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Maximal Augmented Zagreb Index of Trees With at Most Three Branching Vertices

ROBERTO CRUZ, JUAN DANIEL MONSALVE, AND JUAN RADA
Instituto de Matemáticas, Universidad de Antioquia, Medellín 050010, Colombia

Corresponding author: Roberto Cruz (roberto.cruz@udea.edu.co)

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ABSTRACT The Augmented Zagreb index of a graph G is defined to be $\mathcal{AZI}(G) = \sum_{uv\in E(G)} \left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$, where $E(G)$ is the edge set of G, $d(u)$ and $d(v)$ are the degrees of the vertices u and v of edge uv. It is one of the most valuable topological indices used to predict the structure-property correlations of organic compounds. It is well known that the star is the unique tree having minimal $\mathcal{AZI}$ among trees. However, the problem of finding the tree with maximal $\mathcal{AZI}$ is still open and seems to be a very difficult problem. A recent conjecture, posed in the recent paper [IEEE Access, vol. 6, pp. 69335–69341, 2018], states that the balanced double star is the tree with maximal $\mathcal{AZI}$ among all trees with n vertices, for all $n \geq 19$. Let $\Omega(n, p)$ be the set of trees with n vertices and p branching vertices. In this paper we consider the maximal value problem of $\mathcal{AZI}$ over $\Omega(n, p)$. We first show that under a certain condition, the problem reduces to finding the maximal value of $\mathcal{AZI}$ over $\Omega_1(n, p)$, the set of trees in $\Omega(n, p)$ with no vertices of degree 2. Then we rely on this result to find the trees with maximal value of $\mathcal{AZI}$ over $\Omega(n, p)$, when $p = 2$ and 3. In particular, we deduce that the conjecture holds for all trees with at most 3 branching vertices.

INDEX TERMS Augmented Zagreb index, extremal trees.

I. INTRODUCTION

Our graphs in this study are simple (no loops and no multiple edges) and finite. We denote the vertex set and the edge set of a graph G as $V(G)$ and $E(G)$, respectively. We write uv to denote the edge of G which joins the vertices u and v. If $uv \in E(G)$ then we denote by $G - uv$ the graph obtained from G by deleting the edge uv; if $uv \notin E(G)$ then $G + uv$ denotes the graph obtained from G by adding the edge uv. We denote by $d(u) = d_G(u)$ the degree of the vertex u of G and $\Delta = \Delta(G) = \max\{d(u) : u \in V(G)\}$ the maximum degree of G.

Our main interest in this paper are trees (i.e. connected graphs with no cycles). A vertex u of a tree T is called a branching vertex if $d(u) \geq 3$; it is called a leaf if $d(u) = 1$. Let $\pi : v_0v_1 \cdots v_k$ be a path of length k of a tree T such that $d(v_i) = 2$ for all $i = 1, \ldots, k-1$. If v_0 and v_k are branching vertices of T then π is an internal path of T; if v_0 is a branching vertex and v_k is a leaf then π is a pendant path of T.

An n-vertex tree is a tree with n vertices. We denote by $\Omega(n, p)$ the set of all n-vertex trees with exactly p branching vertices. The subset $\Omega_1(n, p)$ of $\Omega(n, p)$ consists of trees with no vertices of degree 2. In other words, an n -vertex tree T belongs to $\Omega_1(n, p)$ if all internal paths and pendant paths of T have length 1.

A topological index is a numeric quantity associated with a graph which is invariant under graph isomorphism. In theoretical chemistry it is used for modeling physico-chemical properties of chemical compounds [5], [10], [11], [16], [17]. The Augmented Zagreb index, introduced by Furtula *et al.* [6], was shown to be the best in correlating abilities among many other topological indices, in the case of standard heats of formation and normal boiling points of octane isomers [7]. Also, it has the greatest structure sensitivity and it is the best for designing quantitative structure-property relations [8].

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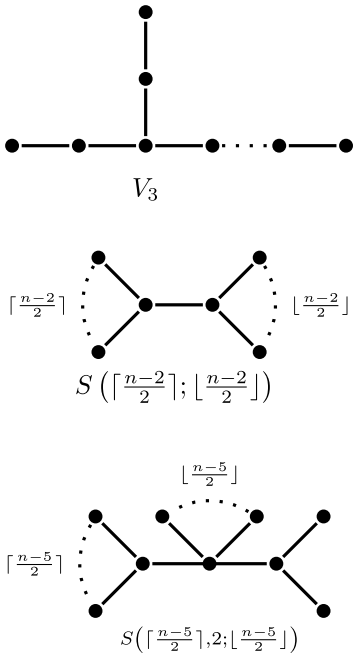


FIGURE 1. Trees with maximum $\mathcal{AZI}$ in $\Omega(n,1)$, $\Omega(n,2)$ and $\Omega(n,3)$, respectively.

As a consequence, researchers are systematically studying its mathematical properties [1], [3], [9], [12], [14], [15], [18].

The Augmented Zagreb index of a graph G, denoted by $\mathcal{AZI}(G)$, is defined as

$$\mathcal{AZI}(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u)+d(v)-2} \right)^3.$$

In [6], the authors show that the star is the unique tree having minimal $\mathcal{AZI}$ among n-vertex trees. The problem of finding the tree with maximal $\mathcal{AZI}$ among n-vertex trees is still open and seems to be a very difficult problem. Recently, Lin et al. [13] develop a very nice algorithm to search for n-vertex trees with maximal $\mathcal{AZI}$, which is based on the so-called breadth-first searching graph maximizing $\mathcal{AZI}$. Using this algorithm they find that the balanced double star $S\left(\left\lceil \frac{n-2}{2} \right\rceil; \left\lfloor \frac{n-2}{2} \right\rfloor\right)$ (see Figure 1) uniquely maximizes $\mathcal{AZI}$ for $19 \leq n \leq 200$. Naturally, they propose the following conjecture:

Conjecture 1: [13, Conjecture 18] If $n \geq 19$, then $S\left(\left\lceil \frac{n-2}{2} \right\rceil; \left\lfloor \frac{n-2}{2} \right\rfloor\right)$ has maximal $\mathcal{AZI}$ among all n-vertex trees.

In this paper we consider the maximal value problem of $\mathcal{AZI}$ over $\Omega(n,p)$. We first show that under a certain condition, the problem reduces to finding the maximal value of $\mathcal{AZI}$ over $\Omega_1(n,p)$. Then we rely on this result to find the trees with maximal value of $\mathcal{AZI}$ over $\Omega(n,p)$, when $p=2$ and 3. In particular, we deduce that the conjecture holds for all trees with at most 3 branching vertices.

More specifically, we show that $S\left(\left\lceil \frac{n-2}{2} \right\rceil; \left\lfloor \frac{n-2}{2} \right\rfloor\right)$ attains the maximal value of $\mathcal{AZI}$ over $\Omega(n,2)$ and $S\left(\left\lceil \frac{n-5}{2} \right\rceil, 2; \left\lfloor \frac{n-5}{2} \right\rfloor\right)$ (see Figure 1) attains the maximal value of $\mathcal{AZI}$ over $\Omega(n,3)$. Bearing in mind that the maximal value of $\mathcal{AZI}$ over $\Omega(n,1)$ occurs in V_3 (see Figure 1) [2], we compare these maximal trees to deduce that

$$\mathcal{AZI}(T) \leq \mathcal{AZI}\left(S\left(\left\lceil \frac{n-2}{2} \right\rceil; \left\lfloor \frac{n-2}{2} \right\rfloor\right)\right)$$

for all trees $T \in \bigcup_{p=1}^{3} \Omega(n,p)$, when $n \geq 19$.

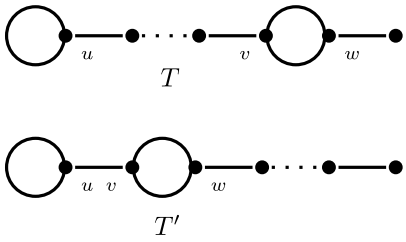


FIGURE 2. Trees used in the proof of Proposition 5.

