$\text{AZI}(\Gamma_{n}^{k,l}) \leq k \frac{\Delta_{r}}{2} \left[\left(\frac{\Delta_{r} + 1}{2 \Delta_{r}}\right)^{3} + \left(\frac{\Delta_{r} (\Delta_{r} + 1)}{2 \Delta_{r} - 1}\right)^{3}\right] + \text{AZI}(\Gamma) - k \frac{\delta_{r}}{2} \left[\left(\frac{\delta_{r} (\delta_{r} + 1)}{2 \delta_{r} - 1}\right)^{3} + \left(\frac{\delta_{r}^{2}}{2 \delta_{r} - 2}\right)^{3}\right] - p \left(\frac{\Delta_{r} + 1}{\Delta_{r}}\right)^{3} + 8k + 8k(l - 2) + 8k + 8p.$$ 

After simplification, we get

$$\text{AZI}(\Gamma_{n}^{k,l}) \leq k \frac{\Delta_{r}}{2} \left[\left(\frac{\Delta_{r} + 1}{2 \Delta_{r}}\right)^{3} + \left(\frac{\Delta_{r} (\Delta_{r} + 1)}{2 \Delta_{r} - 1}\right)^{3}\right] + \text{AZI}(\Gamma) - k \frac{\delta_{r}}{2} \left[\left(\frac{\delta_{r} (\delta_{r} + 1)}{2 \delta_{r} - 1}\right)^{3} + \left(\frac{\delta_{r}^{2}}{2 \delta_{r} - 2}\right)^{3}\right] + 8kl + p \left[8 - \left(\frac{\Delta_{r} + 1}{\Delta_{r}}\right)^{3}\right].$$

Inequality (15) completes the proof.

In Theorem 2, we discussed the effect of successive applications of transformation $A$ as shown in Figure 2 over AZI.

$$\text{AZI}(A_{a}(\Gamma_{n}^{k,l})) \leq k \frac{\Delta_{r}}{2} \left[\left(\frac{\Delta_{r} + \alpha + 1}{2 \Delta_{r} + \alpha}\right)^{3} + \left(\frac{\Delta_{r} (\Delta_{r} + \alpha + 1)}{2 \Delta_{r} + \alpha - 1}\right)^{3}\right] + k \frac{\delta_{r}}{2} \left[\left(\frac{\delta_{r} (\delta_{r} + \alpha + 1)}{2 \delta_{r} + \alpha - 1}\right)^{3} + \left(\frac{\delta_{r}^{2}}{2 \delta_{r} - 2}\right)^{3}\right] + p \left[8 - \left(\frac{\Delta_{r} + 1}{\Delta_{r}}\right)^{3}\right] + 8kl - 8k\alpha + \text{AZI}(\Gamma).$$
Equality holds for a complete graph $\Gamma$ of size $n$ with pendent paths of length $l$ at each vertex, i.e., $k = n$.

**Proof.** Let a simple graph $\Gamma$ of order $n$, Size $m$ having $p \geq 0$ pendent vertices. The augmented Zagreb index of any graph $\Gamma$ is

$$
\text{AZI}(\Gamma) = \sum_{uv \in E(\Gamma)} \left( \frac{\deg_u \deg_v}{\deg_u + \deg_v - 2} \right)^3.
$$

Equality holds for a complete graph $\Gamma$ of size $n$ with pendent paths of length $l$ at each vertex, i.e., $k = n$.

The construction of $\Gamma^{k,l}_n$, $l \geq 2$, implies $|E(\Gamma^{k,l}_n)| = m + kl$. After successive applications of transformation $A$ as $A_n$, $\alpha \leq l - 1$, the edge set of $A_n(\Gamma^{k,l}_n)$ is partitioned as $E_{(\text{deg}_u \cdot \text{deg}_v)}(A_n(\Gamma^{k,l}_n))$ where

$$
E_1(A_n(\Gamma^{k,l}_n)) = \{uv \in \Gamma^{k,l}_n: \deg_u = 1, \deg_v = 2\},
$$

$$
E_2(A_n(\Gamma^{k,l}_n)) = \{uv \in \Gamma^{k,l}_n: \deg_u = \deg_v = 2\},
$$

$$
E_{\text{deg}_u=\alpha+1}(A_n(\Gamma^{k,l}_n)) = \{uv \in \Gamma^{k,l}_n: \alpha \leq \deg_u = \deg_v = 2 \leq \Delta_T + \alpha + 1, \deg_v = 1\},
$$

