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

Huang Yu-fei

(*Department of Mathematics Teaching, Guangzhou Civil Aviation College, Guangzhou, 510403*)

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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

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

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

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

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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E-mail address: fayger@qq.com (Huang Y F).

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 pendent vertex if $d_u = 1$. Let S_n and P_n denote the star and path of order n, respectively. Let $S_l^{n_1,\, n_2}$ be the tree of order $n(\geq 3)$ obtained from the path P_l by attaching n_1 and n_2 pendent 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, $S_1^{n_3,n-n_3-1} \cong S_n$ and $S_{n-2}^{1,1} \cong P_n$, where $1 \leq n_3 \leq \left\lfloor \frac{n-1}{2} \right\rfloor$.

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

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

2.1 The Augmented Zagreb Index of a Tree with Diameter 3

It can be seen that $\mathcal{T}_n^{(3)} = \left\{ S_2^{p-1,n-p-1} \,\middle|\, 2 \leq p \leq \left\lfloor \frac{n}{2} \right\rfloor \right\}$. In the following, we give an order of the augmented Zagreb index of a tree with diameter 3.

Lemma 2.1 *Let*

$$g(x) = \frac{x^2}{(x-1)^2}, \qquad k(x) = \frac{-2x^2}{(x-1)^3}, \qquad m(x) = \frac{-3}{x(x-1)} + \frac{-2x+1}{x^2(x-1)^2}.$$

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 $2 \leq p \leq \left\lfloor \frac{n}{2} \right\rfloor$.

Proof. Let $J(p) = \dfrac{p^3(n-p)^3}{(n-2)^3}$. 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. $2 \leq p \leq \dfrac{2}{5+\sqrt{5}}n$.

In this time, we have

$$n \geq \frac{5+\sqrt{5}}{2}p \geq 8.$$

Hence

$$J'(p) = \frac{3p^2(n-p)^2(n-2p)}{(n-2)^3} > 0, \tag{2.1}$$

and

$$\begin{aligned} f'(p) &= J'(p) + \frac{p^2(p-3)}{(p-1)^3} + \frac{(n-p)^2(-n+p+3)}{(n-p-1)^3} \\ &= J'(p) + \frac{p^2}{(p-1)^2} + \frac{-2p^2}{(p-1)^3} + \frac{-(n-p)^2}{(n-p-1)^2} + \frac{2(n-p)^2}{(n-p-1)^3} \\ &= J'(p) + g(p) - g(n-p) + k(p) + \frac{2(n-p)^2}{(n-p-1)^3}, \end{aligned}$$

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

$$g(p) - g(n-p) \geq 0, \qquad k(p) \geq k(2) = -8.$$

Note that $\dfrac{2(n-p)^2}{(n-p-1)^3} > 0$, 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

$$\begin{aligned} J''(p) &= \frac{6p(n-p)(5p^2-5pn+n^2)}{(n-2)^3} \\ &= \frac{30p(n-p)}{(n-2)^3}\left(p-\frac{2}{5+\sqrt{5}}n\right)\left(p-\frac{2}{5-\sqrt{5}}n\right). \end{aligned} \tag{2.2}$$

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

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

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

$$\begin{aligned} f(p+1) - f(p) =& J(p+1) - J(p) + \left(\frac{3}{p} - \frac{3}{p-1}\right) + \left[\frac{1}{p^2} - \frac{1}{(p-1)^2}\right] \\ &+ \left(\frac{3}{n-p-2} - \frac{3}{n-p-1}\right) + \left[\frac{1}{(n-p-2)^2} - \frac{1}{(n-p-1)^2}\right] \\ >& J(p+1) - J(p) + \frac{-3}{p(p-1)} + \frac{-2p+1}{p^2(p-1)^2} \\ =& J(p+1) - J(p) + m(p), \end{aligned}$$

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,

$$J(p+1)-J(p)\ge J\Big(\Big\lfloor\frac{n}{2}\Big\rfloor\Big)-J\Big(\Big\lfloor\frac{n}{2}\Big\rfloor-1\Big).$$

