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Bounds on Augmented Zagreb Index of Graphs

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Abstract Let $G=(V,E)$ be a simple connected graph with n ($n\geq 3$) vertices and m edges, with vertex degree sequence $\{d_1,d_2,\ldots,d_n\}$. The augmented Zagreb index is defined as $AZI=AZI(G)=\sum_{ij\in E}(\frac{d_id_j}{d_i+d_j-2})^3$. Using the properties of inequality, we investigate the bounds of AZI for connected graphs, in particular unicyclic graphs in this paper, some useful conclusions are obtained.

Keywords augmented Zagreb index; connected graph; unicyclic graph; bound

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1. Introduction

Let $G=(V,E)$ be a simple connected graph with vertex set $V(G)=\{1,2,\ldots,n\}$ and edge set $E(G)$ where $|V(G)|=n$ and $|E(G)|=m$, respectively. Denote by d_i the degree of vertex i, and by Δ the maximum degree. Further, if two vertices i and j are adjacent, or have an edge between them, we write $i\sim j$. Likewise, if they are not adjacent, or do not have an edge between them, we write $i\nsim j$.

In a molecular graph, vertices and edges are represented by atoms and the chemical bonds between two atoms of their carbon-hydrogen skeleton, respectively. A topological index of a graph is a numerical quantity which is invariant under auto-morphisms of the graph. One of the most investigated and widely used such group are the so-called vertex-degree-based indices. These indices are also studied as graph invariant as these values are being preserved under graph automorphism. So far, a lot of topological indices have been introduced using different structural properties for their calculation [1–7].

The oldest vertex-degree-based topological indices, the first and the second Zagreb indices are defined as

$$M_1=M_1(G)=\sum_{i=1}^{n}d_i^2=\sum_{i\sim j}(d_i+d_j),$$

$$M_2=M_2(G)=\sum_{i\sim j}d_id_j.$$

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The atom-bond connectivity index, ABC, introduced in [8–12], is defined as

$$ABC = ABC(G) = \sum_{i\sim j}\sqrt{\frac{d_i + d_j - 2}{d_i d_j}}.$$

Another vertex-degree-based graph invariant, known as augmented Zagreb index (AZI), was introduced by Furtula et al. in [13]

$$AZI(G) = \sum_{i\sim j}(\frac{d_i d_j}{d_i + d_j - 2})^3,$$

it is proven to be a very helpful predictive measure in the study of heat of formation in heptanes and octanes.

In this paper, we will investigate the bounds of AZI of connected graphs. The rest of the paper is organized as follows. In the next section we shall quote some lemmas and properties of inequality. Then in Section 3, we establish the lower and upper bounds of AZI of connected graphs.

2. Some lemmas

In order to obtain our conclusions, we present the following inequality results, as some lemmas which will be used below.

Lemma 2.1 ([14]) *Let $a = (a_i)$, $i = 1, 2, \ldots, n$ be a positive real number sequence. Then, for any real r, $r \le 0$ or $r \ge 1$, there holds*

$$\sum_{i=1}^{n} a_i^r \ge n^{1-r}\Big(\sum_{i=1}^{n} a_i\Big)^r.$$

If $0 \le r \le 1$, then

$$\sum_{i=1}^{n} a_i^r \le n^{1-r}\Big(\sum_{i=1}^{n} a_i\Big)^r$$

with equality holding if and only if $a_1 = a_2 = \cdots = a_m$ or when $r = 0$ and $r = 1$, too.

The following lemma plays a fundamental role in this paper.

Lemma 2.2 ([15]) *Let $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \ldots, n$ be two positive real number sequences. Then, for any $r \ge 0$ there holds*

$$\sum_{i=1}^{n}\frac{a_i^{r+1}}{b_i^r} \ge \frac{(\sum_{i=1}^{n} a_i)^{r+1}}{(\sum_{i=1}^{n} b_i)^r}$$

with equality holding if and only if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \cdots = \frac{a_n}{b_n}$ or when $r = 0$, too.

Lemma 2.3 ([16]) *Let i and j be any two vertices in G.*

If $i \nsim j$, then

$$R_{ij} \ge \frac{1}{d_i} + \frac{1}{d_j};$$

If $i \sim j$, then

$$1 \geq R_{ij} \geq \frac{d_i + d_j - 2}{d_i d_j - 1} \geq \frac{2}{n},$$

where R_{ij} is the effective resistance of the edge $i \sim j$.

