Trees with Given Diameter Minimizing the Augmented Zagreb Index and Maximizing the ABC Index

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Abstract: Let $G$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The augmented Zagreb index of a graph $G$ is defined as

$$AZI(G) = \sum_{u \neq v \in E(G)} \left( \frac{d_ud_v}{d_u + d_v - 2} \right)^3,$$

and the atom-bond connectivity index (ABC index for short) of a graph $G$ is defined as

$$ABC(G) = \sum_{u \neq v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_ud_v}},$$

where $d_u$ and $d_v$ denote the degree of vertices $u$ and $v$ in $G$, respectively. In this paper, trees with given diameter minimizing the augmented Zagreb index and maximizing the ABC index are determined, respectively.

Key words: tree, augmented Zagreb index, ABC index, diameter

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1 Introduction

Let $G$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $N_u$ denote the set of all neighbors of a vertex $u \in V(G)$, and $d_u = |N_u|$ denote the degree of $u$ in $G$. A connected graph $G$ is called a tree if $|E(G)| = |V(G)| - 1$. The length of a shortest path connecting the vertices $u$ and $v$ in $G$ is called the distance between $u$ and $v$, and denoted by $d(u, v)$. The diameter $d$ of $G$ is the maximum distance $d(u, v)$ over all pairs of vertices $u$ and $v$ in $G$. 

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Molecular descriptors have found wide applications in QSPR/QSAR studies (see [1]). Among them, topological indices have a prominent place. Augmented Zagreb index, which was introduced by Furtula et al. [2], is a valuable predictive index in the study of the heat of formation in octanes and heptanes. Another topological index, Atom-bond connectivity index (for short, ABC index), proposed by Estrada et al. [3], displays an excellent correlation with the heat of formation of alkanes (see [3]) and strain energy of cycloalkanes (see [4]).

The augmented Zagreb index of a graph \( G \) is defined as:

\[
AZI(G) = \sum_{uv \in E(G)} \left( \frac{d_u d_v}{d_u + d_v - 2} \right)^3,
\]

and the ABC index of a graph \( G \) is defined as:

\[
ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.
\]

Some interesting problems such as mathematical-chemical properties, bounds and extremal graphs on the augmented Zagreb index and the ABC index for various classes of connected graphs have been investigated in [2], [5] and [6]–[10], respectively. Besides, in the literature, there are many papers concerning the problems related to the diameter (see, e.g., [11]–[13]). In this paper, trees with given diameter minimizing the augmented Zagreb index and maximizing the ABC index are determined, respectively.

2 Trees with Given Diameter Minimizing the Augmented Zagreb Index

A vertex \( u \) is called a pendant vertex if \( d_u = 1 \). Let \( S_n \) and \( P_n \) denote the star and path of order \( n \), respectively. Let \( S_{n_1,n_2} \) be the tree of order \( n(\geq 3) \) obtained from the path \( P_l \) by attaching \( n_1 \) and \( n_2 \) pendant vertices to the end-vertices of \( P_l \) respectively, where \( l, n_1, n_2 \) are positive integers, \( n_1 \leq n_2 \) and \( l + n_1 + n_2 = n \). Especially, \( S_{n_1}^{n_2,n_3,n_4} \cong S_n \) and \( S_{n_2,n_3} \cong P_n \), where \( 1 \leq n_3 \leq \left\lfloor \frac{n - 1}{2} \right\rfloor \).

Let \( T_n^{(d)} \) denote the set of trees with \( n \) vertices and diameter \( d \), where \( 2 \leq d \leq n - 1 \). Obviously, \( T_n^{(2)} = \{S_n\} \) and \( T_n^{(n-1)} = \{P_n\} \). By simply calculating, we have

\[
AZI(S_n) = \frac{(n-1)^4}{(n-2)^3}, \quad AZI(P_n) = 8(n-1).
\]

2.1 The Augmented Zagreb Index of a Tree with Diameter 3

It can be seen that \( T_n^{(3)} = \left\{ S_{n_2,n_3,n_4}^{n_1} \mid 2 \leq p \leq \left\lfloor \frac{n}{2} \right\rfloor \right\} \). In the following, we give an order of the augmented Zagreb index of a tree with diameter 3.