If n is even, then $n\ge 6$ and

$$\begin{aligned}J\Big(\Big\lfloor\frac{n}{2}\Big\rfloor\Big)-J\Big(\Big\lfloor\frac{n}{2}\Big\rfloor-1\Big)&=J\Big(\frac{n}{2}\Big)-J\Big(\frac{n}{2}-1\Big)\\&=\frac{\Big(\frac{n}{2}\Big)^3\Big(\frac{n}{2}\Big)^3}{(n-2)^3}-\frac{\Big(\frac{n}{2}-1\Big)^3\Big(\frac{n}{2}+1\Big)^3}{(n-2)^3}\\&=\frac{3}{16}n+\frac{9}{8}+\frac{15}{4(n-2)}+\frac{3}{(n-2)^2}+\frac{1}{(n-2)^3}\\&>\frac{3}{16}n+\frac{9}{8}\\&\ge\frac{9}{4}.\end{aligned}$$

If n is odd, then $n\ge 5$ and

$$\begin{aligned}J\Big(\Big\lfloor\frac{n}{2}\Big\rfloor\Big)-J\Big(\Big\lfloor\frac{n}{2}\Big\rfloor-1\Big)&=J\Big(\frac{n-1}{2}\Big)-J\Big(\frac{n-1}{2}-1\Big)\\&=\frac{\Big(\frac{n-1}{2}\Big)^3\Big(\frac{n+1}{2}\Big)^3}{(n-2)^3}-\frac{\Big(\frac{n-3}{2}\Big)^3\Big(\frac{n+3}{2}\Big)^3}{(n-2)^3}\\&=\frac{3n^4-30n^2+91}{8(n-2)^3}\\&=\frac{9}{4}+\frac{3}{8}n+\frac{21}{4(n-2)}-\frac{3}{(n-2)^2}+\frac{19}{8(n-2)^3}\\&>\frac{9}{4}.\end{aligned}$$

It leads to $f(p+1)>f(p)$. Hence $f(p)$ is increasing for $\dfrac{2}{5+\sqrt{5}}n<p\le\Big\lfloor\dfrac{n}{2}\Big\rfloor$.

Theorem 2.1 *Let* $\mathcal{T}_n^{(3)}=\Big\{S_2^{p-1,n-p-1}\ \Big|\ 2\le p\le\Big\lfloor\frac{n}{2}\Big\rfloor\Big\}$. *Then for* $n\ge 4$,

$$AZI(S_2^{\lfloor\frac{n-2}{2}\rfloor,\lceil\frac{n-2}{2}\rceil})>\cdots>AZI(S_2^{2,n-4})>AZI(S_2^{1,n-3})=16+\frac{(n-2)^3}{(n-3)^2}.$$

Proof. Note that $\mathcal{T}_4^{(3)}=\{S_2^{1,1}\}$, and for $n\ge 5$,

$$AZI(S_2^{p-1,\ n-p-1})=\frac{p^3(n-p)^3}{(n-2)^3}+\frac{p^3}{(p-1)^2}+\frac{(n-p)^3}{(n-p-1)^2}.$$

Then by Lemma 2.2, we obtain the desired results.

2.2 Trees with Diameter $4\le d\le n-1$ 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 $Z_{ij}=\Big(\dfrac{ij}{i+j-2}\Big)^3$, where i, j are positive integers with $i+j\ne 2$. Clearly, $Z_{ij}=Z_{ji}$. Denote by $\varDelta$ the maximum degree of G. The augmented Zagreb index of G can be rewritten as

$$AZI(G) = \sum_{\substack{1 \le i \le j \le \Delta \\ i+j \ne 2}} x_{ij} Z_{ij}.$$

Lemma 2.3[5] (1) *Z_{1j} is decreasing for $j \ge 2$;*

(2) *$Z_{2j} = 8$ for $j \ge 1$;*

(3) *If $i \ge 3$ is fixed, then Z_{ij} is increasing for $j \ge 1$.*

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 $4 \le d \le n-1$. Clearly,

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

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

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

Then $V(T) = \bigcup\limits_{i=1}^{d} V_i$ and $V_i \cap V_j = \emptyset$ for any $1 \le i < j \le d$. 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 $i = 2, 3, \cdots, d-2$ $(4 \le d \le n-1)$, 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).

