

The Augmented Zagreb Index of Trees with Given Degree Sequence

Fuqin Zhan

School of Mathematics and Statistics, Zhaoqing University, Zhaoqing, Guangdong, China

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Abstract: The augmented Zagreb index $AZI(G)$ of a graph G is defined as the sum of $\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$ over all edges uv of G , where $d(v)$ is the degrees of the vertex v in G . In this paper, we characterize the extremal trees with given degree sequence that maximize and minimize the AZI index.

Keywords: Augmented Zagreb index, Degree sequence, Tree, Extremal graph.

I. INTRODUCTION

All graphs will be simple and finite. Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $v \in V(G)$ in the graph G is denoted by $d(v)$.

The augmented Zagreb index AZI was conceived [1], defined as

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

where uv is an edge of the graph G , $d(u)$ stands for the degree of the vertex u , and the summation goes over all edges of G . The AZI index has proven to be a valuable predictive index in the study of the heat of formation in octanes and heptanes [1], whose prediction power is better than atom-bond connectivity index (please refer to [8-12]).

Delorme et al. [2] described an algorithm that determines a tree of given degree sequence that maximizes the sum of the products of the degrees of adjacent vertices. Wang [3] provided an algorithm to construct the extremal trees with given degree sequence for the Randić index. Then Xing et al. [4] and Gan et al. [5] characterized the extremal trees with fixed degree sequence for ABC index. In this paper, we use the same techniques to characterize the extremal trees with fixed degree sequence to maximize and minimize the AZI index.

II. PRELIMINARIES

For a tree T , the degree sequence of T is the sequence of the degrees of the non-leaf vertices in descending order. Through this paper, for convenience, we let $A(x, y) = \left(\frac{xy}{x+y-2}\right)^3$ for $x, y \geq 1$ with $x+y > 2$. Obviously, $A(x, y) = A(y, x)$.

Lemma 2.1 ([6]): (1) $A(1, y)$ is decreasing for $y \geq 2$.

(2) $A(2, y) = 8$ for $y \geq 2$.

(3) If $y \geq 3$ is fixed, then $A(x, y)$ is increasing for $x \geq 2$.

Lemma 2.2 Let $f(x) = A(x, r) - A(x, s)$ where $x, r, s \geq 2$.

(1) If $r \geq s$, then $f(x)$ is increasing for x ;

(2) If $r < s$, then $f(x)$ is decreasing for x .

Proof By the definition of $A(x, y)$, we have

$$f(x) = \left(\frac{xr}{x+r-2}\right)^3 - \left(\frac{xs}{x+s-2}\right)^3.$$

The derivative of $f(x)$ with respect to x is

$$f'(x) = 3x^2 \left(\frac{r^3(r-2)}{(x+r-2)^4} - \frac{s^3(s-2)}{(x+s-2)^4} \right).$$

Let $g(y) = \frac{y^3(y-2)}{(x+y-2)^4}$ for $y \geq 2$ with $x+y > 2$. Then

$$g'(y) = \frac{2y^2[x(y-3) + y(x-3) + 6]}{(x+y-2)^5}.$$

It is easy to verify that $g'(y) > 0$ for $x, y \geq 2$, from which it follows that $g(y)$ is increasing in y . Therefore, if $r \geq s$, then $f'(x) \geq 0$, implying that $f(x)$ is increasing for x ; if $r < s$, then $f'(x) < 0$, implying that $f(x)$ is decreasing for x .

III. TREE WITH GIVEN DEGREE SEQUENCE WITH MAXIMUM AZI INDEX

Lemma 3.1 Let T be a tree with maximum ABC index among trees with given degree sequence. Let $P = v_0v_1v_2 \cdots v_tv_{t+1}$ be a path in T , where v_0 and v_{t+1} are leaves. Then $d(v_i) \leq d(v_{t+1-i}) \leq d(v_k)$ for $i+1 \leq k \leq t+1-i$.

