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A note on the augmented Zagreb index of cacti with fixed number of vertices and cycles

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Abstract

Recent studies show that augmented Zagreb index (AZI) possess the best correlating ability among various well known topological indices for predicting the certain physicochemical properties of particular types of molecules. Hence, it is meaningful to study the mathematical properties of AZI, especially bounds and characterization of the extremal elements among well known graph families. For $n \geq 4$, let $\mathcal{C}_{n,k}$ be the collection of all cacti with k cycles and n vertices. In this note, the element of $\mathcal{C}_{n,k}$ having the minimum AZI is characterized. Some structural properties of the graph(s) having the maximum AZI over the collection $\mathcal{C}_{n,0}$ are also reported.

Keywords: Augmented Zagreb index; cactus graph; topological index.

1. Introduction

All the graphs considered in the present study are simple, finite, undirected and connected. The vertex set and edge set of a graph G will be denoted by $V(G)$ and $E(G)$ respectively. Undefined notations and terminologies from (chemical) graph theory can be found in (Harary, 1969; Trinajstic′, 1992).

Topological indices are numerical quantities of a graph, which are invariant under graph isomorphisms. There are many topological indices, which may be used to model the physicochemical properties of chemical compounds in quantitative structure-property relation (QSPR) and quantitative structure-activity relation (QSAR) studies (Gutman & Furtula, 2010; Trinajstic′, 1992). The atom-bond connectivity (ABC) index is one of such topological indices. The ABC index was introduced by Estrada *et al.* (1998). This index is defined as:

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

where d_u is the degree of the vertex $u \in V(G)$ and uv is edge connecting the vertices u and v. Details about ABC index can be found in the survey (Gutman *et al.*, 2013), papers (Ashrafi *et al.*, 2016; Dimitrov, 2016; Lin *et al.*, 2015; Palacios, 2014; Raza *et al.*, 2016) and the related references cited therein.

Inspired by the work done on the ABC index, Furtula *et al.* (2010) proposed the following topological index and named it augmented Zagreb index (AZI):

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

The prediction power of AZI is better than ABC index in the study of heat of formation for heptanes and octanes (Furtula *et al.*, 2010). Furtula *et al.* (2013) undertook a comparative study of the structure-sensitivity of twelve topological indices by using trees and they concluded that AZI has the greatest structure sensitivity. In the papers (Gutman & Tošovic′, 2013; Gutman *et al.*, 2014), the correlating ability of several topological indices was tested for the case of standard heats (enthalpy) of formation and normal boiling points of octane isomers, and it was found that the AZI possess the best correlating ability among the examined topological indices. This recent research on AZI motivates us to study the mathematical properties of AZI, especially bounds and characterization of the extremal elements of renowned graph families.

In (Furtula *et al.*, 2010), the extremal n-vertex chemical trees with respect to *AZI* were determined and the n-vertex tree having the minimum *AZI* was characterized. Huang *et al.* (2012) gave various bounds on *AZI* for several families of connected graphs (e.g. chemical graphs, trees, unicyclic graphs, bicyclic graphs, etc.). Wang *et al.* (2012) established some new bounds on *AZI* of connected graphs and improved some results of the papers (Furtula *et al.*, 2010; Huang *et al.*, 2012). The present authors (Ali *et al.*, 2016b) derived tight upper bounds for *AZI* of chemical bicyclic and unicyclic graphs. In (Ali *et al.*, 2016a), the authors characterized the n-vertex graphs having the maximum *AZI* with fixed vertex connectivity (and fixed matching number). Recently, Zhan *et al.* (2015) characterized the n-vertex unicyclic graphs with the first and second minimal *AZI,* and found n-vertex bicyclic graphs with the minimal *AZI*.