In order to present our results, we also need following properties of inequality.

Property 2.4 *Let a, b, m be positive real numbers and $a \geq b$. Then $\frac{b}{a} \leq \frac{b+m}{a+m}$.*

Property 2.5 ([17]) (Jensen's inequality) *Let $a_i > 0, i = 1, 2, \ldots, n$ and $0 < r < s$. Then*

$$\Big(\sum_{k=1}^{n} a_k^s\Big)^{\frac{1}{s}} \leq \Big(\sum_{k=1}^{n} a_k^r\Big)^{\frac{1}{r}}.$$

3. Main results

The literature contains a large collection of upper and lower bounds on the AZI of graphs [18–22]. In this paper, we apply above inequality to study the bounds of AZI of connected graphs, and obtain some results of AZI, especially the results of AZI on unicyclic graphs. A connected graph is unicyclic if its number of vertices and number of edges are the same.

In the following theorem we determine lower bounds for AZI depending on the parameters n, m and the maximum vertex degree Δ, and the index M_2.

Theorem 3.1 *Let $G = (V, E)$ be a connected graph with n $(n \geq 3)$ vertices, m edges and maximum degree Δ. Then*

$$AZI(G) \geq \frac{1}{n^2}(\frac{M_2 + 2m}{2\Delta})^3.$$

Proof Let i, j be two adjacent vertices of G. Since G is connected, d_i, d_j are positive integers. Moreover, as G has $n \geq 3$ vertices then $d_i \geq 2$ or $d_j \geq 2$. So, $d_i + d_j - 2 > 0$.

Consequently, $d_i d_j - (d_i + d_j - 2) > 0$. Since $2 > 0$, by Property 2.4, we have

$$\frac{d_i + d_j - 2}{d_i d_j} \leq \frac{d_i + d_j}{d_i d_j + 2},$$

and hence

$$\frac{d_i d_j}{d_i + d_j - 2} \geq \frac{d_i d_j + 2}{d_i + d_j}.$$

According to Lemma 2.1, let $r = 3$, we have

$$AZI(G) = \sum_{i \sim j}(\frac{d_i d_j}{d_i + d_j - 2})^3 \geq \frac{1}{n^2}\Big(\sum_{i \sim j}\frac{d_i d_j}{d_i + d_j - 2}\Big)^3 \geq \frac{1}{n^2}\Big(\sum_{i \sim j}\frac{d_i d_j + 2}{d_i + d_j}\Big)^3,$$

and since $d_i, d_j \leq \Delta$, so that $\frac{1}{d_i + d_j} \geq \frac{1}{2\Delta}$. Thus, we can write

$$AZI(G) \geq \frac{1}{n^2}(\frac{1}{2\Delta})^3\Big(\sum_{i \sim j}(d_i d_j + 2)\Big)^3 \geq \frac{1}{n^2}(\frac{M_2 + 2m}{2\Delta})^3. \quad \square$$

Corollary 3.2 *Let $G = (V, E)$ be a connected unicyclic graph with n $(n \geq 3)$ vertices and maximum degree Δ. Then*

$$AZI(G) \geq \frac{1}{n^2}(\frac{M_2 + 2n}{2\Delta})^3.$$

The following theorem is another lower bound on the AZI depending on the parameters m, Δ and the indices M_1 and M_2.

Theorem 3.3 *Let $G=(V,E)$ be a connected graph with n $(n\geq 3)$ vertices, m edges and maximum degree Δ. Then*

$$AZI(G)\geq \frac{1}{2(\Delta-1)}\cdot\frac{M_2^3}{(M_1-2m)^2},$$

in particular, when G is a circuit C_n of length n, equality holds.

Proof Obviously, $d_i,d_j\leq\Delta$, so that

$$\frac{1}{d_i+d_j-2}\geq\frac{1}{2(\Delta-1)}.$$

Hence, we have

$$AZI(G)=\sum_{i\sim j}(\frac{d_id_j}{d_i+d_j-2})^3\geq\frac{1}{2(\Delta-1)}\cdot\sum_{i\sim j}\frac{(d_id_j)^3}{(d_i+d_j-2)^2}.$$

By the above Lemma 2.2 and $M_1=\sum_{i=1}^n d_i^2=\sum_{i\sim j}(d_i+d_j)$, we have

$$AZI(G)\geq\frac{1}{2(\Delta-1)}\cdot\frac{(\sum_{i\sim j}d_id_j)^3}{(\sum_{i\sim j}(d_i+d_j-2))^2}\geq\frac{1}{2(\Delta-1)}\cdot\frac{M_2^3}{(M_1-2m)^2}.$$

If G is a circuit C_n of length n, then $d_i=2=\Delta$ for all $i=1,2,\ldots,n$.