II. AUGMENTED ZAGREB INDEX OF TREES WITH A FIXED NUMBER OF BRANCHING VERTICES

In this section we show that finding the maximal value of $\mathcal{AZI}$ over $\Omega(n,p)$ can be reduced to $\Omega_1(n,p)$, when $p \geqslant 2$. We will need the following lemmas that appear in [13].

Lemma 2: [13, Lemma 3] Let $h(x,y) = \left(\frac{xy}{x+y-2}\right)^3$. Then

1) $h(x,1)$ strictly decreases with $x \geq 2$;
2) $h(x,2) = 8$ for all $x \geq 1$;
3) If $y \geq 3$ fixed, then $h(x,y)$ strictly increases for $x \geq 2$.

Lemma 3: [13, Lemma 5] Let $l(x,y) = h(x,y) - h(x-1,y)$. Then

$$l(x,y+1) > l(x,y),$$

for $x \geq 2$, $y \geq 1$ and $x+y \geq 4$.

Lemma 4: [13, Corollary 8] If $3 \leq x \leq y$ and $y \geq 10$ then

$$l(x+1,y) + (x-1)l(x+1,1) + h(x+1,1) - 16 > 0.$$

Now we are ready to prove that a maximal tree in $\Omega(n,p)$ with respect to $\mathcal{AZI}$ has no internal paths nor pendant paths of length > 1.

In our next result we show that given a tree T, it is possible to construct a new tree U with no internal path of length ≥ 2, and $\mathcal{AZI}(T) \leq \mathcal{AZI}(U)$. This is a reformulation of [[1],Theorem 2] (with a simpler proof).

Proposition 5: Consider the trees T and T' given in Figure 2. Assume that $d(w) \geq 2$, $d(u) \geq 3$, $d(v) \geq 3$ and $d = d_T(u,v) \geq 2$, where $d_T(u,v)$ is the distance in T from vertex u to vertex v. Then

$$\mathcal{AZI}(T) \leq \mathcal{AZI}(T').$$

Proof: Let $x = d(u), y = d(v)$ and $z = d(w)$. By Lemma 2 we deduce

$$\begin{aligned}\mathcal{AZI}\left(T'\right) - \mathcal{AZI}\left(T\right) &= h\left(x,y\right) - h\left(1,z\right)\\ &\geq h\left(x,y\right) - h\left(1,2\right)\\ &> h\left(2,y\right) - h\left(1,2\right)\\ &= 0.\end{aligned}$$

■

Proposition 6: Let $p \geq 2$. If T is a maximal tree in $\Omega\left(n,p\right)$ with respect to $\mathcal{AZI}$ and $\Delta\left(T\right) \geq 10$, then $T \in \Omega_1\left(n,p\right)$.

Proof: By Proposition 5, T has no internal paths of length > 1. Suppose T has a pendant path $vv_1v_2\cdots v_k$ with $d(v) \geq 3$ and $k \geq 2$. By Proposition 5 there exists $uv \in E\left(G\right)$ such that $d\left(u\right) \geq 3$. If $k = 2$ then an identical argument as in [13, Theorem 23] gives a contradiction. If $k \geq 3$ we will prove that it is possible to reduce the length of the path by one. In fact, we consider following cases:

1) $y = d\left(v\right) = \Delta\left(T\right) \geq 10$. In this case $d\left(u\right) \leq y$. Let $T_1 = T - v_{k-1}v_k + uv_k$. Then, from Lemmas 3 and 4 we obtain

$$\begin{aligned}&\mathcal{AZI}\left(T_1\right) - \mathcal{AZI}\left(T\right)\\ &\quad= h\left(x+1,y\right) - h\left(x,y\right)\\ &\qquad+ \sum_{w\in N_T(u)-\{v\}} \left[h\left(x+1,d\left(w\right)\right) - h\left(x,d\left(w\right)\right)\right]\\ &\qquad+h\left(x+1,1\right) + 8(k-1) - 8k\\ &\quad= l\left(x+1,y\right) + \sum_{w\in N_T(u)-\{v\}} l\left(x+1,d\left(w\right)\right)\\ &\qquad+h\left(x+1,1\right) - 8\\ &\quad\geq l\left(x+1,y\right) + \left(x-1\right) l\left(x+1,1\right)\\ &\qquad+h\left(x+1,1\right) - 8\\ &\quad\geq 8 > 0.\end{aligned}$$

2) $y = d\left(v\right) < \Delta\left(T\right)$ and $x = d\left(u\right) = \Delta\left(T\right)$. Let $T_2 = T - v_{k-1}v_k + vv_k$. Then, from Lemmas 3 and 4 we obtain

$$\begin{aligned}&\mathcal{AZI}\left(T_2\right) - \mathcal{AZI}\left(T\right)\\ &\quad= h\left(x,y+1\right) - h\left(x,y\right)\\ &\qquad+ \sum_{w\in N_T(v)-\{u\}} \left[h\left(y+1,d\left(w\right)\right) - h\left(y,d\left(w\right)\right)\right]\\ &\qquad+h\left(y+1,1\right) + 8(k-1) - 8k\\ &\quad= l\left(y+1,x\right) - 8\\ &\qquad+ \sum_{w\in N_T(v)-\{u\}} l\left(y+1,d\left(w\right)\right) + h\left(y+1,1\right)\\ &\quad\geq l\left(y+1,x\right) + \left(y-1\right) l\left(y+1,1\right)\\ &\qquad+h\left(y+1,1\right) - 8\\ &\quad\geq 8 > 0.\end{aligned}$$

3) $y = d\left(v\right) < \Delta\left(T\right)$ and $d(u) < \Delta\left(T\right)$ for any $uv \in E\left(T\right)$. Let $rr_1\cdots r_lv$ be a path such that $l \geq 1$, $3 \leq d\left(r_i\right) < d\left(r\right) = \Delta\left(T\right)$ for $i = 1,\ldots l$. Let $T_3 = T - v_{k-1}v_k + r_1v_k$. We denote $x = d\left(r_1\right)$ for and $y = d\left(r\right)$. Again, from Lemmas 3 and 4 we obtain

$$\begin{aligned}&\mathcal{AZI}\left(T_3\right) - \mathcal{AZI}\left(T\right)\\ &\quad= h\left(x+1,y\right) - h\left(x,y\right)\\ &\qquad+h\left(x+1,1\right) + 8(k-1) - 8k\\ &\qquad+ \sum_{w\in N_T(r_1)-\{r\}} \left[h\left(x+1,d\left(w\right)\right) - h\left(x,d\left(w\right)\right)\right]\\ &\quad= l\left(x+1,y\right) - 8\\ &\qquad+ \sum_{w\in N_T(r_1)-\{r\}} l\left(x+1,d\left(w\right)\right) + h\left(x+1,1\right)\\ &\quad\geq l\left(x+1,y\right) + \left(x-1\right) l\left(x+1,1\right)\\ &\qquad+h\left(x+1,1\right) - 8\\ &\quad\geq 8 > 0.\end{aligned}$$

■

Proposition 7: If T is a maximal tree in $\Omega\left(n,p\right)$ with respect to $\mathcal{AZI}$ then

$$\mathcal{AZI}\left(T\right) \leq \left(p-1\right) h\left(\Delta,\Delta\right) + 8\left(n-p\right),$$

where $\Delta = \Delta\left(T\right)$.

