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 $C_{n,k}$ be the collection of all cacti with $k$ cycles and $n$ vertices. In this note, the element of $C_{n,k}$ having the minimum AZI is characterized. Some structural properties of the graph(s) having the maximum AZI over the collection $C_{n,0}$ 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:

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

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):

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

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 $C_{n,k}$ 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 $G^0(n,k) \in C_{n,k}$ be the cactus obtained from $S_n$ by adding $k$ mutually independent edges between the pendent vertices (Figure 1). Note that $G^0(n,0) \equiv S_n$.

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 $C_{n,0}$ 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 $T \equiv G^0(n,0)$.

Observe that the class $C_{n,1}$ 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 $G \equiv G^0(n,1)$.

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

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

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

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

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

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

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

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

**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 $G \in C_{n,k}$ 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 $C_{n-1,k}$. Bearing in mind the Lemma 4, inductive hypothesis and the fact $n \geq 6$, one have

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

**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 $C_{n-2,k-1}$. 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

$$AZI(G) - F(n,k) = AZI(G') - F(n,k) + 24
+ \sum_{i=1}^{x-2} \left[\frac{(x-2)d_{u_i}}{x+d_{u_i}-2} - \frac{(x-2)d_{u_i}}{x+d_{u_i}-4}\right] \geq F(n-2,k-1) - F(n,k) + 24
= (n-2k-1)\left[\frac{(n-3)^3}{n-4} - \frac{(n-1)^3}{n-2}\right] \geq 0.$$
with first equality if and only if \( G^+ \equiv G^0(n-p,k) \) and \( y = n-1 \), and the second equality holds if and only if \( n-p-2k-1 = 0 \). This completes the proof.

\[\square\]

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 its 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 \( G \equiv G^0(n,0) \).

Now, we consider the problem of characterizing graph(s) having the maximum \( AZI \) over the collection \( C_{n,k} \). Let us start from considering the special case \( k = 0 \), that is \( C_{n,0} \) (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 \( C_{n,0} \) 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 \( C_{n,0} \). Hence, the graph having the maximum \( AZI \) in the collection \( C_{n,0} \) 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.](image)

The above inequality suggests that the \( n \)-vertex tree (where \( n \geq 10 \)) with the maximum \( AZI \) must be different from the path \( P_n \). At this time, the problem of finding graph(s) having the maximum \( AZI \) over the class \( C_{n,0} \) (and hence over the class \( C_{n,k} \)) 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 pendant vertex adjacent with a vertex having degree greater than 2 is called star-type pendant vertex.

- A path \( v_1 v_2 \ldots v_{l+1} \) of length \( l \) in a graph \( G \) is called pendant 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 \( v_1 v_2 \ldots v_{l+1} \) of length \( l \) in a graph \( G \) is called internal if both the degrees \( d_{v_2}, d_{v_{l+1}} \) 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 \( T^* \in C_{n,0} \) 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 pendant path of length greater than 3.

iii). \( T^* \) contains at most one pendant path of length 3.

**Proof.** i). Suppose to the contrary that \( T^* \) contains the internal path \( v_1 v_2 \ldots v_{l+1} \) 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 pendant vertex. Let \( u \) be a star-type pendant 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 \( v_1 v_3 \). 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

\[ AZI(T^*) - AZI(T^{(1)}) = \Psi(d_{v_1},d_{v_2}) + \Psi(d_{v_2},d_{v_3}) + \Psi(d_u,d_v) - \Psi(d_{v_1},d_{v_2}) - \Psi(d_{v_2},d_v) = \Psi(1,d_v) - \Psi(d_{v_1},d_{v_3}) < 0, \]

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

**Case 2.** If \( T^* \) does not contain any star-type pendant vertex. Suppose that \( T^{(2)} \) is the tree obtained from \( T^* \) by
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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

\[
AZI(T^*) - AZI(T^{(2)}) = \Psi(d_{v_1}, d_{v_2}) + \Psi(d_{v_2}, d_{v_3}) - \Psi(d_{v_1}, d_{v_3}) - 8
\]

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 \(v_1v_2\ldots v_{i+1}\) of length \(l \geq 4\) where \(d_{v_i} = 1\). 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 one have

\[
AZI(T^*) - AZI(T^{(1)}) = \Psi(d_{v_1}, d_{v_2}) + \Psi(d_{v_2}, d_{v_3}) + \Psi(d_u, d_v) - \Psi(d_{v_1}, d_{v_3}) - \Psi(d_u, d_v) - \Psi(d_{v_2}, d_v)
\]

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 \(N_T(w) = \{v_1, v_2, \ldots, v_D\}\). Note that \(d_{v_i} \geq 2\) for all \(i \geq 1\) where \(1 \leq i \leq D\).

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

\[
AZI(T^{(2)}) - AZI(T^*) = \Psi(d_{v_2}, d_{v_3}) + \Psi(d_{v_2}, d_{v_4}) + \sum_{i=1}^{A} \Psi(d_{w_i}, d_{w_i}) - \Psi(d_{v_2}, d_{w_i}) - \Psi(d_{v_3}, d_{v_4}) - \sum_{i=1}^{A} \Psi(d_{w_i}, d_{w_i})
\]

which is again a contradiction.

Subcase 2.2 If \(d_{w_i} = 2\) for all \(i \leq i \leq A\). Then Part (i) suggests that \(T^*\) must be a starlike tree. Note that each branch of \(T^*\) has length at least 2 and \(w = v_{i+1}\) (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 \(d_{v_i} = d_{u_i} = 1\). Then for the tree \(T'\) obtained from \(T^*\) by deleting the edge \(v_1v_2\) and adding the edge \(v_1u_4\), 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).

\[\square\]

References


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مذكرة حول دليل زغرب الموسع للصابر الذي له عدد ثابت من الرؤوس والدورات

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خلاصة

تين الدراسات الحديثة أن دليل زغرب الموسع (AZI) ميثل أفضل مقددة ترابطية من بين الدلالات الطوبولوجية المعروفة و التي تستخدم للتنبؤ بالخصائص الفيزيوكيميائية لبعض أنواع الجزيئات. لذا يصبح من الأهمية يمكن أن ندرس الخصائص الرياضية للدلائل، و خاصة الحدود و الخصائص للعناصر التفاضلية بين أنواع البيانات المعروفة. لكل k دورات C_n,k تمكن n ≥ 4 لمجموعة الصابرات التي لها k رؤوس. نقوم مذكرون هذه بإيجاد خصائص عناصر AZI AGI التي تأخذ دلالاتها n و البيئية للبيانات التي تأخذ دلالاتها AZI AGI. كما ندرس أيضاً الخصائص غير المعروفة.