**Lemma 2.1** Let

\[
g(x) = \frac{x^2}{(x - 1)^2}, \quad k(x) = \frac{-2x^2}{(x - 1)^3}, \quad m(x) = \frac{-3}{x(x - 1)} + \frac{-2x + 1}{x^2(x - 1)^2}.
\]

Then \( g(x) \) is decreasing for \( x \geq 2 \), and \( k(x), m(x) \) are both increasing for \( x \geq 2 \).
Proof. By directly computing, we have
\[ g'(x) = \frac{-2x}{(x-1)^3} < 0, \]
\[ k'(x) = \frac{2x^2 + 4x}{(x-1)^4} > 0, \]
\[ m'(x) = \frac{3(2x - 1)}{x^2(x - 1)^2} + \frac{2(3x^2 - 3x + 1)}{x^3(x - 1)^3} > 0 \]
for \( x \geq 2 \). The proof is finished.

**Lemma 2.2** Let \( n \geq 5 \) and
\[ f(p) = \frac{p^3(n-p)^3}{(n-2)^3} + \frac{p^3}{(p-1)^2} + \frac{(n-p)^3}{(n-p-1)^2}. \]
Then \( f(p) \) is increasing for \( 2 \leq p \leq \frac{n}{2} \).

**Proof.** Let \( J(p) = \frac{p^3(n-p)^3}{(n-2)^3} \). Then
\[ f(p) = J(p) + \frac{p^3}{(p-1)^2} + \frac{(n-p)^3}{(n-p-1)^2}. \]
Now we consider the following two cases.

Case 1. \( 2 \leq p \leq \frac{2}{5 + \sqrt{5}}n. \)

In this time, we have
\[ n \geq \frac{5 + \sqrt{5}}{2}p \geq 8. \]
Hence
\[ J'(p) = \frac{3p^2(n-p)^2(n-2p)}{(n-2)^3} > 0, \quad (2.1) \]
and
\[ f'(p) = J'(p) + \frac{p^2(p-3)}{(p-1)^3} + \frac{(n-p)^2(-n+p+3)}{(n-p-1)^3} \]
\[ = J'(p) + \frac{p^2}{(p-1)^2} + \frac{-2p^2}{(p-1)^3} + \frac{-(n-p)^2}{(n-p-1)^2} + \frac{2(n-p)^2}{(n-p-1)^3} \]
\[ = J'(p) + g(p) - g(n-p) + k(p) + \frac{2(n-p)^2}{(n-p-1)^3}, \]
where the functions \( g(x) \) and \( k(x) \) are defined in Lemma 2.1. Since \( n-p \geq p \geq 2 \), by Lemma 2.1, we have
\[ g(p) - g(n-p) \geq 0, \quad k(p) \geq k(2) = -8. \]

Note that \( \frac{2(n-p)^2}{(n-p-1)^3} > 0 \), we have
\[ f'(p) \geq J'(p) - 8 + \frac{2(n-p)^2}{(n-p-1)^3} > J'(p) - 8. \]
Now we just need to show that $J'(p) \geq 8$. By directly computing, we have

$$J''(p) = \frac{6p(n-p)(5p^2 - 5pm + n^2)}{(n-2)^3}$$

$$= \frac{30p(n-p)}{(n-2)^3} \left( p - \frac{2}{5 + \sqrt{5}}n \right) \left( p - \frac{2}{5 - \sqrt{5}}n \right). \quad (2.2)$$

Since $p \leq \left\lfloor \frac{n}{2} \right\rfloor < \frac{2}{5 - \sqrt{5}}n \approx 0.724n$ and $p \leq \frac{2}{5 + \sqrt{5}}n$, then $J''(p) > 0$. Therefore,

$$J'(p) \geq J'(2) = \frac{12(n-4)}{n-2} = 12 - \frac{24}{n-2} \geq 8$$

since $n \geq 8$. Thus, $f'(p) > 0$ for $2 \leq p \leq \frac{2}{5 + \sqrt{5}}n$.