A graph G is cactus, if and only if every edge of G lies on at most one cycle. In recent years, many researchers studied the problem of characterizing the extremal cacti with respect to several well known topological indices over the class of all cacti with some fixed parameters. For instance, some extremal results about the cacti can be found in the papers (Lu *et al.*, 2006; Ali *et al.*, 2014; Chen, 2016; Du *et al.*, 2015) and in the related references cited therein. In the present note, the cactus having the minimum *AZI* is determined among all the cacti with fixed number of vertices and cycles. Moreover, some structural properties of the tree(s) having the maximum *AZI* over the set of all trees with fixed number of vertices are reported.

2. The *AZI* of cacti

For $n \geq 4$, let $\mathcal{C}_{n,k}$ be the collection of all cacti with k cycles and n vertices. As usual, denote by S_n and P_n the star graph and path graph (respectively) on n vertices. A vertex of a graph is said to be pendent if it has degree one. Let $G^0(n,k) \in \mathcal{C}_{n,k}$ be the cactus obtained from S_n by adding k mutually independent edges between the pendent vertices (Figure 1). Note that $G^0(n,0) \cong S_n$.

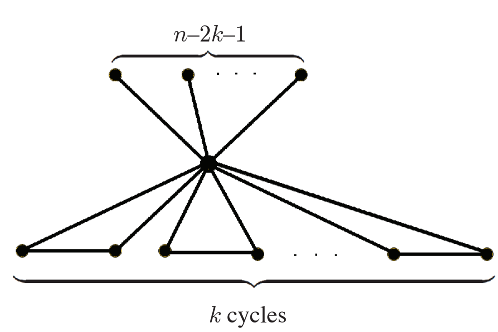

Fig. 1. The cactus $G^0(n,k)$.

Routine calculations show that

$$AZI(G^0(n,k)) = (n-2k-1)\left(\frac{n-1}{n-2}\right)^3 + 24k.$$

Let us take

$$F(n,k) = (n-2k-1)\left(\frac{n-1}{n-2}\right)^3 + 24k.$$

Note that the collection $\mathcal{C}_{n,0}$ consists of all trees on n vertices. Furtula *et al.* (2010) characterized the n-vertex tree having the minimum *AZI*:

Lemma 1. (Furtula *et al.*, 2010). *If T is any tree with $n \geq 3$ vertices, then*

$$AZI(T) \geq F(n,0).$$

The equality holds if and only if $T \cong G^0(n,0)$.

Observe that the class $\mathcal{C}_{n,1}$ consists of all unicyclic graphs on n vertices. The following result about the characterization of unicyclic graph having the minimum *AZI* is due to Huang *et al.* (2012):

Lemma 2. (Huang *et al.*, 2012). *If G is any unicyclic graph with $n \geq 4$ vertices, then*

$$AZI(G) \geq F(n,1).$$

The equality holds if and only if $G \cong G^0(n,1)$.

The main result of this note will be proved with the help of following lemma:

Lemma 3. *For fixed p, let*

$$f(x,y) = \left(\frac{xy}{x+y-2}\right)^3 - \left(\frac{(x-p)y}{x-p+y-2}\right)^3,$$

where $x \geq 2$, $x > p \geq 1$ and $y \geq 2$. The function $f(x,y)$ is increasing for y in the interval $[2,\infty)$.

Proof. Simple computations yield

$$\frac{\partial f(x,y)}{\partial y} = 3y^2\left[\frac{x^3(x-2)}{(x+y-2)^4} - \frac{(x-p)^3(x-p-2)}{(x-p+y-2)^4}\right]. \quad (1)$$

Note that if $0 < x-p \leq 2$ then $\frac{\partial f(x,y)}{\partial y}$ is positive and hence the desired result follows. Let us assume that $x-p > 2$ and $g(x,y) = \frac{x^3(x-2)}{(x+y-2)^4}$. The first order partial derivative of $g(x,y)$ with respect to x, can be written as

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

It can be easily verified that the function $h(x,y) = x(2y-3)-3y+6$ is increasing in both x and y for $x,y \geq 2$ and $h(2,2)$ is positive. Hence $\frac{\partial g(x,y)}{\partial x}$ is positive for all $x \geq 2$ and $y \geq 2$, which means that the function $g(x,y)$ is increasing in x. Therefore, from Equation (1), the desired result follows.

