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THE AUGMENTED ZAGREB INDEX, VERTEX CONNECTIVITY AND MATCHING NUMBER OF GRAPHS

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Abstract. Let $\Gamma_{n,\kappa}$ be the class of all graphs with $n \geq 3$ vertices and $\kappa \geq 2$ vertex connectivity. Denote by $\Upsilon_{n,\beta}$ the family of all connected graphs with $n \geq 4$ vertices and matching number β where $2 \leq \beta \leq \lfloor \frac{n}{2} \rfloor$. In the classes of graphs $\Gamma_{n,\kappa}$ and $\Upsilon_{n,\beta}$, the elements having maximum augmented Zagreb index are determined.

Keywords: Topological index, augmented Zagreb index, vertex connectivity, matching number.
MSC(2010): Primary: 65F05; Secondary: 46L05, 11Y50.

1. Introduction

Let G denote a simple, finite and undirected graph with vertex set $V(G)$ and edge set $E(G)$ such that $|V(G)| = n$, and $|E(G)| = m$. Suppose that d_u is the degree of the vertex $u \in V(G)$ and uv is the edge connecting the vertices u and v. In molecular graphs, vertices correspond to atoms while edges represent covalent bonds between atoms [19]. The numbers reflecting certain structural features of a molecule which are obtained from the corresponding molecular graph are called "molecular structure descriptors" or simply "topological indices" [22]. A great variety of such indices are studied and used in theoretical chemistry [6, 13, 22, 23]. Among which the atom-bond connectivity (ABC) index was proposed by Estrada *et al.* [9]. This index is defined as

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

For chemical applicability of ABC index, see the papers [8, 9, 15] and for more details see the survey [12], recent papers [4, 5, 7, 10, 17, 20] and the references cited therein.

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Inspired by the ABC index, Furtula *et al.* [11] introduced a new topological index known as the augmented Zagreb index (AZI) defined as:

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

AZI is a valuable predictive index in the study of the heat of formation in heptanes and octanes [11]. Gutman and Tošović [14] recently tested the correlation abilities of 20 vertex-degree-based topological indices for the case of standard heats of formation and normal boiling points of octane isomers, and they found that AZI yields the best results. Hence, it is natural and interesting to study the mathematical properties of the AZI.

The union $H \cup K$ of two graphs H and K is the graph with the vertex set $V(H) \cup V(K)$ and the edge set $E(H) \cup E(K)$. The join $H + K$ of two graphs H and K is the graph with the vertex set $V(H) \cup V(K)$ and the edge set $E(H) \cup E(K) \cup \{uv | u \in V(H), v \in V(K)\}$. The vertex connectivity (commonly referred to as connectivity) $\kappa(G) = \kappa$ of a graph G is the minimum number of vertices whose removal gives rise to a disconnected or trivial graph [16]. If G is disconnected then $\kappa(G) = 0$. A matching in a graph is a set of pairwise non-adjacent edges [3]. A maximum matching is one which covers as many vertices as possible. The matching number $\beta(G) = \beta$ of a graph G is the number of edges in a maximum matching. A component of a graph is odd (respectively even) if it has an odd (respectively even) number of vertices. If a graph G has n vertices and $o(G)$ is the number of odd components, then by Tutte-Berge formula [21],

$$n - 2\beta(G) = \max\{o(G - A) - |A| : A \subset V(G)\}. \tag{1.1}$$

For undefined notations and terminologies in graph theory, see [3, 16].

Furtula *et al.* [11] studied the extremal properties of AZI for trees and chemical trees. Huang *et al.* [18] gave various bounds (lower and upper) on AZI for several families of connected graphs and they proved that AZI of a connected graph G strictly increases by adding an edge in G. Wang *et al.* [24] established some bounds on AZI of connected graphs and improved some results of [11, 18]. In [1], the authors derived some inequalities between AZI and several other vertex-degree-based topological indices. In [2], the same authors obtain tight upper bounds for AZI of chemical bicyclic and unicyclic graphs. In this article, sharp upper bounds on AZI of a graph G are given in terms of its order, vertex connectivity or matching number.

2. The augmented Zagreb index and vertex connectivity

Let us denote by $\Gamma_{n,\kappa}$ the collection of all graphs with $n \geq 3$ vertices and $\kappa \geq 2$ vertex connectivity. In this section, we will prove that among all graphs in the collection $\Gamma_{n,\kappa}$, the graph $K_\kappa + (K_1 \cup K_{n-\kappa-1})$ has the maximum AZI. To proceed, we need the following lemma.