Case 2. $\frac{2}{5 + \sqrt{5}}n < p \leq \left\lfloor \frac{n}{2} \right\rfloor$.

Note that

$$f(p) = J(p) + \frac{p^3}{(p-1)^2} + \frac{(n-p)^3}{(n-p-1)^2}$$

$$= J(p) + p + 2 + \frac{3}{p-1} + \frac{1}{(p-1)^2} + (n-p) + 2 + \frac{3}{n-p-1} + \frac{1}{(n-p-1)^2}$$

$$= J(p) + n + 4 + \frac{3}{p-1} + \frac{1}{(p-1)^2} + \frac{3}{n-p-1} + \frac{1}{(n-p-1)^2}.$$

It is easy to get that for $\frac{2}{5 + \sqrt{5}}n < p < p + 1 \leq \left\lfloor \frac{n}{2} \right\rfloor$,

$$f(p + 1) = J(p + 1) + n + 4 + \frac{3}{p} + \frac{1}{p^2} + \frac{3}{n-p-2} + \frac{1}{(n-p-2)^2}.$$

Then from the fact that

$$\left( \frac{3}{n-p-2} - \frac{3}{n-p-1} \right) + \left[ \frac{1}{(n-p-2)^2} - \frac{1}{(n-p-1)^2} \right] > 0,$$

we obtain

$$f(p + 1) - f(p) = J(p + 1) - J(p) + \left( \frac{3}{p} - \frac{3}{p-1} \right) + \left[ \frac{1}{p^2} - \frac{1}{(p-1)^2} \right]$$

$$+ \left( \frac{3}{n-p-2} - \frac{3}{n-p-1} \right) + \left[ \frac{1}{(n-p-2)^2} - \frac{1}{(n-p-1)^2} \right]$$

$$> J(p + 1) - J(p) + \frac{-3}{p(p-1)} + \frac{-2p + 1}{p^2(p-1)^2}$$

$$= J(p + 1) - J(p) + m(p),$$

where the function $m(x)$ is defined in Lemma 2.1. By Lemma 2.1, we get

$$m(p) \geq m(2) = -\frac{9}{4}.$$  

To prove $f(p + 1) > f(p)$, it suffice to prove $J(p + 1) - J(p) \geq \frac{9}{4}$ for $\frac{2}{5 + \sqrt{5}}n < p < p + 1 \leq \left\lfloor \frac{n}{2} \right\rfloor$. From (2.2), when $p > \frac{2}{5 + \sqrt{5}}n$, we have $J''(p) < 0$.

Combining this with inequality (2.1), namely, $J(p)$ is increasing for $p$. It implies that $J(p + 1) - J(p)$ is decreasing for $p$. Therefore,
\[ J(p + 1) - J(p) \geq J\left(\left\lfloor \frac{n}{2} \right\rfloor \right) - J\left(\left\lceil \frac{n}{2} \right\rceil - 1 \right). \]

If \( n \) is even, then \( n \geq 6 \) and
\[
J\left(\left\lfloor \frac{n}{2} \right\rfloor \right) - J\left(\left\lfloor \frac{n}{2} \right\rfloor - 1 \right) = J\left(\frac{n}{2}\right) - J\left(\frac{n}{2} - 1\right) = \frac{\left(\frac{n}{2}\right)^3 - \left(\frac{n}{2} - 1\right)^3}{(n - 2)^3} \geq \frac{9}{16} + \frac{9}{8} > \frac{9}{4}.
\]

If \( n \) is odd, then \( n \geq 5 \) and
\[
J\left(\left\lfloor \frac{n}{2} \right\rfloor \right) - J\left(\left\lfloor \frac{n}{2} \right\rfloor - 1 \right) = J\left(\frac{n - 1}{2}\right) - J\left(\frac{n - 1}{2} - 1\right) = \frac{\left(\frac{n - 1}{2}\right)^3 - \left(\frac{n - 3}{2}\right)^3}{(n - 2)^3} \geq \frac{9}{4}.
\]

It leads to \( f(p + 1) > f(p) \). Hence \( f(p) \) is increasing for \( \frac{2}{5 + \sqrt{5}} n < p \leq \left\lfloor \frac{n}{2} \right\rfloor \).

