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Upper and lower bounds of the fourth geometric-arithmetic index

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Abstract

Let G be a simple connected graph, and d_i be the degree of its vertex v_i. In a recent paper, the geometric-arithmetic index was defined as [1]:

$$GA(G) = \sum \frac{2\sqrt{d_i d_j}}{d_i + d_j} \tag{1}$$

with summation going over all pairs of adjacent vertices. The fourth geometric-arithmetic ($GA_4(G)$) index, which was defined in [2], and the definition is:

$$GA_4(G) = \sum \frac{2\sqrt{e_i e_j}}{e_i + e_j} \tag{2}$$

with summation going over all pairs of adjacent vertices, and e_i denotes the eccentricity of its vertex v_i. In this paper, we give some relations between $GA_4(G)$ index, and other indices like Zagreb indices, and Zagreb eccentricity indices.

Keywords: topological indices, Eccentricity, $GA(G)$ index, $GA_4(G)$ index.

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1. Introduction

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods. Especially graph theory has provided chemist with a variety of useful tools, such as topological indices [3]. Molecules and molecular compounds are often modeled by molecular graph. Topological indices of molecular graphs are one of the oldest and most widely used descriptors in QSPR/QSAR research. Also, graph theory had an important effect on the development of the chemical sciences. Nowadays hundreds of researchers work in this area producing thousands articles annually. Recently, people are studying various topological descriptors [4, 5, 6].

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$ and let $x, y \in V(G)$, then the distance $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y. For a vertex v_i of $V(G)$, its eccentricity e_i is the largest distance between v_i and any other vertex v_k of G, i.e, $e_i = max_{v_j \in V(G)} d_G(v_i, v_j)$. The diameter $d(G)$ of G is defined as the maximum eccentricity of G. Similarly, the radius $r(G)$ is defined as the minimum eccentricity of G.

A class of geometric-arithmetic topological indices are defined as

$$GA_{general}(G) = \sum_{v_i v_j \in E(G)} \frac{2\sqrt{Q_i Q_j}}{Q_i + Q_j} \tag{3}$$

where Q_i is some quantity that in a unique manner can be associated with the vertex v_i of the graph G [11]. The first member of this class was considered by D. Vukičević and B. Furtula [1], by setting Q_i to be d_i which is the degree of its vertex v_i, and it was defined as

$$GA(G) = \sum_{v_i v_j \in E(G)} \frac{2\sqrt{d_i d_j}}{d_i + d_j}. \tag{4}$$

The second member of this class was defined by Fath-Tabar et al. [12], by setting Q_i to be n_i which is the number of vertices of G lying closer to the vertex v_i than to the vertex v_j for the edge $v_i v_j$ of the graph G, and it was defined as

$$GA_2(G) = \sum_{v_i v_j \in E(G)} \frac{2\sqrt{n_i n_j}}{n_i + n_j}. \tag{5}$$

The third member of this class was considered by Bo Zhou et al. [13], by setting Q_i to be m_i which is the number of edges of G lying closer to the vertex v_i than to the vertex v_j for the edge $v_i v_j$ of the graph G, and it was defined as

$$GA_3(G) = \sum_{v_i v_j \in E(G)} \frac{2\sqrt{m_i m_j}}{m_i + m_j}. \tag{6}$$

The fourth member of this class was considered by M. Ghorbani and A. Khaki [2], by setting Q_i to be e_i which is eccentricity of vertex v_i, and it was defined as

$$GA_4(G) = \sum_{v_i v_j \in E(G)} \frac{2\sqrt{e_i e_j}}{e_i + e_j}. \tag{7}$$

Mathematical properties of $GA(G)$, $GA_2(G)$ and $GA_3(G)$ are discussed in [14, 15, 16], [12, 18] and [13, 17], respectively. The $GA(G)$ index is related to the famous Randić index

[5], $GA_2(G)$ index is related to the Szeged [19], and vertex-PI indices [20, 21], and $GA_3(G)$ is related to the conceived edge-Szeged index [22], and edge-PI index [23]. Also, we can find $GA_4(G)$ index is related to the Zagreb indices and the Zagreb eccentricity indices [9, 10, 24].