Proof: By Proposition 5, T has no internal paths of length > 1. Then T has $p-1$ edges u_iv_i joining branching vertices and $n-p$ edges s_it_i, where one of the end-vertices is of degree 1 or 2. Let $x_i = d\left(u_i\right)$, $y_i = d\left(v_i\right)$ for all $i = 1,\ldots,p-1$ and $w_i = d\left(s_i\right)$, $z_i = d\left(t_i\right)$ for all $i = 1,\ldots,n-p$. Note that by Lemma 2, $h\left(w_i,z_i\right) \leq 8$ for all $i = 1,\ldots,n-p$ and

$$\begin{aligned}\mathcal{AZI}\left(T\right) &= \sum_{i=1}^{p-1} h\left(x_i,y_i\right) + \sum_{i=1}^{n-p} h\left(w_i,z_i\right)\\ &\leq \sum_{i=1}^{p-1} h\left(\Delta,\Delta\right) + 8\left(n-p\right)\\ &= \left(p-1\right) h\left(\Delta,\Delta\right) + 8\left(n-p\right).\end{aligned}$$

■

Theorem 8: Let S be a maximal tree in $\Omega_1\left(n,p\right)$ with respect to $\mathcal{AZI}$. Assume further that

$$\mathcal{AZI}\left(S\right) > \left(p-1\right) h\left(9,9\right) + 8\left(n-p\right). \tag{1}$$

Then S is a maximal tree in $\Omega\left(n,p\right)$ with respect to $\mathcal{AZI}$.

Proof: Let T be a maximal tree in $\Omega\left(n,p\right)$. Assume that $\Delta = \Delta\left(T\right) \leq 9$. Then by Proposition 7 and Lemma 2,

$$\begin{aligned}\mathcal{AZI}\left(S\right) &\leq \mathcal{AZI}\left(T\right) \leq \left(p-1\right) h\left(\Delta,\Delta\right) + 8\left(n-p\right)\\ &\leq \left(p-1\right) h\left(9,9\right) + 8\left(n-p\right),\end{aligned}$$

which contradicts (1). Consequently, $\Delta\left(T\right) \geq 10$. It follows from Proposition 6 that $T \in \Omega_1\left(n,p\right)$, which implies $\mathcal{AZI}\left(S\right) = \mathcal{AZI}\left(T\right)$. Hence, S is a maximal tree in $\Omega\left(n,p\right)$ with respect to $\mathcal{AZI}$. ■

Example 9: Let us show that condition (1) is necessary in Theorem 8. For each value of n and p in Table 1 we found computationally the maximal tree with respect to $\mathcal{AZI}$ over the set $\Omega_1(n,p)$, denoted by $S_{n,p}$. For each case, we checked

TABLE 1. Maximal trees in $\Omega_1(n,p)$ with respect to $\mathcal{AZI}$ which are not maximal in $\Omega(n,p)$.

n	p	$\mathcal{AZI}(S_{n,p})$	$(p-1)h(9,9)+8(n-p)$	$\mathcal{AZI}(T_{n,p})$
19	3	157.441	387.49	166.949
20	4	164.872	517.24	174.611
21	5	172.572	646.99	183.296

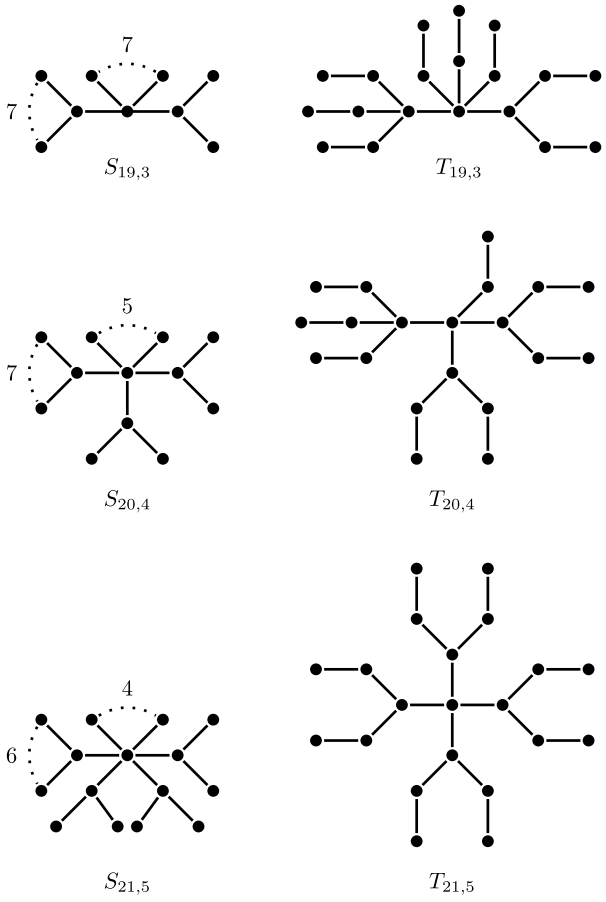


FIGURE 3. Trees in Table 1.

that condition (1) does not hold and found a tree not in $\Omega_1(n,3)$, denoted by $T_{n,p}$, with greater value of $\mathcal{AZI}$. All the trees used in Table 1 are depicted in Figure 3.

Thus, if we want to find the maximal value of $\mathcal{AZI}$ over $\Omega(n,p)$, it is sufficient to find the maximal tree S in $\Omega_1(n,p)$ and show that $\mathcal{AZI}(S)$ is lowerly bounded by the right hand side of (1). We illustrate this idea in $\Omega(n,2)$, the set of trees with n vertices and 2 branching vertices. Recall that $\Omega_1(n,2)$ is the set of double stars $S(r;s)$ where $r \geq s$ and $r+s=n-2$ (see Figure 4).

Corollary 10: The maximal value of $\mathcal{AZI}$ over $\Omega(n,2)$ is attained in $S\left(\left\lceil \frac{n-2}{2} \right\rceil ; \left\lfloor \frac{n-2}{2} \right\rfloor\right)$, for all $n \geq 19$.

Proof: In [4, Corollary 2.1] it was shown that $S\left(\left\lceil \frac{n-2}{2} \right\rceil ; \left\lfloor \frac{n-2}{2} \right\rfloor\right)$ attains the maximal value of $\mathcal{AZI}$ over $\Omega_1(n,2)$, for all $n \geq 6$. On the other hand, if $n \geq 19$ then

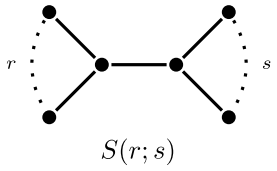


FIGURE 4. Trees in $\Omega_1(n,2)$.

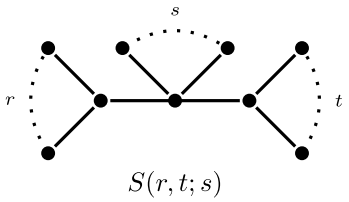


FIGURE 5. Trees in $\Omega_1(n,3)$.

by [13, Lemma 21],

$$\mathcal{AZI}\left(S\left(\left\lceil \frac{n-2}{2} \right\rceil ; \left\lfloor \frac{n-2}{2} \right\rfloor\right)\right) \geq \frac{n^3}{64} + n + 3.$$

Note that the least positive integer m_0 such that

$$\frac{n^3}{64} + n + 3 > h(9,9) + 8(n-2) = \left(\frac{81}{16}\right)^3 + 8(n-2)$$

is $m_0 = 27$. Thus, if $n \geq n_0 = \max\{19, 27\} = 27$, it follows from Theorem 8 that the maximal value of $\mathcal{AZI}$ over $\Omega(n,2)$ is attained in $S\left(\left\lceil \frac{n-2}{2} \right\rceil ; \left\lfloor \frac{n-2}{2} \right\rfloor\right)$. Finally, the result is well known for $19 \leq n \leq 26$ [13]. ■

III. MAXIMAL AUGMENTED ZAGREB INDEX OF TREES WITH THREE BRANCHING VERTICES

In this section we find the maximal value of the Augmented Zagreb index over the set $\Omega(n,3)$. In order to use Theorem 8, we first find the maximal Augmented Zagreb index over $\Omega_1(n,3)$. A tree in $\Omega_1(n,3)$ is denoted by $S(r,t;s)$, where r,s,t are positive integers such that $r+s+t = n-3$, $s \geq 1$ and $r, t \geq 2$ (see Figure 5). Without loosing generality, we assume that $r \geq t$.

We will need the following lemmas in the sequel.

Lemma 11: [13, Lemma 6] For $x \geq 2$ and $y \geq 1$,

1) $l(x,1) < 0$ strictly increases with $x \geq 3$;
2) $l(x,2) = 0$ for $x \geq 3$;
3) If $y \geq 3$ is fixed, then $l(x,y) > 0$ strictly increases with $2 \leq x \leq y-1$ and strictly decreases with $x \geq y$.