Lemma 2.1. *Let* $\phi_1(x) = \frac{x(x-1)}{2}\left(\frac{(x+a-1)^2}{2x+2a-4}\right)^3, \phi_2(x) = ax\left(\frac{(n-1)(x+a-1)}{x+n+a-4}\right)^3$ *and* $\phi(x) = \phi_1(x) + \phi_2(x)$ *where* $x \in [1, \infty)$*,* $a \geq 2$ *and* $a, n \in \mathbb{N}$*. Let* $n' - a - x, n - a - x \in [1, \infty)$ *and* $n' \in \mathbb{N}$ *such that* $n \geq n'$*. Then* $\phi(x) + \phi(n' - a - x)$ *is monotonously decreasing for* $x \in [1, \frac{n'-a}{2}]$ *and monotonously increasing for* $x \in (\frac{n'-a}{2}, n' - a - 1]$*. Moreover, the maximum value of* $\phi(x) + \phi(n' - a - x)$ *in the interval* $[1, n' - a - 1]$ *is* $\phi(1) + \phi(n' - a - 1)$*.*

Proof. After routine calculations, one arrives at

$$\phi_1^{''}(x) = \frac{(x+a-1)^4\phi_3(x)}{8(x+a-2)^5} \tag{2.1}$$

where

$$\begin{aligned}\phi_3(x) &= 10x^4 + (28a-66)x^3 + (27a^2 - 123a + 145)x^2 \\ &\quad + (2a^2(5a-33) + 146a - 111)x + (a-1)(a-2)(a^2 - 6a + 11).\end{aligned}$$

Note that for all $a \geq 2$ and $x \geq 1$, the following inequalities hold:

$$(40x + 84a - 198)x^2 \geq 10, \ (290 + 6a(9a - 41))x \geq 14,$$

$$2a(73 + a(5a - 33)) - 111 \geq -3.$$

Hence, it follows that

$$\begin{aligned}\phi_3^{'}(x) &= (40x + 84a - 198)x^2 + (290 + 6a(9a-41))x \\ &\quad + 2a(73 + a(5a-33)) - 111 > 0,\end{aligned}$$

which implies that $\phi_3(x)$ is monotonously increasing and consequently $\phi_3(x) \geq \phi_3(1) = a^4 + a^3 - 8a^2 + 6a > 0$ as $a \geq 2$. Therefore, from Equation (2.1) it follows that $\phi_1^{''}(x) > 0$. Moreover, it can be easily verified that

$$\phi_2^{''}(x) = \frac{6a(n-3)(n-1)^3 + (x+a-1)((2n+a-7)x + (a-1)(n+a-4))}{(x+n+a-4)^5} > 0$$

and consequently one has $\phi^{''}(x) = \phi_1^{''}(x) + \phi_2^{''}(x) > 0$. It means that $\phi^{'}(x)$ is monotonously increasing in the interval $[1, n'-a-1]$. Therefore, if $x \leq n'-a-x$ then

$$(\phi(x) + \phi(n'-a-x))^{'} = \phi^{'}(x) - \phi^{'}(n'-a-x) \leq 0,$$

and if $x > n' - a - x$ then

$$(\phi(x) + \phi(n'-a-x))^{'} = \phi^{'}(x) - \phi^{'}(n'-a-x) > 0.$$

□

We also need the following result.

Lemma 2.2. (*[18]*) *Let G be a connected graph with $n \geq 3$ vertices, and $G \ncong K_n$. Then*

$$AZI(G) < AZI(G+e),$$

where $e \notin E(G)$.

Now, we are in a position to prove the main result of this section.

Theorem 2.3. *If G is a graph belongs to the class $\Gamma_{n,\kappa}$, then*

$$\begin{aligned} AZI(G) \quad \leq \quad & \frac{\kappa(\kappa-1)}{16}\left(\frac{(n-1)^2}{n-2}\right)^3 + \kappa^4\left(\frac{n-1}{n+\kappa-3}\right)^3 \\ & + \frac{(n-\kappa-1)(n-\kappa-2)}{16}\left(\frac{(n-2)^2}{n-3}\right)^3 \\ & + \kappa(n-\kappa-1)\left(\frac{(n-2)(n-1)}{2n-5}\right)^3, \end{aligned}$$

the equality holds if and only if $G \cong K_\kappa + (K_1 \cup K_{n-\kappa-1})$.