**Theorem 2.1**  Let \( T_4^{(3)} = \{S_2^{p-1,n-p-1} \mid 2 \leq p \leq \left\lfloor \frac{n}{2} \right\rfloor\} \). Then for \( n \geq 4 \),
\[
\text{AZI}(S_2^{p-1,n-p-1}) > \cdots > \text{AZI}(S_2^{2,n-4}) > \text{AZI}(S_2^{1,n-3}) = 16 + \frac{(n - 2)^3}{(n - 3)^3}.
\]
**Proof.** Note that \( T_4^{(3)} = \{S_2^{1,1}\} \), and for \( n \geq 5 \),
\[
\text{AZI}(S_2^{p-1,n-p-1}) = \frac{p^3(n - p)^3}{(n - 2)^3} + \frac{p^3}{(p - 1)^2} + \frac{(n - p)^3}{(n - p - 1)^2}.
\]
Then by Lemma 2.2, we obtain the desired results.

### 2.2 Trees with Diameter 4 ≤ d ≤ n − 1 Minimizing the Augmented Zagreb Index

Let \( G \) be a simple connected graph. Let \( x_{ij} \) be the number of edges in \( G \) connecting vertices of degrees \( i \) and \( j \), and \( Z_{ij} = \left(\frac{ij}{i + j - 2}\right)^3 \), where \( i, j \) are positive integers with \( i + j \neq 2 \).

Clearly, \( Z_{ij} = Z_{ji} \). Denote by \( \Delta \) the maximum degree of \( G \). The augmented Zagreb index
of $G$ can be rewritten as

$$AZI(G) = \sum_{1 \leq i, j \leq \Delta} x_{ij} Z_{ij}.$$

**Lemma 2.3**  
(1) $Z_{1j}$ is decreasing for $j \geq 2$;  
(2) $Z_{2j} = 8$ for $j \geq 1$;  
(3) If $i \geq 3$ is fixed, then $Z_{ij}$ is increasing for $j \geq 1$.

Let $T \in \mathcal{T}_n^{(d)}$ be a tree with a diameter-preserve path $P_{d+1} = v_1 v_2 \cdots v_{d+1}$, where $4 \leq d \leq n - 1$. Clearly,

$$d_{v_1} = d_{v_{d+1}} = 1.$$

Let $V_1 = V(P_{d+1})$. For $i \in \{2, 3, \cdots, d\}$, let 

$$V_i = \{v \in V(T) \mid d(v, v_i) < d(v, v_j), \ 2 \leq j \leq d, \ j \neq i \} \setminus \{v_1, v_i, v_{d+1}\}.$$

Then $V(T) = \bigcup_{i=1}^{d} V_i$ and $V_i \cap V_j = \emptyset$ for any $1 \leq i < j \leq d$. Moreover, since $P_{d+1}$ is a diameter-preserve path, all vertices in $V_2$ and $V_d$ are pendent vertices in $T$. Denote by $T[V^*]$ the subgraph of $T$ induced by $V^*$, where $V^* \subseteq V(T)$. We construct a sequence of trees with diameter $d$ recursively as follows: Let $T_1 \cong T$. For $i = 2, 3, \cdots, d - 2$ ($4 \leq d \leq n - 1$), let $T_i$ be the tree obtained from $T_{i-1}$ by deleting the vertices in $V_{i+1}$ and the edges incident with them, and attaching $|V_{i+1}|$ pendent vertices to the vertex $v_2$ (see Figs. 2.1–2.4).

**Lemma 2.4** $AZI(T_i) \leq AZI(T_{i-1})$ with equality if and only if $V_{i+1} = \emptyset$, where $i = 2, 3, \cdots, d - 2$ and $4 \leq d \leq n - 1$. 

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**Fig. 2.1** $T \cong T_1$  
**Fig. 2.2** $T_2$  
**Fig. 2.3** $T_3$  
**Fig. 2.4** $T_{d-2}$
Proof. Clearly, $AZI(T_i) = AZI(T_{i-1})$ if $V_{i+1} = \emptyset$. It suffice to show that $AZI(T_i) < AZI(T_{i-1})$ if $V_{i+1} \neq \emptyset$.