Proof By induction on i . For $i=1$, we should show that $d(v_1) \leq d(v_t) \leq d(v_k)$ for $2 \leq k \leq t$. Suppose for contradiction that $d(v_1) > d(v_k)$ for some $2 \leq k \leq t-1$. Let $T' = T - \{v_0v_1, v_kv_{k+1}\} + \{v_0v_k, v_1v_{k+1}\}$. Note that the edges in T do not change except for the edges v_0v_1 and v_kv_{k+1} , which are transformed to the edges v_0v_k and v_1v_{k+1} in T' , respectively. Obviously, T' has the same degree sequence as T .

Since $d(v_0) = 1$ and $d(v_1) > d(v_k) \geq 2$, by Lemma 2.1, we have

$$\begin{aligned} AZI(T') - AZI(T) &= A(d(v_0), d(v_k)) + A(d(v_1), d(v_{k+1})) - A(d(v_0), d(v_1)) - A(d(v_k), d(v_{k+1})) \\ &= (A(1, d(v_k)) - A(1, d(v_1))) + (A(d(v_1), d(v_{k+1})) - A(d(v_k), d(v_{k+1}))) > 0 \end{aligned}$$

which is a contradiction. Thus $d(v_1) \leq d(v_k)$. Similarly, we can show $d(v_t) \leq d(v_k)$. Therefore we have $d(v_1) \leq d(v_t) \leq d(v_k)$ for $2 \leq k \leq t$.

Suppose that Lemma 3.1 holds for $i=m \geq 1$. We consider the case $i=m+1$. In other words, we should prove that $d(v_{m+1}) \leq d(v_{t-m}) \leq d(v_k)$ for $m+2 \leq k \leq t-m$. Suppose that $d(v_{m+1}) > d(v_k)$ for some k with $m+2 \leq k \leq t-m$.

Let $T' = T - \{v_mv_{m+1}, v_kv_{k+1}\} + \{v_mv_k, v_{m+1}v_{k+1}\}$.

Note that the edges v_mv_{m+1} and v_kv_{k+1} in T are transformed to the edges v_mv_k and $v_{m+1}v_{k+1}$ in T' , respectively. By the induction hypothesis, we have $d(v_m) \leq d(v_{t+1-m}) \leq d(v_k)$ for $m+1 \leq k \leq t+1-m$. From Lemma 2.2, we know

$$\begin{aligned}
 AZI(T') - AZI(T) &= A(d(v_m), d(v_k)) + A(d(v_{m+1}), d(v_{k+1})) - A(d(v_m), d(v_{m+1})) - A(d(v_k), d(v_{k+1})) \\
 &= (A(d(v_{m+1}), d(v_{k+1})) - A(d(v_m), d(v_{m+1}))) - (A(d(v_k), d(v_{k+1})) - A(d(v_m), d(v_k))) \\
 &= f(d(v_{m+1})) - f(d(v_k)) > 0
 \end{aligned}$$

which is a contradiction. Thus we have $d(v_{m+1}) \leq d(v_k)$. Similarly, we may also have $d(v_{t-m}) \leq d(v_k)$ for $m+2 \leq k \leq t-m$. Clearly, $d(v_{m+1}) \leq d(v_{t-m})$. Therefore, we have $d(v_{m+1}) \leq d(v_{t-m}) \leq d(v_k)$ for $m+2 \leq k \leq t-m$. This completes the proof.

Let L_i be the set of vertices in T , the minimum distance from which to the set of pendent vertices of T is i . In particular, L_0 denote the set of leaves in T .

Remark 1 Let T be as above, every path $v_0 v_1 v_2 \dots v_t v_{t+1}$ in T , where v_0 and v_{t+1} are leaves, has the properties

$$d(v_1) \leq d(v_t) \leq d(v_2) \leq d(v_{t-1}) \leq \dots \leq d(v_{\lfloor \frac{t+1}{2} \rfloor}).$$

Thus, it is easy to see that the vertices of larger degrees have father distances from L_0 than the vertices of smaller degrees.

In the following, we construct the extremal tree T through greedy algorithm [3]. In 2003, Delorme et al. [2] described an algorithm that determines a tree of given degree sequence that maximizes Randić index. In 2008, Wang [4] generalized it to the greedy algorithm. Xing et al. [4] use the same ways to obtain the extremal trees with ABC index.