Proof. If $G \cong K_n$, then $\kappa = n-1$ and hence $K_\kappa + (K_1 \cup K_{n-\kappa-1}) \cong K_n$, so the result is true in this case. If $G \ncong K_n$, then $2 \leq \kappa \leq n-2$. Let $G' \ncong K_n$ be a member of the collection $\Gamma_{n,\kappa}$ with the maximum AZI. Let A be a $\kappa-$element subset of $V(G')$ such that $G' - A$ is disconnected. Then the graph $G' - A$ has only two components (if $G' - A$ has more than two components. Let $G' - A + e$ be a graph obtained from $G' - A$ by adding the edge e between any two components of $G' - A$. Then $\kappa(G') = \kappa(G'+e)$ but $AZI(G') < AZI(G'+e)$, a contradiction to the definition of of G'). Let G_1, G_2 be the components of the graph $G' - A$ such that $|V(G_1)| = n_1, |V(G_2)| = n_2$. Then from Lemma 2.2 and definition of G', it follows that $G_1, G_2, G' - (V(G_1) \cup V(G_2))$ are complete graphs and each vertex of A must be adjacent with all vertices of G_1 and G_2. Hence $G' \cong K_\kappa + (K_{n_1} \cup K_{n_2})$. If $u \in A, v \in V(G_1), w \in V(G_2)$, then

$$d_u = n-1, d_v = n_1 + \kappa - 1, d_w = n_2 + \kappa - 1.$$

By using definition of AZI, one have

$$\begin{aligned} AZI(G') \quad = \quad & \frac{\kappa(\kappa-1)}{16}\left(\frac{(n-1)^2}{n-2}\right)^3 + \frac{n_1(n_1-1)}{2}\left(\frac{(n_1+\kappa-1)^2}{2n_1+2\kappa-4}\right)^3 \\ & + \kappa n_1\left(\frac{(n-1)(n_1+\kappa-1)}{n_1+\kappa+n-4}\right)^3 + \frac{n_2(n_2-1)}{2}\left(\frac{(n_2+\kappa-1)^2}{2n_2+2\kappa-4}\right)^3 \\ & + \kappa n_2\left(\frac{(n-1)(n_2+\kappa-1)}{n_2+\kappa+n-4}\right)^3, \end{aligned}$$

which is equivalent to

$$
\begin{aligned}
AZI(G') &= \frac{\kappa(\kappa-1)}{16}\left(\frac{(n-1)^2}{n-2}\right)^3 + \phi(n_1) + \phi(n_2) \\
&= \frac{\kappa(\kappa-1)}{16}\left(\frac{(n-1)^2}{n-2}\right)^3 + \phi(n_1) + \phi(n-\kappa-n_1),
\end{aligned}
$$

where $\phi(x)$ is defined in Lemma 2.1. By Lemma 2.1 and definition of G', one gets

$$
\begin{aligned}
AZI(G') &= \frac{\kappa(\kappa-1)}{16}\left(\frac{(n-1)^2}{n-2}\right)^3 + \phi(1) + \phi(n-\kappa-1) \\
&= \frac{\kappa(\kappa-1)}{16}\left(\frac{(n-1)^2}{n-2}\right)^3 + \kappa^4\left(\frac{n-1}{n+\kappa-3}\right)^3 \\
&\quad + \frac{(n-\kappa-1)(n-\kappa-2)}{16}\left(\frac{(n-2)^2}{n-3}\right)^3 \\
&\quad + \kappa(n-\kappa-1)\left(\frac{(n-2)(n-1)}{2n-5}\right)^3 \\
&= AZI(K_\kappa + (K_1 \cup K_{n-\kappa-1})).
\end{aligned}
$$

□

Bearing in mind Theorem 2.3 and Lemma 2.2, we have a stronger version of the Theorem 2.3.

Theorem 2.4. *If G is a graph with $n \geq 3$ vertices and vertex connectivity κ' where $2 \leq \kappa' \leq \kappa$, then*

$$
\begin{aligned}
AZI(G) &\leq \frac{\kappa(\kappa-1)}{16}\left(\frac{(n-1)^2}{n-2}\right)^3 + \kappa^4\left(\frac{n-1}{n+\kappa-3}\right)^3 \\
&\quad + \frac{(n-\kappa-1)(n-\kappa-2)}{16}\left(\frac{(n-2)^2}{n-3}\right)^3 \\
&\quad + \kappa(n-\kappa-1)\left(\frac{(n-2)(n-1)}{2n-5}\right)^3,
\end{aligned}
$$

the equality holds if and only if $G \cong K_\kappa + (K_1 \cup K_{n-\kappa-1})$.

3. The augmented Zagreb index and matching number

Let us denote by $\Upsilon_{n,\beta}$, the class of all connected graphs with $n \geq 4$ vertices and matching number β, where $2 \leq \beta \leq \lfloor \frac{n}{2} \rfloor$. In this section, we characterize the graph with the maximum AZI belongs to the calss $\Upsilon_{n,\beta}$.