The Zagreb indices have been introduced more than 30 years ago by I. Gutman and N. Trinajstić [8]. They are defined as

$$M_1(G) = \sum_{v_i \in V(G)} d_i^2$$

$$M_2(G) = \sum_{v_i v_j \in E(G)} d_i d_j.$$

Also, there are similar index called Zagreb eccentricity index [9, 10, 24]. Zagreb eccentricity indices are defined as

$$E_1(G) = \sum_{v_i \in V(G)} e_i^2$$

$$E_2(G) = \sum_{v_i v_j \in E(G)} e_i e_j.$$

The paper is organized as follows. In section 2, we present lower and upper bounds on $GA_4(G)$ index of connected, simple graphs with other indices; the first Zagreb index, the second Zagreb index, and the second Zagreb eccentricity index.

2. Some properties on $GA_4(G)$ index

Theorem 2.1. *Let G be a simple connected graph with m edges, radius r, second Zagreb eccentricity index($E_2(G)$). Then*

$$GA_4(G) \leq \frac{\sqrt{mE_2(G)}}{r} \tag{8}$$

Proof. By the Cauchy-Schwarz inequality,

$$\sum_{v_i v_j \in E(G)} \frac{2\sqrt{e_i e_j}}{e_i + e_j} \leq \sqrt{\sum_{v_i v_j \in E(G)} 4e_i e_j \sum_{v_i v_j \in E(G)} \frac{1}{(e_i + e_j)^2}} \tag{9}$$

and since $e_i \geq r$ for all $v_i \in V(G)$, so we get the result. □

Theorem 2.2. *Let G be a simple connected graph with m edges, radius r, diameter d, second Zagrev eccentricity index $E_2(G)$. Then*

$$\frac{1}{d}\sqrt{E_2(G) + m(m-1)r^2} \leq GA_4(G) \leq \frac{1}{r}\sqrt{E_2(G) + m(m-1)d^2} \tag{10}$$

Proof. We know

$$[GA_4(G)]^2 = \sum_{v_iv_j\in E(G)} \frac{4e_ie_j}{(e_i+e_j)^2} + 2 \sum_{v_iv_j\neq v_rv_s\in E(G)} \frac{2\sqrt{e_ie_j}}{e_i+e_j}\cdot\frac{2\sqrt{e_re_s}}{e_r+e_s}, \tag{11}$$

and $2r \le e_i + e_j \le 2d$ for all edges $v_iv_j \in E(G)$, $r \le e_i \le d$ for all vertices $v_i \in V(G)$. We get the result. □

Theorem 2.3. *Let G be a simple connected graph with n vertices, m edges, second Zagreb eccentricity index $E_2(G)$, first Zagreb index $M_1(G)$, second Zagreb index $M_2(G)$. Then*

$$\frac{2\sqrt{E_2(G)}}{2nm - M_1(G)} \le GA_4(G) \le \sqrt{n^2m^2 - nmM_1(G) + mM_2(G)} \tag{12}$$

Proof.

$$\sum_{v_iv_j\in E(G)} \frac{2\sqrt{e_ie_j}}{e_i+e_j} \ge \frac{\sum_{v_iv_j\in E(G)} 2\sqrt{e_ie_j}}{\sum_{v_iv_j\in E(G)}(e_i+e_j)} \tag{13}$$

and since $e_i \le n - d_i$ for all $v_i \in V(G)$, we get

$$\frac{\sum_{v_iv_j\in E(G)} 2\sqrt{e_ie_j}}{\sum_{v_iv_j\in E(G)}(e_i+e_j)} \ge \frac{\sum_{v_iv_j\in E(G)} 2\sqrt{e_ie_j}}{2nm - M_1(G)} \ge \frac{2\sqrt{E_2(G)}}{2nm - M_1(G)} \tag{14}$$

We complete the first part of proof.