$$
E_{\text{deg}_v=\alpha+1}(A_n(\Gamma^{k,l}_n)) = \{uv \in \Gamma^{k,l}_n: \alpha \leq \deg_u = \deg_v = 2 \leq \Delta_T + \alpha + 1, \deg_u = 1\},
$$

$$
E_{\text{deg}_u=\alpha}(A_n(\Gamma^{k,l}_n)) = \{uv \in \Gamma^{k,l}_n: \alpha \leq \deg_u = \deg_v = 2 \leq \Delta_T + \alpha + 1, \deg_v = 1\},
$$

$$
E_{\text{deg}_v=\alpha}(A_n(\Gamma^{k,l}_n)) = \{uv \in \Gamma^{k,l}_n: \alpha \leq \deg_u = \deg_v = 2 \leq \Delta_T + \alpha + 1, \deg_u = 1\},
$$

The construction of $\Gamma^{k,l}_n$ implies the cardinality

$$
|E_1(A_n(\Gamma^{k,l}_n))| = k,
$$

$$
|E_2(A_n(\Gamma^{k,l}_n))| = k(l - \alpha - 2),
$$

$$
|E_{\text{deg}_u=\alpha+1}(A_n(\Gamma^{k,l}_n))| = k\alpha,
$$

$$
|E_{\text{deg}_v=\alpha+1}(A_n(\Gamma^{k,l}_n))| = k\alpha,
$$

and $|A_n(\text{deg}_u)| = p$. For $\delta_T$, minimum degree of vertices of $\Gamma$ and maximum degree $\Delta_T$, using Lemma 1, we have
\[
\sum_{uv \text{ are pendant edges of } \Gamma} \left( \frac{\deg_u \deg_v}{\deg_u + \deg_v - 2} \right)^3 \leq 8p,
\]
\[
\sum_{uv \in A} \left( \frac{\deg_u \deg_v}{\deg_u + \deg_v + \alpha + 1} \right)^3 \leq \frac{k\Delta + \alpha + 1}{\Delta + \alpha} \left[ \frac{(\Delta + \alpha + 1)^3}{2\Delta + 2\alpha} + \frac{(\Delta + \alpha + 1)^3}{2\Delta + \alpha - 1} \right],
\]
\[
\deg_u, \deg_v \geq 2
\]
\[
\sum_{uv \in A_{\deg_u = 2}} \left( \frac{\deg_u \deg_v}{\deg_u + \deg_v - 2} \right)^3 \leq k\alpha \left( \frac{\Delta + \alpha + 1}{\Delta + \alpha} \right)^3,
\]
\[
\sum_{uv \in A_{\deg_v = 2}} \left( \frac{\deg_u \deg_v}{\deg_u + \deg_v - 2} \right)^3 \leq 8k.
\]

Substituting these changes in equation (19), we have the following inequality.

\[
\text{AZI}(A_n(\Gamma_n^{k,l})) \leq 8k + 8k(l - 2 - \alpha) + 8k + k\alpha \left( \frac{\Delta + \alpha + 1}{\Delta + \alpha} \right)^3 + 8p + k\Delta \left[ \frac{(\Delta + \alpha + 1)^3}{2\Delta + 2\alpha} + \frac{(\Delta + \alpha + 1)^3}{2\Delta + \alpha - 1} \right] \]
\[
+ \text{AZI}(\Gamma) - k \frac{\delta^2}{2} \left[ \frac{(\delta + \alpha + 1)^3}{2\delta + 2\alpha} + \frac{\delta^3}{2\delta + \alpha - 1} \right] - p \left( \frac{\Delta + \alpha + 1}{\Delta + \alpha} \right)^3.
\]

After simplification, we get

\[
\text{AZI}(A_n(\Gamma_n^{k,l})) \leq \frac{k\Delta}{2} \left[ \frac{(\Delta + \alpha + 1)^3}{2\Delta + 2\alpha} + \frac{(\Delta + \alpha + 1)^3}{2\Delta + \alpha - 1} \right] - \frac{k\delta}{2} \left[ \frac{(\delta + \alpha + 1)^3}{2\delta + 2\alpha} + \frac{\delta^3}{2\delta + \alpha - 1} \right] \]
\[
+ p \left[ 8 - \left( \frac{\Delta + 1}{\Delta} \right)^3 \right] + 8kl - 8k\alpha + \text{AZI}(\Gamma).
\]

Inequality (23) completes the proof. \qed

3. Upper Bounds for ABC(\Gamma_n^{k,l}) and ABC(A_n(\Gamma_n^{k,l}))

Lemma 2 (see [39, 40]). Let
\[
\Phi(x, y) = \Phi(y, x)
\]
\[
= \sqrt{\frac{x + y - 2}{xy}} \quad (24)
\]

Then,

(1) \( \Phi(1, y) \) is increasing for \( y \).
(2) \( \Phi(2, y) = \sqrt{2}/2 \) for any real number \( y \).