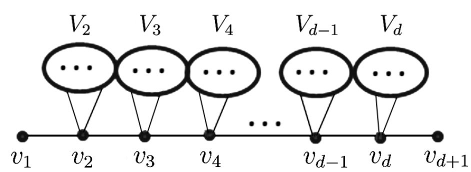

Fig. 2.1 $T \cong T_1$

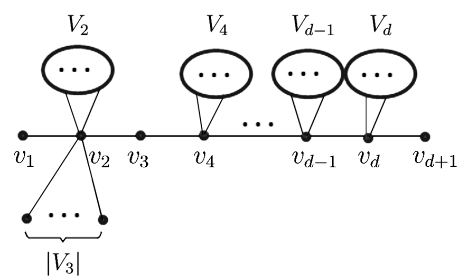

Fig. 2.2 T_2

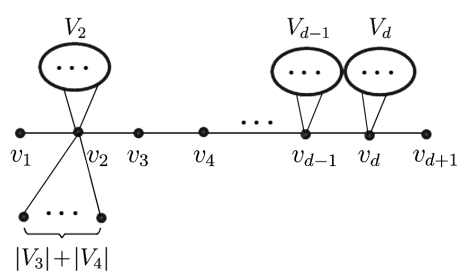

Fig. 2.3 T_3

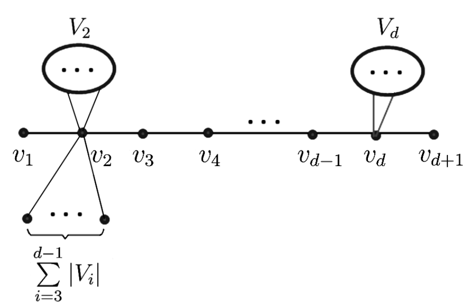

Fig. 2.4 T_{d-2}

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

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

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

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

$$\begin{aligned}
&AZI(T_2) - AZI(T_1)\\
&= [(|V_2| + 1 + |V_3|)Z_{1,|V_2|+|V_3|+2} + Z_{2,|V_2|+|V_3|+2} + Z_{2,d_{v_4}}]\\
&\quad - \left[(|V_2| + 1)Z_{1,|V_2|+2} + \sum_{uv \in E(T[V_3 \cup \{v_3\}])} Z_{d_u,d_v} + Z_{d_{v_2},d_{v_3}} + Z_{d_{v_3},d_{v_4}}\right]\\
&\leq (|V_2| + 1)(Z_{1,|V_2|+|V_3|+2} - Z_{1,|V_2|+2})\\
&< 0.
\end{aligned}$$

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

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

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*

$$AZI(T) \geq \frac{\left(\left\lfloor\frac{n-d+1}{2}\right\rfloor+1\right)^3}{\left\lfloor\frac{n-d+1}{2}\right\rfloor^2} + \frac{\left(\left\lceil\frac{n-d+1}{2}\right\rceil+1\right)^3}{\left\lceil\frac{n-d+1}{2}\right\rceil^2} + 8(d-2),$$

and the equality holds if and only if $T \cong S_{d-1}^{\lfloor\frac{n-d+1}{2}\rfloor, \lceil\frac{n-d+1}{2}\rceil}$.