Lemma 12: Let $f(x) = xh(1,x+1) - (x+1)h(1,x+2)$. For all $x \geq 1$, $-1 < f(x) < 0$ and strictly decreases.

Proof: It follows from the fact that for all $x \geq 1$,

$$f(x) = -1 + \frac{3x^4 + 8x^3 + 6x^2 + x}{x^3(x+1)^3} > -1$$

and

$$f'(x) = -\frac{6x^3 + 15x^2 + 9x + 2}{x^3(x+1)^3} < 0.$$

■

Lemma 13: Let $g(x) = xh(1, x+2) - (x+1)h(1, x+3)$. For all $x \geq 1$, $g(x) < -1$ and strictly increases.

Proof: For all $x \geq 1$,

$$g(x) = -1 - \frac{4x^3 + 21x^2 + 35x + 19}{(x+2)^3 (x+1)^3} < -1$$

and

$$g'(x) = \frac{12x^4 + 84x^3 + 214x^2 + 240x + 101}{(x+2)^2 (x+1)^2} > 0.$$

■

Lemma 14: Let $q(x, y) = h(x+1, y-1) - h(x, y)$. If $y \geq x+1 \geq 1$ then $q(x, y) \geq 0$. If $2 \leq y < x+1$ then $q(x, y) < 0$.

Proof: Note that

$$q(x, y) = \frac{(y-x-1)}{(x+y-2)^3} q_1(x, y),$$

where

$$q_1(x, y) = \left(3y^2 - 3y + 1\right) x^2 + (3y-2)(y-1)x + (y-1)^2.$$

Clearly, $q(x, y) \geq 0$ when $y \geq x+1 \geq 1$ and $q(x, y) < 0$ when $2 \leq y < x+1$. ■

Lemma 15: If $s \geq t \geq 16$, then

$$l(s+3, s+1) + q(s+2, t+1) > 0.$$

Proof: A simple but tedious computation shows that

$$l(s+3, s+1) + q(s+2, t+1) = \frac{Q(s, t)(s-t)^2 + R(s, t)}{8(1+2s)^3(1+s+t)^3},$$

where $Q(s, t)$ and $R(s, t)$ are the polynomials

$$Q(s, t) = \sum_{i=0}^{5} q_i(t) s^i,$$
$$R(s, t) = r_0(t) + r_1(t) s,$$

with the polynomials $q_i(t), r_i(t)$ given in Table 2. We will show that the polynomials $Q(s, t)$ and $R(s, t)$ are positive for $s \geq t \geq 16$. Note that $q_i(t) \geq 0$ for all $i \neq 4$, when $t \geq 16$. Hence

$$\begin{aligned} Q(s, t) &> q_4(t) s^4 + q_5(t) s^5 \geq [q_4(t) + t q_5(t)] s^4 \\ &= 3\left(4t^2 + 128t + 87\right) s^4 > 0. \end{aligned}$$

Similarly, $r_1(t) \geq 0$ if $t \geq 16$. Then

$$\begin{aligned} R(s, t) &\geq r_0(t) + r_1(t) t \\ &= (1+2t)^3 [r(t)(t-16) + 12805739] > 0, \end{aligned}$$

since

$$r(t) = 800365 + 50047t + 3163t^2 + 210t^3 + 12t^4.$$

■

Lemma 16: For $x \geq 1$,

$$4 < xl(x+2, 1) + h(x+2, 3) < 27.$$

Proof: Note that

$$xl(x+2, 1) + h(x+2, 3) - 4 = \frac{A(x)(x-1) + 1416}{x^2(x+1)^3(x+3)^3}$$

and

$$27 - xl(x+2, 1) - h(x+2, 3) = \frac{B(x)}{x^2(x+1)^3(x+3)^3},$$

where

$$\begin{aligned} A(x) = {} & 23x^7 + 215x^6 + 839x^5 + 1792x^4 \\ & + 2344x^3 + 2100x^2 + 1632x + 1443, \end{aligned}$$

and

$$\begin{aligned} B(x) = {} & 84x^7 + 687x^6 + 2175x^5 + 3381x^4 \\ & + 2728x^3 + 1089x^2 + 189x + 27. \end{aligned}$$

■

Lemma 17: If $s \geq r+6$ and $r \geq 1$, then

$$q(r+1, s+2) > 24.$$

Proof: It is easy to see that

$$q(r+1, s+2) - 24 = \frac{P(r, s)}{(1+r+s)^2},$$

where

$$P(r, s) = \left(\sum_{i=0}^{5} p_i(r) s^i\right)(s-r-6) + p_6(r),$$

and the polynomials $p_i(r)$ are given in Table 3. Now the result follows from the fact that $p_i(r) \geq 0$ for all $i = 0, \ldots, 6$ when $r \geq 1$. ■

Now we introduce some operations over the trees in $\Omega_1(n, 3)$ that increases the value of $\mathcal{AZI}$.

Proposition 18: If $r \geq s+2$ then $\mathcal{AZI}(S(r, t; s)) < \mathcal{AZI}(S(r-1, t; s+1))$. If $t \geq s+2$ then $\mathcal{AZI}(S(r, t; s)) < \mathcal{AZI}(S(r, t-1; s+1))$.

Proof: We first note that

$$\begin{aligned} \Delta &= \mathcal{AZI}(S(r-1, t; s+1)) - \mathcal{AZI}(S(r, t; s)) \\ &= f(r-1) - g(s) + l(s+3, t+1) \\ &\quad + q(s+2, r+1). \end{aligned}$$

By Lemma 12, $0 < f(r-1) < -1$ and by Lemma 13, $g(s) < -1$. Consequently, $f(r-1) - g(s) > 0$. On the other hand, $l(s+3, t+1) \geq 0$ by Lemma 11. Since $r+1 \geq s+3 \geq 1$, it follows from Lemma 14 that $q(s+2, r+1) \geq 0$. Hence $\Delta > 0$.

The second inequality is proved similarly. ■

Proposition 19: If $s > r \geq t > 2$ then

$$\mathcal{AZI}(S(r, t; s)) < \mathcal{AZI}(S(r+1, t-1; s)).$$

Proof: We find that

$$\begin{aligned} \Delta &= \mathcal{AZI}(S(r+1, t-1; s)) - \mathcal{AZI}(S(r, t; s)) \\ &= f(t-1) - f(r) + l(r+2, s+2) \\ &\quad - l(t+1, s+2). \end{aligned}$$

Clearly, $1 \leq t-1 < r$. By Lemma 12, f is strictly decreasing when $x \geq 1$. Consequently $f(t-1) - f(r) > 0$. On the other hand, $r+2 > t+1 \geq 3$, so by Lemma 11, $l(r+2, s+2) - l(t+1, s+2) > 0$. In conclusion, $\Delta > 0$. ■

Proposition 20: If $3 \leqslant t \leqslant s$ and $8 \leqslant s$, then

$$\mathcal{AZI}(S(s,t;s)) < \mathcal{AZI}(S(s,t-1;s+1)).$$

Proof: First we assume that $16 \leqslant t \leqslant s$. Note that

$$\begin{aligned}\Delta &= \mathcal{AZI}(S(s,t-1;s+1)) - \mathcal{AZI}(S(s,t;s)) \\ &= f(t-1) - g(s) + l(s+3, s+1) \\ &\quad + q(s+2, t+1).\end{aligned}$$

By Lemmas 12 and 13, $0 < f(t-1) < -1$ and $g(s) < -1$. Hence $f(t-1) - g(s) > 0$. Also, by Lemma 15, $l(s+3, s+1) + q(s+2, t+1) > 0$. Consequently, $\Delta > 0$.