Given the degree sequence $D = \{d_1, d_2, \dots, d_m\}$. Let T be a tree with maximum AZI index among the trees with fixed degree sequence D . Now T can be constructed as:

- (i) Label a vertex with the largest degree d_1 as v (the root);
- (ii) Label the neighbors of v as v_1, v_2, \dots, v_{d_1} such that $d(v_1) \geq d(v_2) \geq \dots \geq d(v_{d_1})$;
- (iii) Label the neighbors of v_1 except v as $v_{11}, v_{12}, \dots, v_{1d_2-1}$ such that $d(v_{11}) \geq d(v_{12}) \geq \dots \geq d(v_{1d_2-1})$, then do the same for v_2, v_3, \dots ;
- (iv) Repeat (iii) for all the newly labeled vertices, and always start with the neighbors of the labeled vertex with the largest degree whose neighbors are not labeled yet.

Example 1 We present an example which is an extremal tree with maximum AZI index obtained by the above greedy algorithm with degree sequence $\{4, 4, 3, 3, 3, 2, 2, 2, 2\}$, see Fig. 1.

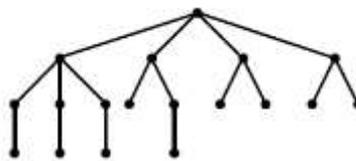


Fig. 1

IV. TREE WITH GIVEN DEGREE SEQUENCE WITH MINIMUM AZI INDEX

We first give a useful elementary result.

Lemma 4.1 Let T be a tree with minimum AZI index among the trees with fixed degree sequence. Let a path $v_0 v_1 v_2 \dots v_t v_{t+1}$ in T , where v_0 and v_{t+1} are leaves. For $1 \leq i \leq \frac{t+1}{2}$, we can always assume

- (i) if i is odd, then $d(v_i) \geq d(v_{i+1-i}) \geq d(v_k)$ for $i+1 \leq k \leq t+1-i$;

(ii) if i is even, then $d(v_i) \leq d(v_{t+1-i}) \leq d(v_k)$ for $i+1 \leq k \leq t+1-i$.

Proof By induction on i . For $i=1$, we prove that $d(v_1) \geq d(v_i) \geq d(v_k)$ for $2 \leq k \leq t$. Suppose for contradiction that $d(v_1) < d(v_k)$ for some $2 \leq k \leq t$. Consider a new tree T' obtained from T by transforming the edges v_0v_1 and v_kv_{k+1} to the edges v_0v_k and v_1v_{k+1} . Note that, T' has the same degree sequence as T . Since $d(v_1) \geq 2$, by Lemma 2.1, we have

$$\begin{aligned} AZI(T') - AZI(T) &= A(d(v_0), d(v_k)) + A(d(v_1), d(v_{k+1})) - A(d(v_0), d(v_1)) - A(d(v_k), d(v_{k+1})) \\ &= (A(1, d(v_k)) - A(1, d(v_1))) + (A(d(v_1), d(v_{k+1})) - A(d(v_k), d(v_{k+1}))) < 0, \end{aligned}$$

which is a contradiction. Thus $d(v_1) \geq d(v_k)$. Similarly, we can show $d(v_i) \geq d(v_k)$. Therefore, we have $d(v_1) \geq d(v_i) \geq d(v_k)$ for $i+1 \leq k \leq t+1-i$.

Suppose that Lemma 4.1 holds for $i = m \geq 1$. We consider the case $i = m+1$. We have the following cases:

Case 1 m is odd.