Proof. Let

(3) For fixed \( y \geq 2 \), \( \Phi(x, y) \) is decreasing for \( x \).

Proposition 2 is related to the ABC index.

Proposition 2. Let

\[
\Phi(\eta, \zeta) = \Phi(\zeta, \eta)
\]
\[
= \sqrt{\frac{\eta + \zeta - 2}{\eta \zeta}} \quad (25)
\]

For \( \eta, \zeta, \Delta \in \mathbb{R}, \eta, \zeta \leq \Delta \) and \( \eta, \zeta, \Delta \geq 2 \).

\[
\Phi(\eta, \zeta) \geq \Phi(\Delta, \Delta). \quad (26)
\]

Proof. Let
\[ \Phi(\eta, \zeta) = \Phi(\zeta, \eta) \]
\[ = \sqrt{\frac{\eta + \zeta - 2}{\eta\zeta}} \quad (27) \]

By Lemma 2, for \( \eta = 2 \) or \( \zeta = 2 \) and \( \Delta = 2 \),
\[ \Phi(\eta, \zeta) = \Phi(\Delta, \Delta) \]
\[ = \Phi(\Delta, \zeta) \]

Now for \( \eta \geq 3 \) or \( \zeta \geq 3 \) and \( \Delta = \zeta \), let \( \alpha, \beta, \gamma \geq 1, \alpha \leq \gamma, \beta = \gamma \) and \( \eta = 2 + \alpha \) or \( \zeta = 2 + \beta, \Delta = 2 + \gamma \),
\[ \Phi(\eta, \zeta) - \Phi(\Delta, \Delta) = \frac{\sqrt{\Delta + \Delta - 2}}{\Delta\Delta} \]
\[ = \frac{\alpha + 2 + \beta}{(\alpha + 2)(\beta + 2)} \sqrt{\frac{2}{\gamma + 2}} \]
\[ = \frac{1}{\sqrt[4]{\alpha + 2 + \beta/(\alpha + 2)(\beta + 2) + 2}(\gamma + 2)^2} \left[ \frac{\alpha + 2 + \beta}{(\alpha + 2)(\beta + 2)} - \frac{2}{\gamma + 2} \right] \]
\[ = \frac{1}{\sqrt[4]{\alpha + 2 + \beta/(\alpha + 2)(\beta + 2) + 2}(\gamma + 2)^2} \left[ \frac{\gamma - \beta}{(\beta + 2)} + \frac{\beta}{(\alpha + 2)(\beta + 2)} - \frac{1}{\gamma + 2} \right] \]
\[ = \frac{1}{\sqrt[4]{\alpha + 2 + \beta/(\alpha + 2)(\beta + 2) + 2}(\gamma + 2)^2} \left[ \frac{\gamma - \beta}{(\beta + 2)} + \frac{\beta y(\gamma - \alpha)}{(\alpha + 2)(\beta + 2)(\gamma + 2)^2} \right] \]
\[ = \frac{1}{\sqrt[4]{\alpha + 2 + \beta/(\alpha + 2)(\beta + 2) + 2}(\gamma + 2)^2} \left[ \frac{\beta y(\gamma - \alpha) + 2y(\beta - \alpha) + 4(\beta - \gamma)}{(\alpha + 2)(\beta + 2)(\gamma + 2)^2} \right] \]
\[ = \frac{1}{\sqrt[4]{\alpha + 2 + \beta/(\alpha + 2)(\beta + 2) + 2}(\gamma + 2)^2} \left[ \frac{(\Delta - 2)((\zeta - 2)(\Delta - \eta) + 2(\zeta - \eta))}{\eta\zeta^2} + \frac{(\Delta - \zeta)(\eta^2 - 4)}{\eta\zeta^2} \right] \]
\[ = \frac{1}{\sqrt[4]{\alpha + 2 + \beta/(\alpha + 2)(\beta + 2) + 2}(\gamma + 2)^2} \left[ \frac{(\Delta - 2)((\zeta - 2)(\Delta - \eta) + 2(\zeta - \eta))}{\eta\zeta^2} + \frac{(\Delta - \zeta)(\eta^2 - 4)}{\eta\zeta^2} \right] \]
\[ = \frac{1}{\sqrt[4]{\alpha + 2 + \beta/(\alpha + 2)(\beta + 2) + 2}(\gamma + 2)^2} \left[ \frac{(\Delta - 2)((\zeta - 2)(\Delta - \eta) + 2(\zeta - \eta))}{\eta\zeta^2} + \frac{(\Delta - \zeta)(\eta^2 - 4)}{\eta\zeta^2} \right] \]
\[ = \frac{1}{\sqrt[4]{\alpha + 2 + \beta/(\alpha + 2)(\beta + 2) + 2}(\gamma + 2)^2} \left[ \frac{(\Delta - 2)((\zeta - 2)(\Delta - \eta) + 2(\zeta - \eta))}{\eta\zeta^2} + \frac{(\Delta - \zeta)(\eta^2 - 4)}{\eta\zeta^2} \right] \]
\[ (29) \]
Since $\Phi(\eta, \zeta)$ is a symmetric function, one can let $\eta \geq \zeta$ or $\zeta \geq \eta$, so the factor $(\zeta - \eta) \geq 0$ along with $\eta - 2 \geq 0$, $\zeta - 2 \geq 0$, $\Delta - 2 \geq 0$, and $\Delta - \zeta \geq 0$. All the factors involved in equation (29) are positive. This implies
\[ \Phi(\eta, \zeta) - \Phi(\Delta, \Delta) \geq 0. \] (30)