Secondly, suppose that $3 \leqslant t \leqslant 15$, $26 \leqslant s$ and $t \leqslant s$. Then, for $t = 3, \ldots, 15$,

$$\Delta = \frac{(s-26)\left(\sum_{i=0}^{13} q_{t,i} s^i\right) + r_t}{8(s+1)^3(s+2)^3(2s+1)^3(t-1)^2 t^2(s+t+1)^3},$$

where r_t, and $q_{t,i}$ are the values in Table 4. Bearing in mind that all of these polynomials have positive coefficients for $3 \leq t \leq 15$ and $0 \leq i \leq 13$, we deduce that $\Delta > 0$.

For the remainder cases $3 \leqslant t \leqslant 15$ and $t \leqslant s \leqslant 26$, it was checked by hand that $\Delta > 0$. ■

Proposition 21: If $3 \leqslant t \leqslant s$ and $8 \leqslant s$, then

$$\mathcal{AZI}(S(s+1,t;s)) < \mathcal{AZI}(S(s+1,t-1;s+1)).$$

Proof: We know that

$$\begin{aligned}\Delta &= \mathcal{AZI}(S(s+1,t-1;s+1)) - \mathcal{AZI}(S(s+1,t;s)) \\ &= f(t-1) - g(s) + l(s+3, s+2) \\ &\quad + q(s+2, t+1).\end{aligned}$$

By Lemma 3, $l(s+3, s+2) > l(s+3, s+1)$. Hence

$$\Delta > f(t-1) - g(s) + l(s+3, s+1) + q(s+2, t+1).$$

Now we proceed as in the proof of Proposition 20 to deduce that $\Delta > 0$. ■

Proposition 22: If $s > r$ then

$$\mathcal{AZI}(S(r,2;s)) < \mathcal{AZI}(S(s,2;r)).$$

Proof: Note that

$$\begin{aligned}\Delta &= \mathcal{AZI}(S(s,2;r)) - \mathcal{AZI}(S(r,2;s)) \\ &= rl(r+2,1) - sl(s+2,1) + q(r+1, s+2) \\ &\quad + h(r+2,3) - h(s+2,3).\end{aligned}$$

Now by Lemma 16, $rl(r+2,1) + h(r+2,3) > 4$ and $sl(s+2,1) + h(s+2,3) < 27$. Furthermore, if $s \geqslant r+6$ and $r \geqslant 2$ then, by Lemma 17, $q(r+1, s+2) > 24$. Hence $\Delta > 0$ in this case. Now suppose that $s = r + k$, with $k = 1, \ldots, 5$ and $r \geqslant 2$. An easy computation shows that

$$\Delta = \frac{(r-2)q_k(r) + p_k}{r^2(r+1)^3(r+3)^3 C_k(r)},$$

where $q_k(r)$, and p_k are the polynomials in Table 5 and

$$C_k(r) = (k+r)^2(k+r+1)^3(k+r+3)^3(k+2r+1)^3.$$

Since $q_k(r) > 0$ and $p_k > 0$, for all $k = 1, \ldots, 5$ and $r \geqslant 2$, it follows that $\Delta > 0$. ■

In our next result we find the maximal tree over $\Omega_1(n, 3)$ with respect to $\mathcal{AZI}$.

Theorem 23: If $n \geq 13$ then $S\left(\left\lceil \frac{n-5}{2} \right\rceil, 2; \left\lfloor \frac{n-5}{2} \right\rfloor\right)$ is the unique maximal tree with respect to $\mathcal{AZI}$ over $\Omega_1(n, 3)$.

Proof: Let $n \geq 27$ and suppose that $T = S(r,t;s)$ is a maximal tree over $\Omega_1(n, 3)$ with respect to $\mathcal{AZI}$. If $r \geq s+2$ then by Proposition 18 we get a contradiction. Hence

$$2 \leq t \leq r \leq s+1.$$

Note that $s \geq 8$, otherwise

$$n = r + s + t + 3 \leq 3s + 5 \leq 26.$$

Assume first that $t > 2$. If $t \leq r < s$ then by Proposition 19 we get a contradiction. So $r = s$ or $r = s+1$. In any case, we get a contradiction by Propositions 20 and 21. Thus $t = 2$. Now, if $r < s$ then by Proposition 22 we get a contradiction. Consequently, $T = S(s+x, 2; s)$ with $x \in \{0, 1\}$. Since $2s + x = n - 5$ it follows that $S(s+x, 2; s)$ is precisely $S\left(\left\lceil \frac{n-5}{2} \right\rceil, 2; \left\lfloor \frac{n-5}{2} \right\rfloor\right)$.

For $13 \leq n \leq 26$ the result is obtained by computer search. ■

Example 24: Let us illustrate how Propositions 18 - 22 are used as operations to increase $\mathcal{AZI}$. In each step we indicate the proposition used over the inequality sign. The trees used are depicted in Figure 6.

$$\begin{aligned}&\mathcal{AZI}(S(98,6;95)) \overset{18}{<} \mathcal{AZI}(S(97,6;96)) \overset{21}{<} \\ &\mathcal{AZI}(S(97,5;97)) \overset{20}{<} \mathcal{AZI}(S(97,4;98)) \overset{19}{<} \\ &\mathcal{AZI}(S(98,3;98)) \overset{20}{<} \mathcal{AZI}(S(98,2;99)) \overset{22}{<} \\ &\qquad \mathcal{AZI}(S(99,2;98))\end{aligned}$$

Now we can find the maximal value of $\mathcal{AZI}$ over $\Omega(n, 3)$.

Corollary 25: The maximal value of $\mathcal{AZI}$ over $\Omega(n, 3)$ is attained in $S\left(\left\lceil \frac{n-5}{2} \right\rceil, 2; \left\lfloor \frac{n-5}{2} \right\rfloor\right)$ for all $n \geq 35$.

Proof: By Theorem 8 we only have to prove that for $n \geq 35$,

$$\mathcal{AZI}\left(S\left(\left\lceil \frac{n-5}{2} \right\rceil, 2; \left\lfloor \frac{n-5}{2} \right\rfloor\right)\right) > 2h(9,9) + 8(n-3).$$

Using Lemma 2 it follows that

$$\begin{aligned}&\mathcal{AZI}\left(S\left(\left\lceil \frac{n-5}{2} \right\rceil, 2; \left\lfloor \frac{n-5}{2} \right\rfloor\right)\right) \\ &\quad \geq \frac{n-5}{2} h\left(\frac{n-1}{2}, 1\right) + \frac{n-7}{2} h\left(\frac{n-1}{2}, 1\right) \\ &\qquad + 2h(3,1) + h\left(\frac{n-3}{2}, \frac{n-3}{2}\right)\end{aligned}$$

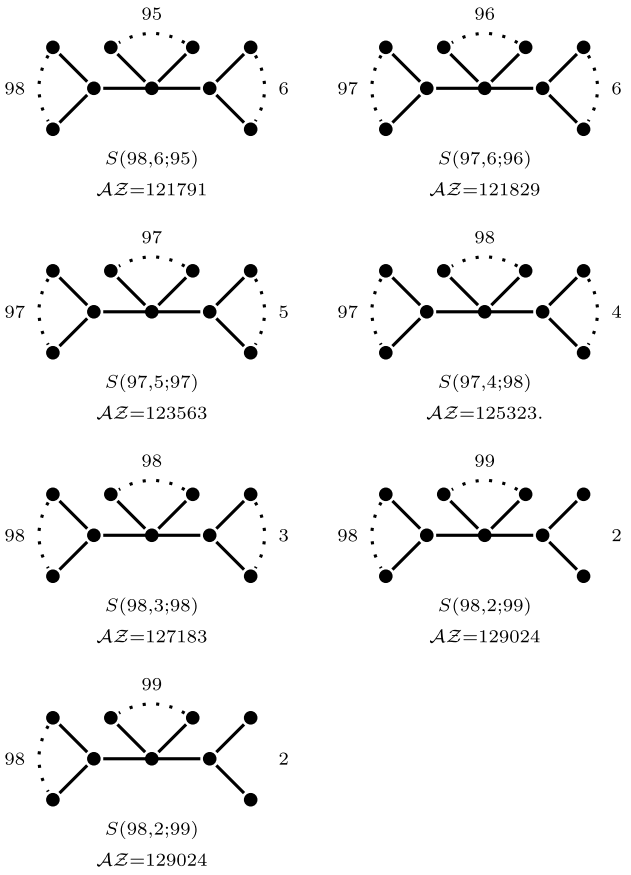


FIGURE 6. Trees used in example 24.

$$= 2h(3,1) + (n-6)\frac{(n-1)^3}{(n-3)^3} + \frac{1}{64}\frac{(n-3)^6}{(n-5)^3}$$
$$\geq 2h(3,1) + (n-6) + \frac{1}{64}(n-3)^3.$$

Now it is easy to see that

$$2h(3,1) + (n-6) + \frac{1}{64}(n-3)^3 > 2h(9,9) + 8(n-3)$$

for all $n \geq 35$. ■

One important consequence of our previous results is that Conjecture 1 holds for all trees with at most 3 branching vertices.