$$\sum_{v_iv_j\in E(G)} \frac{2\sqrt{e_ie_j}}{e_i+e_j} \le \sum_{v_iv_j\in E(G)} \sqrt{e_ie_j} \tag{15}$$

and by using the Cauchy-Schwarz inequality, we get

$$\sum_{v_iv_j\in E(G)} \sqrt{e_ie_j} \le \sqrt{\sum_{v_iv_j\in E(G)} 1 \cdot \sum_{v_iv_j\in E(G)} e_ie_j} \tag{16}$$

and since $e_i \le n - d_i$ for all $v_i \in V(G)$,

$$\sqrt{\sum_{v_iv_j\in E(G)} 1 \cdot \sum_{v_iv_j\in E(G)} e_ie_j} \le \sqrt{n^2m^2 - nmM_1(G) + mM_2(G)}. \tag{17}$$

This completes the proof. □

We refer the reader to the book [7, p. 71-72, 253-255] for a classical result, the Pólya-Szegö inequality. From this result, we can find the following result and it will be used to find the lower bound on $GA_4(G)$ index.

Lemma 2.4. [7] *Let $(a_1, a_2, \ldots, a_n)$ be positive n-tuples such that there exist positive numbers $A\,, a$ satisfying:*

$$0 < a \leq a_i \leq A\,.$$

Then

$$\frac{n\sum_{i=1}^{n} a_i^2}{\left(\sum_{i=1}^{n} a_i\right)^2} \leq \frac{1}{4}\left(\sqrt{\frac{A}{a}} + \sqrt{\frac{a}{A}}\right)^2 . \tag{18}$$

The inequality becomes an equality if and only if $a = A$ or

$$q = \frac{A/a}{A/a+1} n$$

is an integer and q of the numbers a_i coincide with a and the remaining $n-q$ of the a_i's coincide with A ($\neq a$).

Theorem 2.5. *Let G be a simple connected graph with m edges, radius r, diameter d, second Zagreb eccentricity index $E_2(G)$. Then*

$$GA_4(G) \geq \frac{\sqrt{8(d+r)\sqrt{dr}}}{(\sqrt{d}+\sqrt{r})^2}\sqrt{m^2 - \frac{m}{4r^2}\Big(\sum_{v_i \in V(G)} d_i e_i^2 - 2E_2(G)\Big)} \tag{19}$$

Proof. Since $r \leq e_i, e_j \leq d$, we have $\frac{d}{r} \geq \frac{e_i}{e_j} \geq \frac{r}{d}$, so we get

$$\begin{aligned} \Big(\sqrt{\frac{e_i}{e_j}} + \sqrt{\frac{e_j}{e_i}}\Big)^2 &= \Big(\sqrt{\frac{e_i}{e_j}} - \sqrt{\frac{e_j}{e_i}}\Big)^2 + 4 \\ &\leq \Big(\sqrt{\frac{d}{r}} - \sqrt{\frac{r}{d}}\Big)^2 + 4 \\ &= \Big(\sqrt{\frac{d}{r}} + \sqrt{\frac{r}{d}}\Big)^2 \end{aligned} \tag{20}$$

This implies

$$\frac{2\sqrt{dr}}{d+r} \leq \frac{2\sqrt{e_i e_j}}{e_i + e_j} \leq 1. \tag{21}$$

Since

$$\frac{2\sqrt{e_i e_j}}{e_i + e_j} = \sqrt{1 - \Big(\frac{e_i - e_j}{e_i + e_j}\Big)^2} \tag{22}$$

and m is the number of edges in G, using Lemma 2.4 we have

$$\Big(\sum_{v_iv_j\in E(G)}\frac{2\sqrt{e_ie_j}}{e_i+e_j}\Big)^2\geq\frac{8m(d+r)\sqrt{dr}}{(\sqrt{d}+\sqrt{r})^4}\sum_{v_iv_j\in E(G)}\Big[1-\Big(\frac{e_i-e_j}{e_i+e_j}\Big)^2\Big] \tag{23}$$

Now,

$$\begin{aligned}\sum_{v_iv_j\in E(G)}\Big(1-\Big(\frac{e_i-e_j}{e_i+e_j}\Big)^2\Big) &\geq m-\frac{1}{4r^2}\sum_{v_iv_j\in E(G)}(e_i-e_j)^2\\ &= m-\frac{1}{4r^2}\Big(\sum_{v_i\in V(G)}d_ie_i^2-2E_2(G)\Big) \qquad (24)\end{aligned}$$

So we get the theorem. □

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