Proof. For $T \in \mathcal{T}_n^{(d)}$ $(4 \leq d \leq n-1)$, 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,

$$T_{d-2} \cong S_{d-1}^{|V_d|+1, n-|V_d|-d},$$

where $0 \leq |V_d| \leq \left\lfloor\frac{n-d-1}{2}\right\rfloor$. Note that

$$AZI(S_{d-1}^{|V_d|+1,\ n-|V_d|-d}) = \frac{(|V_d|+2)^3}{(|V_d|+1)^2} + \frac{(n-|V_d|-d+1)^3}{(n-|V_d|-d)^2} + 8(d-2).$$

Let $t(x) = \frac{(x+1)^3}{x^2}$. Thus

$$AZI(S_{d-1}^{|V_d|+1,\ n-|V_d|-d}) = t(|V_d|+1) + t(n-|V_d|-d) + 8(d-2).$$

Since for $x \geq 2$,

$$t'(x) = \frac{(x+1)^2(x-2)}{x^3} \geq 0, \qquad t''(x) = \frac{6(x+1)}{x^4} > 0,$$

the function $t(x)$ is convex increasing for $x \geq 2$.

Besides, $t(1) = 8 > t(2) = \frac{27}{4}$, and it follows that

$$t(1) + t(n-d) > t(2) + t(n-d-1) \geq \cdots \geq t\left(\left\lfloor\frac{n-d+1}{2}\right\rfloor\right) + t\left(\left\lceil\frac{n-d+1}{2}\right\rceil\right).$$

It leads to

$$\frac{(|V_d|+2)^3}{(|V_d|+1)^2} + \frac{(n-|V_d|-d+1)^3}{(n-|V_d|-d)^2} \geq \frac{\left(\left\lfloor\frac{n-d+1}{2}\right\rfloor+1\right)^3}{\left\lfloor\frac{n-d+1}{2}\right\rfloor^2} + \frac{\left(\left\lceil\frac{n-d+1}{2}\right\rceil+1\right)^3}{\left\lceil\frac{n-d+1}{2}\right\rceil^2},$$

and the equality holds if and only if $|V_d| = \left\lfloor\frac{n-d-1}{2}\right\rfloor$. Consequently,

$$AZI(T) \geq \frac{\left(\left\lfloor\frac{n-d+1}{2}\right\rfloor+1\right)^3}{\left\lfloor\frac{n-d+1}{2}\right\rfloor^2} + \frac{\left(\left\lceil\frac{n-d+1}{2}\right\rceil+1\right)^3}{\left\lceil\frac{n-d+1}{2}\right\rceil^2} + 8(d-2),$$

and the equality holds if and only if $T \cong S_{d-1}^{\lfloor\frac{n-d+1}{2}\rfloor, \lceil\frac{n-d+1}{2}\rceil}$.

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 pendent 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 $T \cong S_{n-p}^{1,p-1}$.*

It is known from Section 2 that

$$\mathcal{T}_n^{(2)} = \{S_n\},$$
$$\mathcal{T}_n^{(3)} = \left\{S_2^{p-1,n-p-1} \mid 2 \le p \le \left\lfloor \frac{n}{2} \right\rfloor\right\},$$
$$\mathcal{T}_n^{(n-1)} = \{P_n\}.$$

By simply computing, we have

$$ABC(S_n) = \sqrt{(n-1)(n-2)}, \qquad ABC(P_n) = \frac{\sqrt{2}}{2}(n-1).$$

Note that $S_2^{p-1,\ n-p-1}$ $\left(2 \le p \le \left\lfloor \frac{n}{2} \right\rfloor\right)$ have exactly $n-2$ pendent vertices, it follows from Lemma 3.1 that

Corollary 3.1 *Let $T \in \mathcal{T}_n^{(3)}$ $(n \ge 4)$. Then $ABC(T) \le \sqrt{2} + (n-3)\sqrt{\frac{n-3}{n-2}}$ with equality if and only if $T \cong S_2^{1,n-3}$.*

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

$$ABC(G) = \sum_{1 \le i \le j \le \Delta} x_{ij} A_{ij},$$

where x_{ij} denotes the number of edges in G connecting vertices of degrees i and j, and Δ denotes the maximum degree of G.

Lemma 3.2[8],[9] (1) *A_{1j} is increasing for $j \ge 1$;*

(2) $A_{2j} = \frac{\sqrt{2}}{2}$ *for $j \ge 1$;*

(3) *If $i \ge 3$ is fixed, then A_{ij} is decreasing for $j \ge 1$.*

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

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 $V_{i+1} \ne \emptyset$.