So, according to definition of AZI, we get $AZI(G)=8n$.

On the other hand, we have $M_1=\sum_{i=1}^n d_i^2=4n$, $M_2=\sum_{i\sim j}d_id_j=4n$. Therefore,

$$\frac{1}{2(\Delta-1)}\cdot\frac{M_2^3}{(M_1-2m)^2}=\frac{1}{2}\cdot\frac{(4n)^3}{(2n)^2}=8n.$$

Thus, we get $AZI(G)=\frac{1}{2(\Delta-1)}\cdot\frac{M_2^3}{(M_1-2m)^2}$. $\square$

Corollary 3.4 *Let $G=(V,E)$ be a connected unicyclic graph with n $(n\geq 3)$ vertices and maximum degree Δ. Then*

$$AZI(G)\geq\frac{1}{2(\Delta-1)}\cdot\frac{M_2^3}{(M_1-2n)^2}.$$

Now, we consider the upper bound for AZI in the following theorem, it depends on the index M_2.

Theorem 3.5 *Let $G=(V,E)$ be a connected graph with n $(n\geq 3)$ vertices and maximum degree Δ. Then $AZI(G)\leq M_2^3$.*

Proof Suppose that vertex i is adjacent to vertex j, then, at least one of d_i, d_j is greater than 1. Hence, we get

$$d_i+d_j-2\geq 1,$$

i.e.,

$$\frac{d_id_j}{d_i+d_j-2}\leq d_id_j.$$

Therefore, by Property 2.5, we deduce

$$AZI(G) = \sum_{i\sim j}(\frac{d_i d_j}{d_i + d_j - 2})^3 \le \sum_{i\sim j}(d_i d_j)^3 \le \Big(\sum_{i\sim j} d_i d_j\Big)^3,$$

i.e., $AZI(G) \le M_2^3$. Thus we have proved theorem. $\square$

In the next theorem we apply Lemma 2.3 to establish another upper bound on AZI.

Theorem 3.6 *Let $G = (V, E)$ be a connected graph with n $(n \ge 3)$ vertices, m edges. Then there is $\alpha_{ij} \in (0, 1]$ such that*

$$AZI(G) \le (\frac{n}{2})^3 m(1 + \alpha_{ij})^3.$$

Proof Without loss of generality, we assume that vertices i and j are adjacent in G. Then there must be

$$1 < \frac{d_i d_j}{d_i d_j - 1} \le 2.$$

That is, there is $\alpha_{ij} \in (0, 1]$ such that

$$\frac{d_i d_j}{d_i d_j - 1} = 1 + \alpha_{ij}.$$

Applying Lemma 2.3, we have

$$1 \le \frac{d_i d_j - 1}{d_i + d_j - 2} \le \frac{n}{2}.$$

Hence, we deduce

$$\begin{aligned} AZI(G) &= \sum_{i\sim j}(\frac{d_i d_j}{d_i + d_j - 2})^3 = \sum_{i\sim j}(\frac{d_i d_j - 1}{d_i + d_j - 2} \cdot \frac{d_i d_j}{d_i d_j - 1})^3 \\ &= \sum_{i\sim j}(\frac{d_i d_j - 1}{d_i + d_j - 2})^3(\frac{d_i d_j}{d_i d_j - 1})^3 \\ &\le (\frac{n}{2})^3 \sum_{i\sim j}(\frac{d_i d_j}{d_i d_j - 1})^3 \le (\frac{n}{2})^3 m(1 + \alpha_{ij})^3. \end{aligned}$$

More generally, when $\alpha = \max\{\alpha_{ij} : i \sim j\} = 1$. Then, we have

$$AZI(G) \le (\frac{n}{2})^3 m(1 + \alpha)^3 \le m \cdot n^3,$$

which proves the theorem. $\square$

Corollary 3.7 *Let $G = (V, E)$ be a connected unicyclic graph with n $(n \ge 3)$ vertices. Then there is $\alpha \in (0, 1]$ such that*

$$AZI(G) \le \frac{n^4}{8}(1 + \alpha)^3.$$

In particular, when G is a circuit of length 3 and $\alpha = \frac{1}{3}$, equality holds.

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