Hence, for all $\eta, \zeta \geq 2$ and $\eta, \zeta \leq \Delta$,
\[ \Phi(\eta, \zeta) \geq \Phi(\Delta, \Delta). \] (31)

In Theorem 3, we discuss the effect of pendent paths over ABC index and determine its upper bound. \hfill \Box

**Theorem 3.** Let graph $\Gamma$ and $\Gamma$ having order $n$, size $m$, and $p \geq 0$ pendent vertices. Then, the construction of $\Gamma^{kl}_n$, $l \geq 2$, implies $|E(\Gamma^{kl}_n)| = m + kl$, and for $uv \in E(\Gamma^{kl}_n)$,
\[ (\deg_u + \deg_v) \in [3, 4, \deg_u + 3, \deg_v + \deg_u + 1, \deg_v]. \] (34)

We use edge set partition of $\Gamma^{kl}_n$ defined in Theorem 1:

\[ ABC(\Gamma^{kl}_n) = \sum_{uv \in E(\Gamma^{kl}_n)} \sqrt{\frac{\deg_u + \deg_v - 2}{\deg_u \deg_v}} + \sum_{uv \in \Delta} \sqrt{\frac{\deg_u + \deg_v - 2}{\deg_u \deg_v}}, \] (35)

The construction of $\Gamma^{kl}_n$ implies that the cardinality of $A_{u}$ is $k$, i.e., $|A_u| = k$, $|A_{v}| = k(1 - 2)$, $|A_{\deg_u \geq 2}| = k$, and $|A_{\deg_v \geq 2}| = k$. For $\Delta$, minimum degree of vertices of $\Gamma$ and maximum degree $\Delta$, using Lemma 2 and Proposition 2, we have

\[ \sum_{uv \text{ are pendent edges of } \Gamma} \sqrt{\frac{\deg_u + \deg_v - 2}{\deg_u \deg_v}} \leq \frac{\sqrt{\Delta}}{\Delta + 1} p, \]

\[ \sum_{uv \in A \text{ or } \deg_u \geq 2} \sqrt{\frac{\deg_u + \deg_v - 2}{\deg_u \deg_v}} \leq k \Delta \frac{1}{\sqrt{2}}. \]
\[
\sum_{uv \in A} \deg_u + \deg_v - 2 \begin{cases}
\deg_u, \deg_v \geq 2
\end{cases} \leq ABC(\Gamma) - p \frac{1}{\sqrt{2}} - \frac{k\delta}{2} \left[ \frac{2\Delta - 1}{(\Delta + 1)^2} + \frac{2\Delta - 1}{\Delta(\Delta + 1)} \right].
\]