Case 1. $i = 2$.

Notice that $|E(T[V_3 \cup \{v_3\}])| = |V_3|$. By Lemma 2.3, for any $uv \in E(T[V_3 \cup \{v_3\}])$ (since $d_u + d_v > 2$, without loss of generality, assume that $d_v > 1$), we obtain

$$Z_{d_u,d_v} \geq Z_{1,d_v} \geq Z_{1,|V_3|+2} \geq Z_{1,|V_2|+|V_3|+2}.$$ 

Since $V_3 \neq \emptyset$, one has $d_{v_3} > 2$. It follows from $d_{v_2}, d_{v_4} \geq 2$ and Lemma 2.3 that

$$Z_{d_{v_2},d_{v_3}} \geq Z_{2,d_{v_3}} = Z_{2,|V_2|+|V_3|+2} = 8, \quad Z_{d_{v_3},d_{v_4}} \geq Z_{2,d_{v_4}}.$$ 

Therefore, bearing in mind that $V_3 \neq \emptyset$,

$$AZI(T_2) - AZI(T_1) = \left(\left(\sum_{t=2}^{4} |V_t| + 1 + |V_{i+1}\right)Z_{1,|V_{i+1}|+2} + Z_{2,d_{v_4}}\right) - \left(\left(\sum_{t=2}^{4} |V_t| + 1\right)Z_{1,\sum_{t=2}^{i+1} |V_t|+2} + \sum_{uv \in E(T[V_3 \cup \{v_3\}])} Z_{d_u,d_v} + Z_{d_{v_2},d_{v_3}} + Z_{d_{v_3},d_{v_4}}\right) \leq (|V_2| + 1)(Z_{1,|V_2|+|V_3|+2} - Z_{1,|V_2|+2}) < 0.$$ 

Case 2. $3 \leq i \leq d - 2$.

Clearly,

$$|E(T[V_{i+1} \cup \{v_{i+1}\}])| = |V_{i+1}|.$$ 

For any $uv \in E(T[V_{i+1} \cup \{v_{i+1}\}])$ (since $d_u + d_v > 2$, without loss of generality, suppose $d_v > 1$), by Lemma 2.3, we have

$$Z_{d_u,d_v} \geq Z_{1,d_v} \geq Z_{1,|V_{i+1}|+2} \geq Z_{1,\sum_{t=2}^{i+1} |V_t|+2}.$$ 

Besides, since $d_{v_{i+1}} \geq 2$ and $d_{v_{i+2}} \geq 2$, by Lemma 2.3, one has

$$Z_{d_{v_{i+1}},d_{v_{i+2}}} \geq Z_{2,d_{v_{i+2}}}.$$ 

Then

$$AZI(T_i) - AZI(T_{i-1}) = \left(\left(\sum_{t=2}^{i} |V_t| + 1 + |V_{i+1}\right)Z_{1,\sum_{t=2}^{i+1} |V_t|+2} + Z_{2,d_{v_4}}\right) - \left(\left(\sum_{t=2}^{i} |V_t| + 1\right)Z_{1,\sum_{t=2}^{i+1} |V_t|+2} + \sum_{uv \in E(T[V_{i+1} \cup \{v_{i+1}\}])} Z_{d_u,d_v} + Z_{d_{v_{i+1}},d_{v_{i+2}}}\right) \leq \left(\sum_{t=2}^{i} |V_t| + 1\right)(Z_{1,\sum_{t=2}^{i+1} |V_t|+2} - Z_{1,\sum_{t=2}^{i+1} |V_t|+2}) < 0,$$

and the last inequality holds since $V_{i+1} \neq \emptyset$.

**Theorem 2.2** Let $T \in \mathcal{T}_n^{(d)}$, where $4 \leq d \leq n - 1$. Then
Lemma 3.1 [10] In this section, we continue to use the marks in Section 2. T and the equality holds if and only if \( T \cong S^{\left\lfloor \frac{n-d+1}{2} \right\rfloor, \left\lfloor \frac{n-d+1}{2} \right\rfloor} \).