Case 1. $i = 2$.

Clearly,

$$|E(T[V_3 \cup \{v_3\}])| = |V_3|.$$

By Lemma 3.2, for any $uv \in E(T[V_3 \cup \{v_3\}])$ (since $d_u + d_v > 2$, without loss of generality, assume that $d_v > 1$), we have

$$A_{d_u,d_v} \le A_{1,d_v} \le A_{1,|V_3|+2} \le A_{1,|V_2|+|V_3|+2}.$$

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

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

Consequently,

$$\begin{aligned}
&ABC(T_2) - ABC(T_1) \\
=\ &[(|V_2| + 1 + |V_3|)A_{1,|V_2|+|V_3|+2} + A_{2,|V_2|+|V_3|+2} + A_{2,d_{v_4}}] \\
&- \left[(|V_2| + 1)A_{1,\ |V_2|+2} + \sum_{uv\in E(T[V_3\cup\{v_3\}])} A_{d_u,\ d_v} + A_{d_{v_2},\ d_{v_3}} + A_{d_{v_3},\ d_{v_4}}\right] \\
\geq\ &(|V_2| + 1)(A_{1,|V_2|+|V_3|+2} - A_{1,|V_2|+2}) \\
>\ &0,
\end{aligned}$$

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 $d_v > 1$), it follows from Lemma 3.2 that

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

Moreover, since $d_{v_{i+1}} \geq 2$ and $d_{v_{i+2}} \geq 2$, by Lemma 3.2 we have

$$A_{d_{v_{i+1}},d_{v_{i+2}}} \leq A_{2,d_{v_{i+2}}}.$$

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

$$\begin{aligned}
&ABC(T_i) - ABC(T_{i-1}) \\
=\ &\left[\left(\sum_{t=2}^{i}|V_t| + 1 + |V_{i+1}|\right)A_{1,\sum\limits_{t=2}^{i+1}|V_t|+2} + A_{2,d_{v_{i+2}}}\right] \\
&- \left[\left(\sum_{t=2}^{i}|V_t| + 1\right)A_{1,\sum\limits_{t=2}^{i}|V_t|+2} + \sum_{uv\in E(T[V_{i+1}\cup\{v_{i+1}\}])} A_{d_u,d_v} + A_{d_{v_{i+1}},d_{v_{i+2}}}\right] \\
\geq\ &\left(\sum_{t=2}^{i}|V_t| + 1\right)\left(A_{1,\sum\limits_{t=2}^{i+1}|V_t|+2} - A_{1,\sum\limits_{t=2}^{i}|V_t|+2}\right) \\
>\ &0.
\end{aligned}$$

This completes the proof of Lemma 3.3.

Theorem 3.1 *Let $T \in \mathcal{T}_n^{(d)}$, 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 $T \cong S_{d-1}^{1,n-d}$.

Proof. For $T \in \mathcal{T}_n^{(d)}$ $(4 \leq d \leq n - 2)$, 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 $T_{d-2} \cong S_{d-1}^{|V_d|+1,n-|V_d|-d}$, and they have exactly $n-d+1$ pendent vertices, where $0 \le |V_d| \le \left\lfloor \dfrac{n-d-1}{2} \right\rfloor$. Then by Lemma 3.1, we have

$$\begin{aligned} ABC(T) &\le ABC(S_{d-1}^{|V_d|+1,n-|V_d|-d}) \\ &\le ABC(S_{d-1}^{1,n-d}) \\ &= \frac{\sqrt{2}}{2}(d-1) + (n-d)\sqrt{\frac{n-d}{n-d+1}}, \end{aligned}$$

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 $(4 \le d \le n-3)$ minimizing the augmented Zagreb index (that is, $S_{d-1}^{\lfloor \frac{n-d+1}{2} \rfloor, \lceil \frac{n-d+1}{2} \rceil}$) is different from that maximizing the ABC index (that is, $S_{d-1}^{1,\ n-d}$).

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