Lemma 3.1. *Let* $H_1 = K_\beta + \bigcup_{i=1}^{r} K_{n_i}$ *and*

$H_2 = K_\beta + (K_{n_1} \cup ... \cup K_{n_{s-1}} \cup K_{n_s - 1} \cup K_{n_{s+1}} \cup ... \cup K_{n_{t-1}} \cup K_{n_t + 1} \cup K_{n_{t+1}} \cup ... \cup K_{n_r})$

where $1 \leq s < t \leq r,\ n_t \geq n_s \geq 2;\ r, \beta \geq 2, \sum_{i=1}^{r} n_i + \beta = n,\ r, \beta, n_i \in \mathbb{N}$. *Then*

$$AZI(H_2) > AZI(H_1).$$

Proof. Let $\Theta = AZI(H_2) - AZI(H_1)$. Then By using the definitions of AZI and $\phi(x)$, one has

$$\begin{aligned}
\Theta &= \frac{(n_s-1)(n_s-2)}{2}\left(\frac{(n_s+\beta-2)^2}{2n_s+2\beta-6}\right)^3 \\
&\quad +\beta(n_s-1)\left(\frac{(n-1)(n_s+\beta-2)}{n_s+n+\beta-5}\right)^3 \\
&\quad +\frac{n_t(n_t+1)}{2}\left(\frac{(n_t+\beta)^2}{2n_t+2\beta-2}\right)^3 + \beta(n_t+1)\left(\frac{(n-1)(n_t+\beta)}{n_t+n+\beta-3}\right)^3 \\
&\quad -\frac{n_s(n_s-1)}{2}\left(\frac{(n_s+\beta-1)^2}{2n_s+2\beta-4}\right)^3 - \beta n_s\left(\frac{(n-1)(n_s+\beta-1)}{n_s+n+\beta-4}\right)^3 \\
&\quad -\frac{n_t(n_t-1)}{2}\left(\frac{(n_t+\beta-1)^2}{2n_t+2\beta-4}\right)^3 - \beta n_t\left(\frac{(n-1)(n_t+\beta-1)}{n_t+n+\beta-4}\right)^3 \\
&= \phi(n_s-1) + \phi(n_t+1) - \phi(n_s) - \phi(n_t).
\end{aligned}$$

Let us take $N = n_s + n_t + \beta$. Then $n_t \geq n_s$ implies that $n_s \leq \frac{N-\beta}{2}$ and hence by using Lemma 2.1, we have

$$\Theta = \phi(n_s-1) + \phi(N-\beta-(n_s-1)) - (\phi(n_s) + \phi(N-\beta-n_s)) > 0$$

□

Now, we are ready to prove the main result of this section.

Theorem 3.2. *Let* G *be a graph belongs to the class* $\Upsilon_{n,\beta}$.

(i) *If* $\beta = \lfloor \frac{n}{2} \rfloor$, *then* $AZI(G) \leq \frac{n(n-1)^7}{16(n-2)^3}$, *the equality holds if and only if* $G \cong K_n$.

(ii) *If* $2 \leq \beta < \lfloor \frac{n}{2} \rfloor$, *then* $AZI(G) \leq \frac{\beta(\beta-1)(n-1)^6}{16(n-2)^3} + \beta^4(n-\beta)\left(\frac{n-1}{n+\beta-3}\right)^3$, *the equality holds if and only if* $G \cong K_\beta + \overline{K_{n-\beta}}$.

Proof. Part (i) is a direct consequence of Lemma 2.2. To prove the part (ii), let us denote by $\Upsilon^1_{n,\beta}$ the collection of all graphs belongs to $\Upsilon_{n,\beta}$ for which

$2 \leq \beta < \lfloor \frac{n}{2} \rfloor$. Let G' be a member of $\Upsilon^1_{n,\beta}$ having the maximum AZI. Then by Tutte-Berge formula (1.1) there must be a set $B_1 \subset V(G')$ such that

$$n - 2\beta = \max\{o(G-B) - |B| : B \subset V(G')\} = o(G' - B_1) - |B_1|.$$

Let us take $|B_1| = b$ and $o(G' - B_1) = r$. Then $n - 2\beta = r - b$ and $n \geq r + b$ implies that $\beta \geq b$. If $b = 0$, then $n - 2\beta = r = 0$ or 1 because G' is connected. In both cases, $\beta = \lfloor \frac{n}{2} \rfloor$, a contradiction. Hence $b \geq 1$, which implies that $r \geq 3$.