□

The following elementary result will also be helpful in proving the main result of the present note.

Lemma 4. *The function* $f(x) = \left(\frac{x}{x-1}\right)^3$ *is decreasing in the interval* $[2,\infty)$.

For a vertex u of a graph G, denote by $N_G(u)$ (the neighborhood of u) the set of all vertices adjacent with u. Now, we are in position to prove that the unique graph $G^0(n,k)$ has the minimum *AZI* among all cacti in the collection $\mathcal{C}_{n,k}$.

Theorem 1. *If G is any cactus belongs to the collection* $\mathcal{C}_{n,k}$, *then*

$$AZI(G) \geq F(n,k)$$

with equality if and only if $G \cong G^0(n,k)$.

Proof. We will prove the theorem by double induction on n and k. For $k=0$ and $k=1$, the result holds due to Lemma 1 and Lemma 2 respectively. Note that if $k \geq 2$ then $n \geq 5$. For $n=5$ there is only one cactus which is isomorphic to $G^0(5,2)$ and hence the theorem holds in this case. Let us assume that $G \in \mathcal{C}_{n,k}$ where $k \geq 2$ and $n \geq 6$. Then there are two possibilities.

Case 1. G does not contain any pendent vertex. In this case, there must exist three vertices u, v and w on some cycle of G such that u is adjacent with both the vertices v, w where $d_u = d_v = 2$ and $d_w = x \geq 3$. Here we consider two subcases.

Subcase 1.1. There is no edge between v and w. Note that the graph G' obtained from G by removing the vertex u and adding the edge vw, belongs to the collection $\mathcal{C}_{n-1,k}$. Bearing in mind the Lemma 4, inductive hypothesis and the fact $n \geq 6$, one have

$$AZI(G) - F(n,k) = AZI(G') + 8 - F(n,k)$$
$$\geq F(n-1,k) - F(n,k) + 8$$
$$= (n-2k-1)\left[\left(\frac{n-2}{n-3}\right)^3 - \left(\frac{n-1}{n-2}\right)^3\right]$$
$$+\left[8 - \left(\frac{n-2}{n-3}\right)^3\right] \geq 8 - \left(\frac{n-2}{n-3}\right)^3 > 0.$$

Subcase 1.2. There is an edge between v and w. Let G^* be the graph obtained from G by removing both the vertices u, v, then G^* belongs to the class $\mathcal{C}_{n-2,k-1}$. Let $N_G(w) = \{u, v, u_1, u_2, \ldots, u_{x-2}\}$. By virtue of Lemma 3, Lemma 4 and inductive hypothesis, one have

$$AZI(G) - F(n,k) = AZI(G^*) - F(n,k) + 24$$
$$+\sum_{i=1}^{x-2}\left[\left(\frac{x d_{u_i}}{x + d_{u_i} - 2}\right)^3 - \left(\frac{(x-2) d_{u_i}}{x + d_{u_i} - 4}\right)^3\right]$$
$$\geq F(n-2,k-1) - F(n,k) + 24$$
$$= (n-2k-1)\left[\left(\frac{n-3}{n-4}\right)^3 - \left(\frac{n-1}{n-2}\right)^3\right] \geq 0.$$

The equality $AZI(G) - F(n,k) = 0$ holds if and only if $G^* \cong G^0(n-2,k-1)$, $d_{u_i} = 2$ for all i (where $1 \leq i \leq x-2$) and $n-2k-1 = 0$.