Proof. For \( T \in T_n^d \) (\( 4 \leq d \leq n - 1 \)), by Lemma 2.4, we obtain
\[
AZI(T) = AZI(T_1) \geq \cdots \geq AZI(T_{d-2})
\]
with equality if and only if \( T \cong T_{d-2} \). Actually,
\[
T_{d-2} \cong S^{V_{d+1}, n - |V_d| - d}_d,
\]
where \( 0 \leq |V_d| \leq \left\lfloor \frac{n-d-1}{2} \right\rfloor \). Note that
\[
AZI(S^{V_{d+1}, n - |V_d| - d}_d) = \frac{(|V_d| + 2)^3}{(|V_d| + 1)^2} + \frac{(n - |V_d| - d + 1)^3}{(n - |V_d| - d)^2} + 8(d - 2).
\]
Let \( t(x) = \frac{(x + 1)^3}{x^2} \). Thus
\[
AZI(S^{V_{d+1}, n - |V_d| - d}_d) = t(|V_d| + 1) + t(n - |V_d| - d) + 8(d - 2).
\]
Since for \( x \geq 2 \),
\[
t'(x) = \frac{(x + 1)^3}{x^2} \geq 0, \quad t''(x) = \frac{6(x + 1)^3}{x^4} > 0,
\]
the function \( t(x) \) is convex increasing for \( x \geq 2 \).

Besides, \( t(1) = 8 > t(2) = \frac{27}{4} \), and it follows that
\[
t(1) + t(n - d) > t(2) + t(n - d - 1) \geq \cdots \geq t(n - \left\lfloor \frac{n-d+1}{2} \right\rfloor) + t(n - \left\lfloor \frac{n-d+1}{2} \right\rfloor).
\]
It leads to
\[
\frac{(|V_d| + 2)^3}{(|V_d| + 1)^2} + \frac{(n - |V_d| - d + 1)^3}{(n - |V_d| - d)^2} \geq \frac{(n - \left\lfloor \frac{n-d+1}{2} \right\rfloor)}{2} \left\lfloor \frac{n-d+1}{2} \right\rfloor + \frac{(n - \left\lfloor \frac{n-d+1}{2} \right\rfloor)}{2} \left\lfloor \frac{n-d+1}{2} \right\rfloor,
\]
and the equality holds if and only if \( |V_d| = \left\lfloor \frac{n-d-1}{2} \right\rfloor \). Consequently,
\[
AZI(T) \geq \frac{(n - \left\lfloor \frac{n-d+1}{2} \right\rfloor)}{2} \left\lfloor \frac{n-d+1}{2} \right\rfloor + \frac{(n - \left\lfloor \frac{n-d+1}{2} \right\rfloor)}{2} \left\lfloor \frac{n-d+1}{2} \right\rfloor + 8(d - 2),
\]
and the equality holds if and only if \( T \cong S^{\left\lfloor \frac{n-d+1}{2} \right\rfloor, \left\lfloor \frac{n-d+1}{2} \right\rfloor} \).

3 Trees with Given Diameter Maximizing the ABC Index

In this section, we continue to use the marks in Section 2.

Lemma 3.1 [10] Let \( T \) be a tree with \( n \) vertices and \( p \) pendant vertices, where \( 2 \leq p \leq n - 2 \).

Then \( ABC(T) \leq \frac{\sqrt{2}}{2} (n - p) + (p - 1) \sqrt{\frac{p-1}{p}} \) with equality if and only if \( T \cong S^{1,p-1}_n \).
It is known from Section 2 that
\[ T_n^{(2)} = \{S_n\}, \]
\[ T_n^{(3)} = \{S_{2^{p-1}, n-p-1} \mid 2 \leq p \leq \left\lfloor \frac{n}{2} \right\rfloor \}, \]
\[ T_n^{(n-1)} = \{P_n\}. \]
By simply computing, we have
\[ ABC(S_n) = \sqrt{(n-1)(n-2)}, \quad ABC(P_n) = \frac{\sqrt{2}}{2} (n-1). \]
Note that \( S_{2^{p-1}, n-p-1} \) have exactly \( n-2 \) pendant vertices, it follows from Lemma 3.1 that

**Corollary 3.1** Let \( T \in T_n^{(3)} \) \((n \geq 4)\). Then \( ABC(T) \leq \sqrt{2} + (n-3) \sqrt{\frac{n-3}{n-2}} \) with equality if and only if \( T \cong S_{2^{1,n-3}}^{1,n-3} \).