Suppose that $G_1, G_2, G_3, \ldots, G_r$ be the all odd components of $G' - B_1$. We claim that $G' - B_1$ has no even component(s). Contrarily suppose that G_{r+1} be an even component of $G' - B_1$. Let G^+ be the graph obtained from G' by adding an edge e between G_1 and G_{r+1}. Then $\beta(G^+) \geq \beta(G')$. But

$$n - 2\beta(G^+) \geq o(G^+ - B_1) - |B_1| = o(G' - B_1) - |B_1| = n - 2\beta(G'),$$

which implies $\beta(G^+) \leq \beta(G')$ and hence $\beta(G^+) = \beta(G')$. On the other hand, from the Lemma 2.2 it follows that $AZI(G^+) > AZI(G')$, a contradiction to the definition of G'.

Let $|V(G_i)| = n_i$ where $i = 1, 2, \ldots, r$. Without loss of generality, we can assume that $n_r \geq n_{r-1} \geq \ldots \geq n_1$. By using Lemma 2.2, we deduce that all the graphs $G_1, G_2, G_3, \ldots, G_r, G' - (\bigcup_{i=1}^r V(G_i))$ are complete and each vertex of B_1 is adjacent with all vertices of $G_1, G_2, G_3, \ldots, G_r$. Hence $G' \cong K_b + (\bigcup_{i=1}^r K_{n_i})$. Now, we have the following three possibilities:

Case 1. If $n_r = 1$, then $\beta = b$ and

$$G' \cong K_b + \left(\bigcup_{i=1}^{r} K_{n_i}\right) \cong K_b + \overline{K_r} \cong K_b + \overline{K_{n-2\beta+b}} \cong K_\beta + \overline{K_{n-\beta}}.$$

Case 2. If $n_i = 1$ for $i = 1, 2, \ldots, r-1$ and $n_r \geq 3$. Then we have

$$G' \cong K_b + \left(\bigcup_{i=1}^{r} K_{n_i}\right) \cong K_b + \left(\overline{K_{r-1}} \cup K_{n_r}\right) \cong K_b + \left(\overline{K_{n-2\beta+b-1}} \cup K_{2\beta-2b+1}\right).$$

But $K_b + \left(\overline{K_{n-2\beta+b-1}} \cup K_{2\beta-2b+1}\right)$ is a spanning subgraph of $K_\beta + \overline{K_{n-\beta}}$ and hence from Lemma 2.2, it follows that $AZI(G') < AZI(K_\beta + \overline{K_{n-\beta}})$, a contradiction to the definition of G'.

Case 3. If there are some $i, j \in \{1, 2, \ldots, r\}$ such that $n_j \geq n_i \geq 3$. Then by using Lemma 3.1 and Lemma 2.2, we have

$$\begin{aligned} AZI(G') &= AZI\left(K_b + \left(\bigcup_{i=1}^{r} K_{n_i}\right)\right) \\ &< AZI\left(K_b + \left(\overline{K_{n-2\beta+b-1}} \cup K_{2\beta-2b+1}\right)\right) \\ &< AZI\left(K_\beta + \overline{K_{n-\beta}}\right), \end{aligned}$$

again a contradiction to the definition of G'.

In the last two cases, contradiction is obtained and only the case 1 is true. Hence $G' \cong K_\beta + \overline{K_{n-\beta}}$ and by simple calculations, one has

$$AZI(G') = \frac{\beta(\beta-1)(n-1)^6}{16(n-2)^3} + \beta^4(n-\beta)\left(\frac{n-1}{n+\beta-3}\right)^3.$$

□

Keeping in view of the Theorem 3.2 and Lemma 2.2, we have the stronger version of the Theorem 3.2.

Theorem 3.3. *Let G be a graph with $n \geq 4$ vertices and matching number β', where $2 \leq \beta' \leq \beta \leq \lfloor \frac{n}{2} \rfloor$.*

(i) *If $\beta = \lfloor \frac{n}{2} \rfloor$, then $AZI(G) \leq \frac{n(n-1)^7}{16(n-2)^3}$, the equality holds if and only if $G \cong K_n$.*

(ii) *If $2 \leq \beta' \leq \beta < \lfloor \frac{n}{2} \rfloor$, then $AZI(G) \leq \frac{\beta(\beta-1)(n-1)^6}{16(n-2)^3} + \beta^4(n-\beta)\left(\frac{n-1}{n+\beta-3}\right)^3$, the equality holds if and only if $G \cong K_\beta + \overline{K_{n-\beta}}$.*

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