Case 2. G has at least one pendent vertex. Let u_0 be the pendent vertex adjacent with a vertex v_0 and assume that $N_G(v_0) = \{u_0, u_1, u_2, \ldots, u_{y-1}\}$. Without loss of generality, one can assume that $d_{u_i} = 1$ for $0 \leq i \leq p-1$ and $d_{u_i} \geq 2$ for $p \leq i \leq y-1$. Let G^+ be the graph obtained from G by removing the pendent vertices $u_0, u_1, u_2, \ldots, u_{p-1}$, then $G^+ \in \mathcal{C}_{n-p,k}$ and hence one have

$$AZI(G) - F(n,k)$$
$$= AZI(G^+) + p\left(\frac{y}{y-1}\right)^3 - F(n,k)$$
$$+\sum_{i=p}^{y-1}\left[\left(\frac{y d_{u_i}}{y + d_{u_i} - 2}\right)^3 - \left(\frac{(y-p) d_{u_i}}{y + d_{u_i} - p - 2}\right)^3\right].$$

By virtu of Lemma 3 and inductive hypothesis, we have

$$AZI(G) - F(n,k) \geq F(n-p,k) - F(n,k) + p\left(\frac{y}{y-1}\right)^3, \quad (2)$$

with equality if and only if $G^+ \cong G^0(n-p,k)$ and $d_{u_i} = 2$ for all i (where $p \leq i \leq y-1$). From Lemma 4 and Inequality (2), it follows that

$$AZI(G) - F(n,k)$$
$$\geq (n-p-2k-1)\left[\left(\frac{n-p-1}{n-p-2}\right)^3 - \left(\frac{n-1}{n-2}\right)^3\right]$$
$$\geq 0,$$

with first equality if and only if $G^+ \cong G^0(n-p,k)$ and $y = n-1$, and the second equality holds if and only if $n-p-2k-1 = 0$. This completes the proof.

□

Note that $\frac{\partial F(n,k)}{\partial k} = -2\left(\frac{n-1}{n-2}\right)^3 + 24$ is positive for all $n \geq 4$, which means that $F(n,k)$ is increasing in k (where $k \geq 0$). Hence, $F(n,k)$ attains it minimum value at $k = 0$ and therefore from Theorem 1, one have:

Corollary 1. *If G is any cactus with* $n \geq 4$ *vertices, then*

$$AZI(G) \geq F(n,0)$$

with equality if and only if $G \cong G^0(n,0)$.

Now, we consider the problem of characterizing graph(s) having the maximum *AZI* over the collection $\mathcal{C}_{n,k}$. Let us start from considering the special case $k = 0$, that is $\mathcal{C}_{n,0}$ (which is the class of all n-vertex trees). It can be easily checked that for $n = 4,5,6$, the path P_n has the maximum *AZI* in $\mathcal{C}_{n,0}$ and for $n = 7,8,9$, all those n-vertex trees in which every edge is incident with at least one vertex of degree 2, have the maximum *AZI* in $\mathcal{C}_{n,0}$. Hence, the graph having the maximum *AZI* in the collection $\mathcal{C}_{n,0}$ needs not to be unique. Also, note that for the n-vertex tree T^+ depicted in Figure 2, one have

$$AZI(T^+) = \left(\frac{9}{4}\right)^3 + 8(n-2)$$

$$> 8(n-1) = AZI(P_n) \text{ for all } n \geq 10.$$

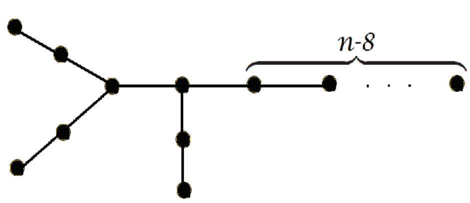

Fig. 2. The n-vertex tree T^+ where $n \geq 10$.

The above inequality suggests that the n-vertex tree (where $n \geq 10$) with the maximum *AZI* must be different fromthe path P_n. At this time, the problem of finding graph(s) having the maximum *AZI* over the class $\mathcal{C}_{n,0}$ (and hence over the class $\mathcal{C}_{n,k}$) seems to be hard and we leave it for future work. However, here we prove some results related to the structure of the n-vertex tree(s) having the maximum *AZI*. In order to prove these results, we need the following lemma.

Lemma 5 (Huang *et al.*, 2012). *If* $\Psi(x,y) = \left(\frac{xy}{x+y-2}\right)^3$, *then*

i). $\Psi(1,y)$ is decreasing for $y \geq 2$.

ii). $\Psi(2,y) = 8$ for all $y \geq 2$.