Let \( A_{ij} = \sqrt{\frac{i+j-2}{ij}} \), where \( i, j \) are positive integers. It is obvious that \( A_{ij} = A_{ji} \), and the ABC index of a simple connected graph \( G \) can be restated as
\[ ABC(G) = \sum_{1 \leq i \leq j \leq \Delta} x_{ij} A_{ij}, \]
where \( x_{ij} \) denotes the number of edges in \( G \) connecting vertices of degrees \( i \) and \( j \), and \( \Delta \) denotes the maximum degree of \( G \).

**Lemma 3.2** \([8],[9]\)

1. \( A_{1j} \) is increasing for \( j \geq 1 \);
2. \( A_{2j} = \frac{\sqrt{2}}{2} \) for \( j \geq 1 \);
3. If \( i \geq 3 \) is fixed, then \( A_{ij} \) is decreasing for \( j \geq 1 \).

Let \( T \in T_n^{(d)} \) be a tree with a diameter-preserve path \( P_{d+1} = v_1 v_2 \cdots v_{d+1} \), where \( 4 \leq d \leq n-2 \). Let \( V_i \) \((i = 1, \cdots, d)\) be the vertices sets and \( T_j \) \((j = 1, \cdots, d-2)\) be the sequences of trees with diameter \( d \) defined in Subsection 2.2.

**Lemma 3.3** \( ABC(T_i) \geq ABC(T_{i-1}) \) with equality if and only if \( V_{i+1} = \emptyset \), where \( i = 2, 3, \cdots, d-2 \) and \( 4 \leq d \leq n-2 \).

**Proof.** It is obvious that \( ABC(T_i) = ABC(T_{i-1}) \) if \( V_{i+1} = \emptyset \). We need to show that \( ABC(T_i) > ABC(T_{i-1}) \) if \( V_{i+1} \neq \emptyset \).

Case 1. \( i = 2 \).
Clearly,
\[ |E(T[V_3 \cup \{v_3\}])| = |V_3|. \]
By Lemma 3.2, for any \( uv \in E(T[V_3 \cup \{v_3\}] \) \( (\text{since } d_u + d_v > 2, \text{ without loss of generality, assume that } d_v > 1) \), we have
\[ A_{d_u,d_v} \leq A_{1,d_v} \leq A_{1,|V_3|+2} \leq A_{1,|V_2|+|V_3|+2}. \]
Since $V_3 \neq \emptyset$, we know $d_{v_3} > 2$, and combining this with $d_{v_2}, d_{v_4} \geq 2$ and Lemma 3.2, we get

$$A_{d_{v_2}d_{v_3}} \leq A_{2,|V_2|+|V_3|+2}, \quad A_{d_{v_3}d_{v_4}} \leq A_{2,d_{v_4}}.$$  

Consequently,

$$ABC(T_2) - ABC(T_1) \leq \left( |V_2| + 1 + |V_3| \right) A_{1,|V_2|+|V_3|+2} + A_{2,|V_2|+|V_3|+2} + A_{2,d_{v_4}}$$

$$\quad - \left( |V_2| + 1 \right) A_{1,|V_2|+2} + \sum_{uv \in E(T[V_3 \cup \{v_3\}])} A_{d_u, d_v} + A_{d_{v_2}, d_{v_3}} + A_{d_{v_3}, d_{v_4}}$$

$$\geq (|V_2| + 1) (A_{1,|V_2|+|V_3|+2} - A_{1,|V_2|+2}) > 0,$$

and the last inequality holds since $V_3 \neq \emptyset$.

Case 2. $3 \leq i \leq d - 2$.