Theorem 26: Let $n \geq 19$. If T is an n-vertex tree with at most three branching vertices, then

$$\mathcal{AZI}(T) \leq \mathcal{AZI}\left(S\left(\left\lceil \frac{n-2}{2} \right\rceil; \left\lfloor \frac{n-2}{2} \right\rfloor\right)\right). \quad (2)$$

Proof: It was shown in [13] that inequality (2) holds for all n -vertex trees when $19 \leq n \leq 200$. So we may assume that $n > 200$. By [2], for any tree $T \in \Omega(n,1)$

$$\mathcal{AZI}(T) \leq \mathcal{AZI}(V_3) = 8(n-1),$$

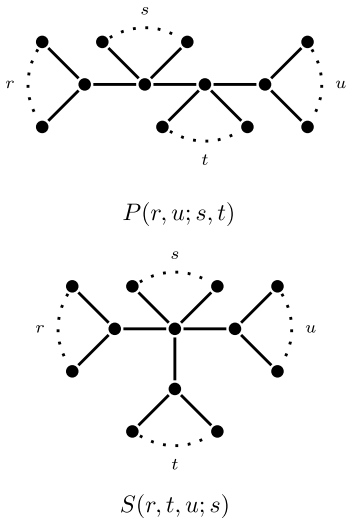


FIGURE 7. Trees in $\Omega_1(n,4)$.

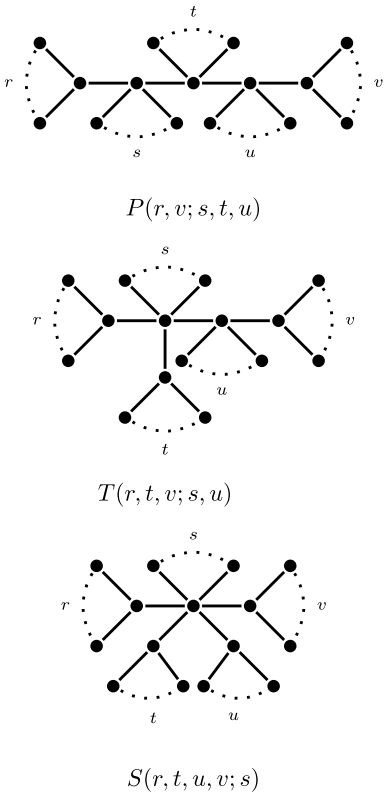


FIGURE 8. Trees in $\Omega_1(n,5)$.

where V_3 is shown in Figure 1. In Corollary 10 we established that for any tree $T \in \Omega(n,2)$,

$$\mathcal{AZI}(T) \leq \mathcal{AZI}\left(S\left(\left\lceil \frac{n-2}{2} \right\rceil; \left\lfloor \frac{n-2}{2} \right\rfloor\right)\right).$$

Note that if $n = 2k$

$$\mathcal{AZI}\left(S\left(\left\lceil \frac{n-2}{2} \right\rceil; \left\lfloor \frac{n-2}{2} \right\rfloor\right)\right) = \frac{k^6}{8(k-1)^3} + \frac{2k^3}{(k-1)^2},$$

TABLE 2. Polynomials in the proof of lemma 15.

$q_0(t)$	=	$336t^6+120t^5-6968t^4-19590t^3$ $-20529t^2-9584t-1833$
$q_1(t)$	=	$240t^5-168t^4-5680t^3-12858t^2$ $-8604t-2302$
$q_2(t)$	=	$144t^4-456t^3-4392t^2-3591t$ -1251
$q_3(t)$	=	$48t^3-744t^2-213t-30$
$q_4(t)$	=	$-48t^2+282t+261$
$q_5(t)$	=	$60t+102$
$r_0(t)$	=	$-336t^8-120t^7+6968t^6+19590t^5$ $+20529t^4+9699t^3+1530t^2-303t$ -101
$r_1(t)$	=	$432t^7+408t^6-8256t^5-26322t^4$ $-31521t^3-18714t^2-5625t$ -690

TABLE 3. Polynomials in the proof of lemma 17.

$p_0(r)$	=	$12r^7+534r^6+7226r^5+45300r^4+139200r^3$ $+168110r^2-62790r-216696$
$p_1(r)$	=	$12r^6+471r^5+4637r^4+18918r^3+29526r^2$ $-3901r-35967$
$p_2(r)$	=	$15r^5+426r^4+2642r^3+5556r^2+1023r$ -5758
$p_3(r)$	=	$21r^4+330r^3+1094r^2+702r-771$
$p_4(r)$	=	$18r^3+150r^2+206r-54$
$p_5(r)$	=	$6r^2+24r+2$
$p_6(r)$	=	$12r^8+606r^7+10399r^6+88380r^5$ $+410001r^4+1001430r^3+943929r^2$ $-594480r-1300405$

while if $n=2k+1$

$$\mathcal{AZI}\left(S\left(\left\lceil\frac{n-2}{2}\right\rceil;\left\lfloor\frac{n-2}{2}\right\rfloor\right)\right)=\frac{k^3(k+1)^3}{(2k-1)^3}+\frac{(k+1)^3}{k^2}+\frac{k^3}{(k-1)^2}.$$

Finally, in Corollary 25 we found that for any tree $T\in\Omega(n,3)$

$$\mathcal{AZI}(T)\leq\mathcal{AZI}\left(S\left(\left\lceil\frac{n-5}{2}\right\rceil,2;\left\lfloor\frac{n-5}{2}\right\rfloor\right)\right).$$

Note that if $n=2k$

$$\mathcal{AZI}\left(S\left(\left\lceil\frac{n-5}{2}\right\rceil,2;\left\lfloor\frac{n-5}{2}\right\rfloor\right)\right)=\frac{(k-1)^6}{8(k-2)^3}+\frac{(2k-5)(k-1)^3}{(k-2)^3}+\frac{27(k-1)^3}{k^3}+\frac{27}{4}$$

while if $n=2k+1$

$$\mathcal{AZI}\left(S\left(\left\lceil\frac{n-5}{2}\right\rceil,2;\left\lfloor\frac{n-5}{2}\right\rfloor\right)\right)=\frac{k^3(k-1)^3}{(2k-3)^3}+\frac{k^3(k-2)}{(k-1)^3}+\frac{27k^3}{(k+1)^3}+\frac{(k-1)^3}{(k-2)^2}+\frac{27}{4}.$$

TABLE 4. Coefficients of the polynomials $\sum_{i=0}^{13}q_{t,i}s^i+r_t$, with $3\leqslant t\leqslant 15$, in the proof of proposition 20.