By the induction hypothesis, we have $d(v_m) \geq d(v_{t+1-m}) \geq d(v_k)$ for $m+1 \leq k \leq t+1-m$. We should prove that $d(v_{m+1}) \leq d(v_{t-m}) \leq d(v_k)$ for $m+2 \leq k \leq t-m$. Suppose that $d(v_{m+1}) > d(v_k)$ for some k with $m+2 \leq k \leq t-m$. Let $T' = T - \{v_mv_{m+1}, v_kv_{k+1}\} + \{v_mv_k, v_{m+1}v_{k+1}\}$. Since $k+1 \leq t+1-m$, we have $d(v_m) \geq d(v_{k+1})$. By Lemma 2.2, we have

$$\begin{aligned} AZI(T') - AZI(T) &= A(d(v_m), d(v_k)) + A(d(v_{m+1}), d(v_{k+1})) - A(d(v_m), d(v_{m+1})) - A(d(v_k), d(v_{k+1})) \\ &= (A(d(v_{m+1}), d(v_{k+1})) - A(d(v_m), d(v_{m+1}))) - (A(d(v_k), d(v_{k+1})) - A(d(v_m), d(v_k))) \\ &= f(d(v_{m+1})) - f(d(v_k)) < 0 \end{aligned}$$

which is a contradiction. Then we get $d(v_{m+1}) \leq d(v_k)$. By the same argument, we can prove that $d(v_{t-m}) \leq d(v_k)$ for $m+2 \leq k \leq t-m$.

Case 2 m is even.

By the same reasoning as above, the result follows.

Remark 2 Let T be as above. From Lemma 4.1, for $v_i \in L_i$ and $j > i \geq 1$, we have $d(v_i) \geq d(v_j)$ if i is odd or $d(v_i) \leq d(v_j)$ if i is even. It is easy to verify that the vertices in L_1 take the largest degrees and they are adjacent to the vertices in L_2 with the smallest degrees.

In 2008, Wang [3] provides an algorithm to construct the extremal trees with given degree sequence for the Randić index. Xing et al. [4] also provide algorithms to obtain the extremal trees with ABC index. Now, we construct the extremal trees through the recursive algorithm [3].

Given the degree sequence $D = \{d_1, d_2, \dots, d_m\}$, we construct a tree T with minimum AZI index among the trees with fixed degree sequence D .

(i) If $d_m \geq m-1$, by Lemma 4.1, then we get an extremal tree T by rooting at vertex r with d_m children with degrees d_1, d_2, \dots, d_{m-1} and $\underbrace{1, \dots, 1}_{d_m - m + 1 \text{ times}}$;

(ii) If $d_m \leq m-2$, by Remark 2, we construct subtree T_1 : rooted at vertex r_1 with $d_m - 1$ children with degrees $d_1, d_2, \dots, d_{d_m - 1}$, where $r_1 \in L_2$ and the children of r_1 are all in L_1 . Then removing T_1 except the root r_1 from T results in a new tree S_1 with degree sequence $D_1 = \{d_m, \dots, d_{m-1}\}$. Then do the same to S_1 to get T_2 and S_2 , and so on, until S_k satisfied the condition of (i);

(iii) We construct T as: identifying the root r_i of T_i with a leaf v_i of S_i , let v be the only neighbor of v_i of S_i such that $v \in L_1$ and $d(v) = \min\{d(u), u \in L_1\}$.

Example 2 We present the procedure to construct extremal trees of degree sequence $\{6,5,5,4,4,4,3,3,2,2,2\}$ with minimum *AZI* index.

First, by the above algorithm (ii), we have the following subtree T_i and $D_i (i=1,2,3,4)$ and S_4 , see Fig. 2.