Now, from equation (35),

\[
ABC(\Gamma^{k,l}_n) \leq ABC(\Gamma) + p\sqrt{\frac{\Delta - 1}{\Delta + 1}} + k\Delta \sqrt{\frac{1}{2} + \frac{\sqrt{2}}{2} k - \frac{k\delta}{2}} \left[ \frac{2\Delta - 1}{(\Delta + 1)^2} + \frac{2\Delta - 1}{\Delta(\Delta + 1)} \right] - \frac{\sqrt{2}}{2} p + \frac{\sqrt{2}}{2} k(l - 2) + \frac{\sqrt{2}}{2} k.
\]

After simplification,

\[
ABC(\Gamma^{k,l}_n) \leq k\Delta \sqrt{\frac{1}{2} - \frac{k\delta}{2}} \left[ \frac{2\Delta - 1}{(\Delta + 1)^2} + \frac{2\Delta - 1}{\Delta(\Delta + 1)} \right] + \frac{\sqrt{2}}{2} kl + p \left( \frac{\Delta}{(\Delta + 1)} - \frac{\sqrt{2}}{2} \right) + ABC(\Gamma).
\]

Inequality (38) completes the proof.

Theorem 4 gives the discussion about the effect of successive applications of transformation A as shown in Figure 2 over ABC index.

Proof. Let \( \Gamma^{k,l}_n \) graph having pendent paths and \( A_\alpha \) be the \( \alpha \) time repetition of transformation A. ABC(\( \Gamma \)) is
\[ ABC(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\frac{\deg_u + \deg_v - 2}{\deg_u \deg_v}} \]  

(40) After successive applications of transformation \( A \) as \( A_\alpha \), \( \alpha \leq l - 1 \), the edge set of \( A_\alpha (\Gamma^k_n) \) is partitioned as \( E_{(\deg_u, \deg_v)} (A_\alpha (\Gamma^k_n)) \) where

\[ (\deg_u + \deg_v) \in \{3, 4, \deg_u + \alpha + 2, \deg_u + \alpha + 3, \deg_u + \deg_v, \deg_u + \alpha + 1 + \deg_v\}. \]  

(41)

The construction of \( A_\alpha (\Gamma^k_n) \) shows

\[
\begin{align*}
E_1(A_\alpha (\Gamma^k_n)) = & \{uv \in \Gamma^k_n : \deg_u = 1, \deg_v = 2\}, \\
E_\alpha(A_\alpha (\Gamma^k_n)) = & \{uv \in \Gamma^k_n : \deg_u = \deg_v = 2\}, \\
E_{\deg_u, \alpha + 2}(A_\alpha (\Gamma^k_n)) = & \{uv \in \Gamma^k_n : \delta_l + 1 \leq \deg_u = \deg_v = \deg_u + \alpha + 1 \leq \Delta_\Gamma + \alpha + 1, \deg_v = 1\}, \\
E_{\deg_v, \alpha + 3}(A_\alpha (\Gamma^k_n)) = & \{uv \in \Gamma^k_n : \delta_l + 1 \leq \deg_v = \deg_u = \deg_u + \alpha + 1 \leq \Delta_\Gamma + \alpha + 1, \deg_v = 2\}, \\
E_{\deg_u, \deg_v}(A_\alpha (\Gamma^k_n)) = & \{uv \in \Gamma^k_n : \delta_l \leq \deg_u = \deg_v, \deg_v = \deg_v = \deg_u + \alpha + 1\}, \\
E_{\deg_{u+1}}(A_\alpha (\Gamma^k_n)) = & \{uv \in \Gamma^k_n : \delta_l \leq \deg_v = \deg_v, \deg_v \leq \Delta_\Gamma, \deg_{u+1} = \deg_u + \alpha + 1\}.
\end{align*}
\]  

(42)

The construction of \( A_\alpha (\Gamma^k_n) \) implies that

\[
\begin{align*}
|E_1(A_\alpha (\Gamma^k_n))| &= k, \\
|E_\alpha(A_\alpha (\Gamma^k_n))| &= k(l - \alpha - 2), \\
|E_{\deg_u, \alpha + 2}(A_\alpha (\Gamma^k_n))| &= k\alpha, \\
|E_{\deg_{u+1}}(A_\alpha (\Gamma^k_n))| &= k.
\end{align*}
\]  