It can be seen that

$$|E(T[V_{i+1} \cup \{v_{i+1}\})]| = |V_{i+1}|.$$

For any $uv \in E(T[V_{i+1} \cup \{v_{i+1}\}])$ (since $d_u + d_v > 2$, without loss of generality, suppose $d_u > 1$), it follows from Lemma 3.2 that

$$A_{d_u,d_v} \leq A_{1,d_v} \leq A_{1,|V_{i+1}|+2} \leq A_{1,\sum_{t=2}^{i} |V_t| + 2}.$$

Moreover, since $d_{v_{i+3}} \geq 2$ and $d_{v_{i+4}} \geq 2$, by Lemma 3.2 we have

$$A_{d_{v_{i+3}},d_{v_{i+2}}} \leq A_{2,d_{v_{i+2}}}.$$

Then bearing in mind that $V_{i+1} \neq \emptyset$, we have

$$ABC(T_i) - ABC(T_{i-1})$$

$$= \left( \sum_{i=2}^{i} |V_i| + 1 + |V_{i+1}| \right) A_{1,\sum_{t=2}^{i+1} |V_t|+2} + A_{2,d_{v_{i+2}}}$$

$$\quad - \left( \sum_{i=2}^{i} |V_i| + 1 \right) A_{1,\sum_{t=2}^{i} |V_t|+2} + \sum_{uv \in E(T[V_{i+1} \cup \{v_{i+1}\}])} A_{d_u,d_v} + A_{d_{v_{i+1}},d_{v_{i+2}}}$$

$$\geq \left( \sum_{i=2}^{i} |V_i| + 1 \right) (A_{1,\sum_{t=2}^{i} |V_t|+2} - A_{1,\sum_{t=2}^{i} |V_t|+2})$$

$$> 0.$$

This completes the proof of Lemma 3.3.

**Theorem 3.1** Let $T \in T_n^{(d)}$, where $4 \leq d \leq n - 2$. Then

$$ABC(T) \leq \frac{\sqrt{2}}{2} (d-1) + (n-d) \sqrt{\frac{n-d}{n-d+1}}$$

with equality holding if and only if $T \cong S_{d-1}^1$.

**Proof.** For $T \in T_n^{(d)}$ ($4 \leq d \leq n - 2$), it follows from Lemma 3.3 that

$$ABC(T) = ABC(T_1) \leq \cdots \leq ABC(T_{d-2})$$
with equality if and only if \( T \cong T_{d-2} \). Note that \( T_{d-2} \cong S_{d-1}^{1|V_d|+1,n-|V_d|-d} \), and they have exactly \( n - d + 1 \) pendent vertices, where \( 0 \leq |V_d| \leq \left\lfloor \frac{n-d-1}{2} \right\rfloor \). Then by Lemma 3.1, we have

\[
ABC(T) \leq ABC(S_{d-1}^{1|V_d|+1,n-|V_d|-d}) \\
\leq ABC(S_{d-1}^{1,n-d}) \\
= \frac{\sqrt{2}}{2} (d-1) + (n-d)\sqrt{\frac{n-d}{n-d+1}},
\]

with equality holding if and only if \( |V_d| = 0 \), that is, \( T \cong S_{d-1}^{1,n-d} \).

**Remark 3.1** From the main results of this paper (e.g. Theorems 2.1, 2.2, 3.1 and Corollary 3.1), the tree with diameter \( d \) (resp. \( d = 2, 3, n-2, n-1 \)) minimizing the augmented Zagreb index and maximizing the ABC index are the same (resp. \( S_n, S_2^{1,n-3}, S_{n-3}^{1,2}, P_n \)). However, for general cases (excluding special \( n \) value), the tree with diameter \( d \) (4 \( \leq d \leq n-3 \)) minimizing the augmented Zagreb index (that is, \( S_{d-1}^{\left\lfloor \frac{n-d+1}{2} \right\rfloor,\left\lceil \frac{n-d+1}{2} \right\rceil} \)) is different from that maximizing the ABC index (that is, \( S_{d-1}^{1,n-d} \)).

**References**