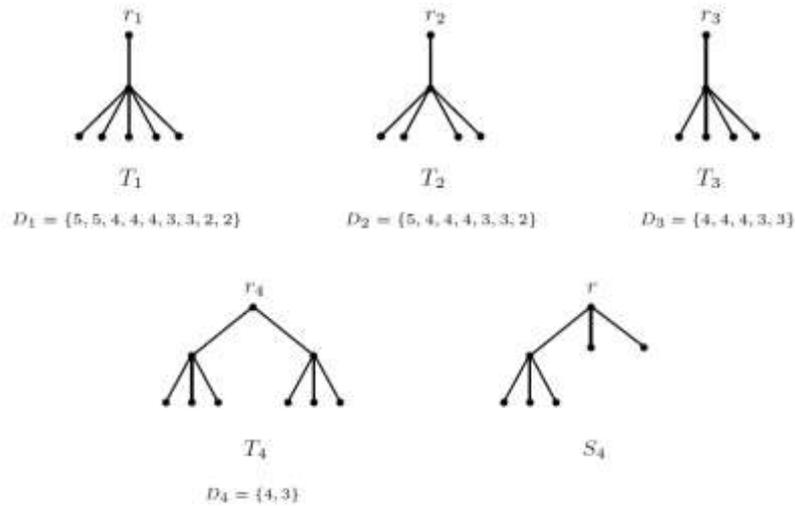


Fig. 2

Second, by (ii), attaching T_4 to S_4 yields the extremal tree S_3 for the degree sequence $D_3 = \{4, 4, 4, 3, 3\}$, then attaching T_3 to S_3 , similarly, by attaching T_2 to S_2 yields S_1 , attaching T_1 to S_1 yields the tree S for $\{6, 5, 5, 4, 4, 4, 3, 3, 2, 2, 2\}$, see Fig. 3 and Fig. 4.

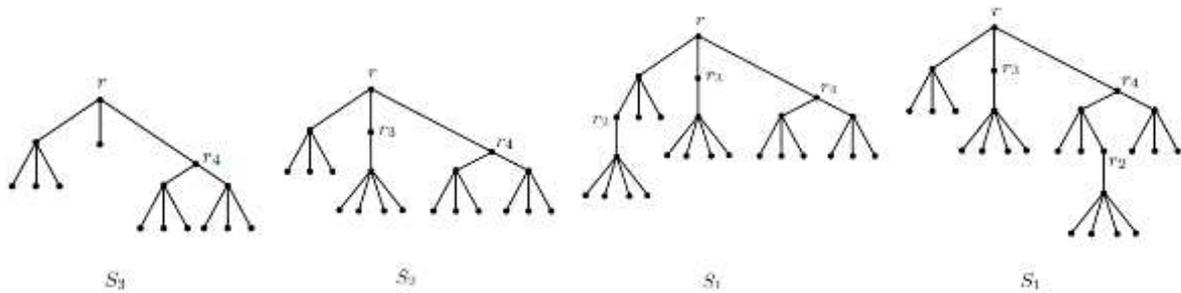


Fig. 3 Attaching subtree T_2 to S_2 to get two types of S_1

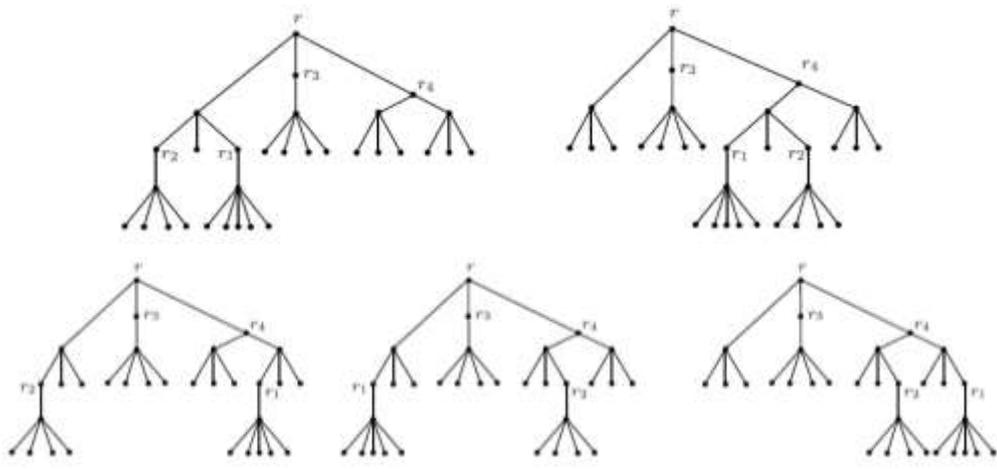


Fig. 4 Attaching subtree T_1 to S_1 to get five extremal trees

From the above example, we know that the extremal tree is not necessarily unique. But it does if the degrees of non-leaf vertices are different from each other.

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