$q_{3,0}$	2296119577315519788800	$q_{4,0}$	9080289826209294790880
$q_{3,1}$	88312291435212152512	$q_{4,1}$	34924191639266295212 8
$q_{3,2}$	3396626593661240192	$q_{4,2}$	1343238139970631380 0
$q_{3,3}$	130639484369537296	$q_{4,3}$	516630053802658224
$q_{3,4}$	5024595549509168	$q_{4,4}$	19870386629347752
$q_{3,5}$	193253672178292	$q_{4,5}$	764245578441936
$q_{3,6}$	7432832492608	$q_{4,6}$	29394017741544
$q_{3,7}$	285878658596	$q_{4,7}$	1130521700928
$q_{3,8}$	10996155232	$q_{4,8}$	43479277656
$q_{3,9}$	423376148	$q_{4,9}$	1673514448
$q_{3,10}$	16401208	$q_{4,10}$	65004368
$q_{3,11}$	640724	$q_{4,11}$	2595184
$q_{3,12}$	22680	$q_{4,12}$	95904
$q_{3,13}$	432	$q_{4,13}$	1728
r_3	5969910901020351477 1200	r_4	2360875354814416690 24128
$q_{5,0}$	246098720660106097 38496	$q_{6,0}$	534781936426768502 24720
$q_{5,1}$	946533541000393201280	$q_{6,1}$	205685360164135254 9616
$q_{5,2}$	364051361922465575 52	$q_{6,2}$	791097539089511589 56
$q_{5,3}$	1400197545639104704	$q_{6,3}$	304268284170459593 2
$q_{5,4}$	53853751372298736	$q_{6,4}$	117026261445265472
$q_{5,5}$	2071297685806632	$q_{6,5}$	4501008048234688
$q_{5,6}$	79664955831480	$q_{6,6}$	173114105735824
$q_{5,7}$	3063870761096	$q_{6,7}$	6657410330696
$q_{5,8}$	117795464248	$q_{6,8}$	255792934504
$q_{5,9}$	4527134880	$q_{6,9}$	9798645824
$q_{5,10}$	175771872	$q_{6,10}$	378379780
$q_{5,11}$	7179216	$q_{6,11}$	15809564
$q_{5,12}$	280800	$q_{6,12}$	664200
$q_{5,13}$	4800	$q_{6,13}$	10800
r_5	6398566737162758838 76352	r_6	1390433034709598241 475872
$q_{7,0}$	1006050774776231 45564672	$q_{8,0}$	1714172384705191 39806880
$q_{7,1}$	3869426056831442770240	$q_{8,1}$	6592907710403977 949312
$q_{7,2}$	1488240791077934 28416	$q_{8,2}$	2535757965509104 54552
$q_{7,3}$	5724003039430842192	$q_{8,3}$	9752915243085562336
$q_{7,4}$	220153957323907488	$q_{8,4}$	375112108654790568
$q_{7,5}$	8467453042705236	$q_{8,5}$	14427369428823312
$q_{7,6}$	325665751102224	$q_{8,6}$	554883060105288
$q_{7,7}$	12522653460228	$q_{8,7}$	21333072410816
$q_{7,8}$	480646296240	$q_{8,8}$	817512330232
$q_{7,9}$	18306176692	$q_{8,9}$	30852421968
$q_{7,10}$	697674536	$q_{8,10}$	1147362528
$q_{7,11}$	29765812	$q_{8,11}$	49770624
$q_{7,12}$	1365336	$q_{8,12}$	2540160
$q_{7,13}$	21168	$q_{8,13}$	37632
r_7	2615732014418202242287872	r_8	4456848200233498918338560
$q_{9,0}$	2727317193923838607 19360	$q_{10,0}$	4146000721523625715 60976
$q_{9,1}$	1048968151509021179 2768	$q_{10,1}$	1594615662124146360 0880
$q_{9,2}$	4034492890343961958 40	$q_{10,2}$	6133137161849973744 92
$q_{9,3}$	1551728032579973 5744	$q_{10,3}$	2358898903623892 2204
$q_{9,4}$	596818434663849392	$q_{10,4}$	907268721999173376
$q_{9,5}$	22954507492659256	$q_{10,5}$	34894845090422112
$q_{9,6}$	882826570354744	$q_{10,6}$	1342022251079760
$q_{9,7}$	33933322267928	$q_{10,7}$	51567798540936
$q_{9,8}$	1297456623256	$q_{10,8}$	1965866964648
$q_{9,9}$	48309983888	$q_{10,9}$	71853821920
$q_{9,10}$	1724775328	$q_{10,10}$	2407738772
$q_{9,11}$	75457664	$q_{10,11}$	104727196
$q_{9,12}$	4385664	$q_{10,12}$	7144200
$q_{9,13}$	62208	$q_{10,13}$	97200
r_9	7091024704201983523 258368	r_{10}	1077960187596143380 9601952
$q_{11,0}$	6133709903215694904 48640	$q_{12,0}$	8962290987973802621 30912
$q_{11,1}$	2359119193543837446 1376	$q_{12,1}$	3447034995373282521 1840
$q_{11,2}$	9073535359446815275 96	$q_{12,2}$	1325782690464046571 336
$q_{11,3}$	3489821282376483152	$q_{12,3}$	5099164175593853771 2
$q_{11,4}$	1342238777396126352	$q_{12,4}$	1961216652552810728
$q_{11,5}$	51624352407570708	$q_{12,5}$	7543099724896609 6
$q_{11,6}$	1985373294810144	$q_{12,6}$	2900849790775144
$q_{11,7}$	76260569772356	$q_{12,7}$	111378726180608
$q_{11,8}$	2896569421504	$q_{12,8}$	4212863007640
$q_{11,9}$	103383417204	$q_{12,9}$	146177260112
$q_{11,10}$	3154574040	$q_{12,10}$	3908258896
$q_{11,11}$	132989364	$q_{12,11}$	152295152
$q_{11,12}$	11107800	$q_{12,12}$	16622496
$q_{11,13}$	145200	$q_{12,13}$	209088
r_{11}	1594764574836082090 3922432	r_{12}	2330195656873191379 00077312
$q_{13,0}$	1307467606491558066 978560	$q_{14,0}$	1916752527925975252 002640
$q_{13,1}$	5028721563426804772 2112	$q_{14,1}$	7372125107402246104 7408
$q_{13,2}$	1934123678125541242112	$q_{14,2}$	2835432733417465761580
$q_{13,3}$	74389371902198486976	$q_{14,3}$	1090551045575829399 64
$q_{13,4}$	2861129078603886768	$q_{14,4}$	4194426047580757632
$q_{13,5}$	110042680675669032	$q_{14,5}$	161322792803986176
$q_{13,6}$	4231790432240568	$q_{14,6}$	6203650410004944
$q_{13,7}$	162411185360136	$q_{14,7}$	237994996062728
$q_{13,8}$	6116688861432	$q_{14,8}$	8927149847656
$q_{13,9}$	205822269088	$q_{14,9}$	291460748928
$q_{13,10}$	4605777248	$q_{14,10}$	5193685188
$q_{13,11}$	150355024	$q_{14,11}$	109445244
$q_{13,12}$	24092640	$q_{14,12}$	33985224
$q_{13,13}$	292032	$q_{14,13}$	397488
q_{13}	3399415776878055841 1243520	r_{14}	4983556572606561240 1119008

$q_{15,0}$	28296361796166683687 10656
$q_{15,1}$	10883216075442276400 2880
$q_{15,2}$	41858523363797220936 32
$q_{15,3}$	16099431968032087470 4
$q_{15,4}$	6192087478246130816
$q_{15,5}$	238155078582368692
$q_{15,6}$	9158029644275440
$q_{15,7}$	351221181083876
$q_{15,8}$	13129596498448
$q_{15,9}$	417397496660
$q_{15,10}$	5650921672
$q_{15,11}$	5201876
$q_{15,12}$	46834200
$q_{15,13}$	529200
r_{15}	7357054067003351645478 8352

TABLE 5. Polynomials in the proof of propostion 22.