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

To proceed, we require the following definitions which are taken from the paper (Gutman *et al.*, 2012):

- A pendent vertex adjacent with a vertex having degree greater than 2 is called star-type pendent vertex.
- A path $v_1v_2 \ldots v_{l+1}$ of length l in a graph G is called pendent if one of the degrees $d_{v_1}, d_{v_{l+1}}$ is 1 and other is greater than 2, and $d_{v_i} = 2$ for all i where $2 \leq i \leq l$.
- A path $v_1v_2 \ldots v_{l+1}$ of length l in a graph G is called internal if both the degrees $d_{v_1}, d_{v_{l+1}}$ are greater than 2 and $d_{v_i} = 2$ for all i where $2 \leq i \leq l$.

Theorem 2. *For* $n \geq 10$, *let* $T^* \in \mathcal{C}_{n,0}$ *be the tree with the maximum AZI. Then*

i). T^* does not contain any internal path of length greater than 1.

ii). T^* does not contain any pendent path of length greater than 3.

iii). T^* contains at most one pendent path of length 3.

Proof. i). Suppose to the contrary that T^* contains the internal path $v_1v_2 \ldots v_{l+1}$ of length $l \geq 2$ where $d_{v_1}, d_{v_{l+1}} \geq 3$. We consider two cases.

Case 1. If T^* contains at least one star-type pendent vertex. Let u be a star-type pendent vertex adjacent with a vertex v (then $d_v \geq 3$) and suppose that $T^{(1)}$ is the tree obtained from T^* by moving the vertex v_2 on the edge uv and adding the edge v_1v_3. Observe that both the trees $T^{(1)}$ and T^* have same degree sequence. By virtue of Lemma 5(i) and Lemma 5(ii), we have

$$AZI(T^*) - AZI(T^{(1)})$$

$$= \Psi(d_{v_1}, d_{v_2}) + \Psi(d_{v_2}, d_{v_3}) + \Psi(d_u, d_v)$$

$$-\Psi(d_{v_1}, d_{v_3}) - \Psi(d_u, d_{v_2}) - \Psi(d_{v_2}, d_v)$$

$$= \Psi(1, d_v) - \Psi(d_{v_1}, d_{v_3}) < 0,$$

which is a contradiction to the maximality of $AZI(T^*)$.

Case 2. If T^* does not contain any star-type pendent vertex. Suppose that $T^{(2)}$ is the tree obtained from T^* by moving the vertex v_2 on any pendent edge and adding the edge v_1v_3. If $l = 2$ then by using Lemma 5(i) and Lemma 5. (iii), one have

$$AZI(T^*) - AZI\big(T^{(2)}\big)$$

$$= \Psi\big(d_{v_1}, d_{v_2}\big) + \Psi\big(d_{v_2}, d_{v_3}\big)$$

$$-\Psi\big(d_{v_1}, d_{v_3}\big) - 8$$

$$= \Psi(d_{v_1}, 2) - \Psi(d_{v_1}, d_{v_3}) < 0,$$

which is a contradiction.

If $l \geq 3$, then it can be easily checked that $AZI(T^*) - AZI(T^{(2)}) = 0$. After repeating the above transformation (defined in *Case 2*) sufficient number of times, one arrives at a tree $T^{(3)}$ such that $AZI(T^*) - AZI(T^{(3)}) < 0$. This contradicts the maximality of $AZI(T^*)$, which completes the proof of Part (i).

ii). Let us suppose to the contrary that T^* contains the pendent path $v_1v_2...v_{l+1}$ of length $l \geq 4$ where $d_{v_1} = 1$. We consider two cases.