(43)
and $|A_{1\text{-deg}}| = p$. For $\delta_\Gamma$ minimum degree of vertices of $\Gamma$ and maximum degree $\Delta_\Gamma$, using Lemma 2 and Proposition 2, we have

\[ \sum_{u,v \text{ are pendant edges of } \Gamma} \frac{\deg_u + \deg_v - 2}{\deg_u \deg_v} \leq p \frac{\Delta_\Gamma + \alpha}{\left(\Delta_\Gamma + \alpha + 1\right)} \]

\[ \sum_{u,v \in A} \frac{\deg_u + \deg_v - 2}{\deg_u \deg_v} \leq k \Delta_\Gamma \frac{2\delta_\Gamma + 2\alpha - 1}{\left(\delta_\Gamma + \alpha\right)\left(\delta_\Gamma + \alpha + 1\right)} \]

for $\deg_u, \deg_v \geq 2$

\[ \sum_{u,v \in A_{\deg_u + v < 2}} \frac{\deg_u + \deg_v - 2}{\deg_u \deg_v} \leq k \alpha \frac{\Delta_\Gamma + \alpha}{\left(\Delta_\Gamma + \alpha + 1\right)} \]

\[ \sum_{u,v \in A_{\deg_u + v < 3}} \frac{\deg_u + \deg_v - 2}{\deg_u \deg_v} = \frac{1}{\sqrt{2}} k, \]

for $\deg_u, \deg_v \geq 2$

Substituting these changes in equation (42), we have following inequality.

\[
ABC(A_n(\Gamma_{k,l})) \leq p \frac{\Delta_\Gamma + \alpha}{\left(\Delta_\Gamma + \alpha + 1\right)} + \frac{1}{\sqrt{2}} k \left(1 - \alpha\right) + \frac{1}{\sqrt{2}} k + k \Delta_\Gamma \frac{\Delta_\Gamma + \alpha}{\left(\Delta_\Gamma + \alpha + 1\right)} + k \Delta_\Gamma \frac{2\delta_\Gamma + 2\alpha - 1}{\left(\delta_\Gamma + \alpha\right)\left(\delta_\Gamma + \alpha + 1\right)} + ABC(\Gamma)
\]

\[- \frac{1}{\sqrt{2}} \sqrt{\frac{2 \Delta_\Gamma + 2 \alpha}{\left(\Delta_\Gamma + \alpha + 1\right)^2} + \frac{2 \Delta_\Gamma + 2 \alpha - 1}{\left(\Delta_\Gamma + \alpha\right)\left(\Delta_\Gamma + \alpha + 1\right)}} \]

After simplification, we get

\[
ABC(A_n(\Gamma_{k,l})) \leq \frac{1}{\sqrt{2}} k l + k \alpha \sqrt{\frac{\Delta_\Gamma + \alpha}{\left(\Delta_\Gamma + \alpha + 1\right)}} + k \Delta_\Gamma \sqrt{\frac{2 \Delta_\Gamma + 2 \alpha - 1}{\left(\Delta_\Gamma + \alpha\right)\left(\Delta_\Gamma + \alpha + 1\right)}} - \frac{k \Delta_\Gamma}{2} \left[ \sqrt{\frac{2 \Delta_\Gamma + 2 \alpha}{\left(\Delta_\Gamma + \alpha + 1\right)^2} + \frac{2 \Delta_\Gamma + 2 \alpha - 1}{\left(\Delta_\Gamma + \alpha\right)\left(\Delta_\Gamma + \alpha + 1\right)}} \right]
\]

\[ + p \left( \sqrt{\frac{\Delta_\Gamma + \alpha}{\left(\Delta_\Gamma + \alpha + 1\right)}} - \frac{1}{\sqrt{2}} \right) + ABC(\Gamma). \]

(46)
4. Conclusion

The study of mathematical aspect regarding topological indices is a partially open problem: for which members of graph family, certain index has minimal or maximal value? In this work, we deal with this fundamental question. We considered graphs of family $\Gamma_{n}^{k,l}$ with $0 \leq k \leq n$, length $l \geq 2$ and transformed family $A_{\alpha}(\Gamma_{n}^{k,l})$ where transformation $A_{\alpha}$ is the graph transformation. The concluding key points concerning our study are given as follows. We studied the fact of pendent paths over the increase and decrease of $\alpha$ZI and ABC index in addition to defining upper bounds for these indices and mentioned graphs with maximum values of these indices. We discussed the fact of defined transformation as $A_{\alpha}; 0 \leq \alpha \leq 1 – 2, 0 \leq k \leq n$ over AZI and ABC indices. We determined upper bounds and characterized extremal graphs for such bounds.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors’ Contributions

All authors contributed equally to this study.

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