$q_1(r)$	$3r^{19}+126r^{18}+2487r^{17}+30048r^{16}+247879r^{15}$ $+1487734r^{14}+6786444r^{13}+24339294r^{12}$ $+70712283r^{11}+171624272r^{10}+361123529r^{9}$ $+690994362r^{8}+1271692219r^{7}+2362555748r^{6}$ $+4525593988r^{5}+8892822176r^{4}+17694729680r^{3}$ $+35352667584r^{2}+70695433152r+141389290368$
p_1	282778470144
$q_2(r)$	$6r^{19}+312r^{18}+7614r^{17}+114696r^{16}+1190702r^{15}$ $+9051288r^{14}+52400558r^{13}+237742208r^{12}$ $+865422248r^{11}+2585207376r^{10}+6503547048r^{9}$ $+14253768540r^{8}+28469177618r^{7}+54554516128r^{6}$ $+104598086582r^{5}+204206480392r^{4}$ $+404714404070r^{3}+807574532488r^{2}$ $+1614547206950r+3228980252500$
p_2	6457950663500
$q_3(r)$	$9r^{19}+558r^{18}+16191r^{17}+290394r^{16}+3596985r^{15}$ $+32656122r^{14}+225524952r^{13}+1215665178r^{12}$ $+5217428721r^{11}+18149274528r^{10}+52179063573r^{9}$ $+127221493380r^{8}+272942660973r^{7}$ $+541218938832r^{6}+1044354519540r^{5}$ $+2029776508656r^{4}+4006507703616r^{3}$ $+7982552678400r^{2}+15954185613312r$ $+31906131738624$
p_3	63812048486400
$q_4(r)$	$12r^{19}+864r^{18}+29028r^{17}+602232r^{16}+8624044r^{15}$ $+90418288r^{14}+719444820r^{13}+4449996888r^{12}$ $+21775839840r^{11}+85556446880r^{10}+274075485104r^{9}$ $+730535006616r^{8}+1670696551372r^{7}$ $+3430466738384r^{6}+6685967961412r^{5}$ $+12961538205416r^{4}+25486805128652r^{3}$ $+50696911017504r^{2}+101288262407508r$ $+20255400074001$
p_4	6405105686230032
$q_5(r)$	$15r^{19}+1230r^{18}+46935r^{17}+1103940r^{16}$ $+17893595r^{15}+211930830r^{14}+1899688100r^{13}$ $+13184573510r^{12}+71990216735r^{11}$ $+313165097280r^{10}+1098921578985r^{9}$ $+3161911591710r^{8}+7655523844535r^{7}$ $+16258956445420r^{6}+32066443023980r^{5}$ $+62099890860880r^{4}+121687319555120r^{3}$ $+241652072413120r^{2}+482618054582720r$ $+965086556156800$
p_5	1930156988000000

Now a simple computation shows that $\mathcal{AZI}(V_3)$ and $\mathcal{AZI}\left(S\left(\left\lceil\frac{n-5}{2}\right\rceil,2,\left\lfloor\frac{n-5}{2}\right\rfloor\right)\right)$ are less or equal than

$$\mathcal{AZI}\left(S\left(\left\lceil\frac{n-2}{2}\right\rceil;\left\lfloor\frac{n-2}{2}\right\rfloor\right)\right).$$

■

IV. CONCLUSION

In conclusion, we show that the maximum value problem of $\mathcal{AZI}$ over $\Omega(n,p)$ reduces to $\Omega_1(n,p)$ under a certain condition. Relying on this result, we find the trees with maximal value of $\mathcal{AZI}$ over $\Omega(n,p)$, when $p=2$ and 3. In particular, we deduce that the Conjecture 1 holds for all trees with at most 3 branching vertices.

The problem of finding the tree with maximal value of $\mathcal{AZI}$ over $\Omega(n,p)$ when $p>3$ is far more complicated. For example, if $p=4$ there are two different types of trees in $\Omega_1(n,4)$ (see Figure 7). We found computationally that for $20\leq n\leq 200$, the maximal tree with respect to $\mathcal{AZI}$ over $\Omega_1(n,4)$ is $S\left(\left\lceil\frac{n-7}{2}\right\rceil,2,2;\left\lfloor\frac{n-5}{2}\right\rfloor\right)$. Since for all $n\geq 35$.

$$\mathcal{AZI}\left[S\left(\left\lceil\frac{n-7}{2}\right\rceil,2,2;\left\lfloor\frac{n-9}{2}\right\rfloor\right)\right]>3h(9,9)+8(n-4),$$

then by Theorem 10, it is reasonable to conjecture that the maximal value of $\mathcal{AZI}$ over $\Omega(n,4)$ is attained at $S\left(\left\lceil\frac{n-7}{2}\right\rceil,2,2;\left\lfloor\frac{n-5}{2}\right\rfloor\right)$, for all $n\geq 35$.

If $p=5$ there are three different types of trees in $\Omega_1(n,5)$ (see Figure 8). In this case we also found computationally that for $20\leq n\leq 200$, the maximal tree with respect to AZ over $\Omega_1(n,5)$ is $S\left(\left\lceil\frac{n-9}{2}\right\rceil,2,2,2;\left\lfloor\frac{n-13}{2}\right\rfloor\right)$. Similary, for $n\geq 39$

$$\mathcal{AZI}\left[S\left(\left\lceil\frac{n-9}{2}\right\rceil,2,2,2;\left\lfloor\frac{n-13}{2}\right\rfloor\right)\right]>4h(9,9)+8(n-5),$$

and so by Theorem 8, it is natural to conjecture that the maximal value of $\mathcal{AZI}$ over $\Omega(n,5)$ is attained at $S\left(\left\lceil\frac{n-7}{2}\right\rceil,2,2;\left\lfloor\frac{n-5}{2}\right\rfloor\right)$, for all $n\geq 39$.

In general, if $p>3$, then the problem of finding the maximal value of $\mathcal{AZI}$ over $\Omega(n,p)$ remains open.

APPENDIX

In this appendix we give a list of polynomials that appeared in the proofs of Lemmas 15 and 17, and in the proofs of Propositions 20 and 22.

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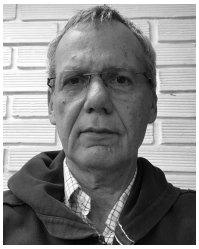
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ROBERTO CRUZ was born in La Habana, Cuba, in 1962. He received the B.S. degree in applied mathematics from Lomonosov Moscow State University, Russia, in 1986, and the Ph.D. degree in mathematics from the Instituto de Cibernética, Matemática y Física, Cuba, in 2000. From 1986 to 2002, he was an Assistant Professor with the Department of Basic Sciences, Instituto Superior de Ciencias y Tecnologias Nucleares, La Habana, Cuba. Since 2003, he has been a Full Professor with the Institute of Mathematics, Universidad de Antioquia, Medellín, Colombia. His research interests include mathematical chemistry and graph theory.



JUAN DANIEL MONSALVE received the B.S. and M.S. degrees in mathematics from the Universidad Nacional de Colombia Sede Medellín, Colombia, in 2008 and 2010, respectively, and the Ph.D. degree in mathematics from the Universidad de Antioquia, Colombia, in 2018, where he is currently a Postdoctoral Researcher with the Instituto de Matemáticas. He has been a Visiting Student with the Center for Combinatorics, Nankai University, Tianjin, China, in 2017. He was a Postdoctoral Researcher with the Instituto de Matemática e Estatística Programa de Pós-graduação em Matemática Aplicada, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil, in 2018. His research interest includes graph theory and its applications.



JUAN RADA was born in Mérida, Venezuela, in 1959. He received the B.S. and M.S. degrees in mathematics from the Universidad de Los Andes, Venezuela, in 1989, and the Ph.D. degree in algebra from the Universidad de Murcia, Spain, in 1996. From 1998 to 2008, he was a Full Professor with the Deparment of Mathematics, Universidad de Los Andes. Then, he moved to Caracas, Venezuela, where he was a Full Professor with Mathematics Deparment, Universidad Simón Bolívar, from 2008 to 2012. He was also a Visiting Professor with the University of Kentucky, Lexington, USA, in 2001. Since 2012, he has been a Full Professor with the Institute of Mathematics, Universidad de Antioquia, Medellín, Colombia. He is the author of 2 books, 2 chapters of books, and more than 90 articles. His research interests include algebra, spectral graph theory, and chemical graph theory. He is a member of the Editorial Board of *Communications in Mathematical and in Computer Chemistry* (MATCH), the *Kragujevac Journal of Mathematics*, and *Mathematical Aspects of Topological Indices* (MATI).