Case 1. If T^* contains at least one star-type pendent vertex. Let u be a star-type pendent vertex adjacent with a vertex v. Let $T^{(1)}$ be the tree obtained from T^* by moving the vertex v_2 on the edge uv and adding the edge v_1v_3. Bearing in mind the Lemma 5(i), Lemma 5(ii) and the fact $d_v \geq 3$, one have

$$AZI(T^*) - AZI\big(T^{(1)}\big)$$

$$= \Psi(d_{v_1}, d_{v_2}) + \Psi(d_{v_2}, d_{v_3}) + \Psi(d_u, d_v)$$

$$-\Psi(d_{v_1}, d_{v_3}) - \Psi(d_u, d_{v_2}) - \Psi(d_{v_2}, d_v)$$

$$= \Psi(1, d_v) - 8 < 0,$$

which is a contradiction to the maximality of $AZI(T^*)$.

Case 2. If T^* does not contain any star-type pendent vertex. Suppose that $w \in V(T^*)$ has the maximum degree and $N_{T^*}(w) = \{w_1, w_2, ..., w_\Delta\}$. Note that $d_{w_i} \geq 2$ for all i where $1 \leq i \leq \Delta$.

Subcase 2.1 If at least one neighbor of w has degree greater than 2. Suppose that $T^{(2)}$ is the tree obtained from T^* by removing the edge v_2v_3 and adding the edge v_2w. By using Lemma 5(ii) and Lemma 5(iii), one have

$$AZI(T^*) - AZI\big(T^{(2)}\big)$$

$$= \Psi(d_{v_2}, d_{v_3}) + \Psi(d_{v_3}, d_{v_4}) + \sum_{i=1}^{\Delta} \Psi(d_w, d_{w_i})$$

$$-\Psi\big(d_{v_2}, d_w + 1\big) - \Psi\big(d_{v_3} - 1, d_{v_4}\big)$$

$$-\sum_{i=1}^{\Delta} \Psi(d_w + 1, d_{w_i})$$

$$= \sum_{i=1}^{\Delta} \big[\Psi(d_w, d_{w_i}) - \Psi(d_w + 1, d_{w_i})\big] < 0,$$

which is again a contradiction.

Subcase 2.2 If $d_{w_i} = 2$ for all i where $1 \leq i \leq \Delta$. Then Part (i) suggests that T^* must be a starlike tree. Note that each branch of T^* has length at least 2 and $w = v_{l+1}$ (in this case), hence

$$AZI(T^*) = 8(n-1)$$

$$< \left(\frac{9}{4}\right)^3 + 8(n-2) = AZI(T^+)$$

where the tree T^+ is depicted in the Figure 2. This is a contradiction to the maximality of $AZI(T^*)$. This completes the proof of Part (ii).

iii). Suppose to the contrary that T^* contains two pendent paths $v_1v_2v_3v_4$ and $u_1u_2u_3u_4$ of length three, where $d_{v_1} = d_{u_1} = 1$. Then for the tree T' obtained from $T^{(*)}$ by deleting the edge v_1v_2 and adding the edge v_1u_1, one have $AZI(T^*) = AZI(T')$, which means that T' has also the maximum *AZI*. But, T' contains a pendent path of length 4, namely $v_1u_1u_2u_3u_4$. This contradicts the Part (ii).

□

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مذكرة حول دليل زغرب الموسع للصبار الذي له عدد ثابت من الرؤوس و الدورات

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خلاصة

تبين الدراسات الحديثة أن دليل زغرب الموسع (AZI) يمتلك أفضل مقدرة ترابطية من بين الدلائل الطوبولوجية المعروفة و التي تستخدم للتنبؤ بالخصائص الفيزيوكوكيميائية لبعض أنواع الجزئيات. لذا يصبح من الأهمية بمكان أن ندرس الخصائص الرياضية للدلائل AZI، و خاصة الحدود و الخصائص للعناصر التطرفية بين أنواع البيانات المعروفة. لكل $n \geq 4$ لتكن $\mathcal{C}_{n,k}$ مجموعة الصبارات التي لها k دورات و n رؤوس. نقوم بمذكرتنا هذه بإيجاد خصائص عناصر $\mathcal{C}_{n,k}$ التي تأخذ دلائلها AZI قيمها الصغرى. كما ندرس أيضاً الخصائص البنيوية للبيانات التي تأخذ دلائلها AZI قيمها العظمى.