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# A note on the fourth version of geometric-arithmetic index

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The geometric-arithmetic index is another topological index was defined as $GA(G)=\sum_{uv\in E}\frac{2\sqrt{dudv}}{du+dv}$, in which degree of vertex u denoted by *du*. Now we define a new version of *GA* index as $GA_4(G)=\sum_{uv\in E}\frac{2\sqrt{\varepsilon_u\varepsilon_v}}{\varepsilon_u+\varepsilon_v}$, in which *ε*(*u*) is the eccentricity of vertex *u*. The goal of this paper is to further the study of the $GA_4$ 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 without necessarily referring to quantum mechanics [1-3]. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [4]. This theory had an important effect on the development of the chemical sciences. Nowadays hundreds of researchers work in this area producing thousands articles annually.

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. By IUPAC terminology, a topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity [5-11].

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. If *e* is an edge of *G*, connecting the vertices u and v, then we write *e* = *uv* and say "*u* and *v* are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices.

Let $\sum$ be the class of finite graphs. A topological index is a function Top from $\sum$ into real numbers with this property that *Top*(*G*) = *Top*(*H*), if *G* and *H* are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The Wiener index is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. If $x, y \in V(G)$ 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 *u* of *V*(*G*) its eccentricity $\varepsilon_G(u)$ is the largest distance between *u* and any other vertex *v* of *G*, $\varepsilon_G(u)=\max_{v\in V(G)} d_G(u,v)$. The maximum eccentricity over all vertices of *G* is called the diameter of *G* and denoted by *D*(*G*). The eccentric connectivity index $\xi(G)$ of a graph *G* is defined as

$$\xi(G)=\sum_{u\in V(G)}\deg_G(u)\varepsilon_G(u).$$

Where, $\deg_G(u)$ denotes the degree of vertex *u* in *G*, i. e., the number of its neighbors in *G*.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestic [1]. They are defined as:

$$M_1(G)=\sum_{v\in V(G)}\left(\deg_G(v)\right)^2 \text{ and}$$

$$M_1(G)=\sum_{uv\in E(G)}\deg_G(u)\deg_G(v)\cdot$$

Now we define a new version of Zagreb indices as follows:

$$M_1^*(G)=\sum_{uv\in E(G)}\varepsilon(u)+\varepsilon(v) \text{ and}$$

$$M_2^*(G)=\sum_{uv\in E(G)}\varepsilon(u)\varepsilon(v).$$

It is easy to see that for every connected graph *G*, $M_2^*(G)=\xi(G)$.

A class of geometric–arithmetic topological indices may be defined as $GA_{general} = \sum_{uv\in E}\frac{2\sqrt{Q_uQ_v}}{Q_u+Q_v}$, where $Q_u$ is some quantity that in a unique manner can be associated with the vertex $u$ of the graph $G$, see [13]. The first member of this class was considered by Vukicevic and Furtula [14], by setting $Q_u$ to be the

$$GA(G) = \sum_{uv\in E}\frac{2\sqrt{dudv}}{du+dv},$$

in which degree of vertex u denoted by $du$. The second member of this class was considered by Fath-Tabar et al. [15] by setting $Q_u$ to be the number $n_u$ of vertices of $G$ lying closer to the vertex $u$ than to the vertex $v$ for the edge $uv$ of the graph $G$:

$$GA_2(G) = \sum_{uv\in E}\frac{2\sqrt{n_un_v}}{n_u+n_v}.$$

The third member of this class was considered by Bo Zhou et al. [16] by setting $Q_u$ to be the number $m_u$ of edges of $G$ lying closer to the vertex $u$ than to the vertex $v$ for the edge $uv$ of the graph $G$:

$$GA_3(G) = \sum_{uv\in E}\frac{2\sqrt{m_um_v}}{m_u+m_v}.$$

Here, we define the forth member of this class as follows:

$$GA_4(G) = \sum_{uv\in E}\frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)},$$

in which $\varepsilon(u)$ denote to the eccentricity of vertex $u$. The goal of this paper is computing some bounds for $GA_4$ index. Throughout this paper our notation is standard and mainly taken from standard books of graph theory [18-23]. All graphs considered in this paper are simple and connected.

## 2. Results and discussions

In this section we first compute some bounds for $GA_4$ index. Next we introduce the conception of transitive and edge-transitive acting on vertices of graph $G$. Finally by using this definition and some Lemmas we compute the $GA_4$ index of hypercube graph.

**Theorem 1.** Let $G = (V, E)$ be a graph. Then

$$\frac{2M_2^*(G)}{M_1^*(G)} \le GA_4(G) \le \frac{2}{3}M_2^*(G).$$

**Proof.** It is easy to see that for every $e = uv$ in $E(G)$, $\varepsilon(u)+\varepsilon(v)\ge 3$. By the definition of $GA_4$ index we have

$$GA_4(G) = \sum_{uv\in E}\frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)} \le \frac{2}{3}\sum_{uv\in E}\sqrt{\varepsilon(u)\varepsilon(v)}$$
$$\le \frac{2}{3}\sum_{uv\in E}\varepsilon(u)\varepsilon(v) = \frac{2}{3}M_2^*(G).$$

On the other hand,

$$GA_4(G) = \sum_{uv\in E}\frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)} \ge 2\frac{\sum_{uv\in E}\sqrt{\varepsilon(u)\varepsilon(v)}}{M_1^*(G)} = \frac{2M_2^*(G)}{M_1^*(G)}.$$

This completes the proof.

**Theorem 2**.

$$GA_4(G) \ge \frac{\sqrt{M_2^*(G)}}{M_1^*(G)}.$$

**Proof.**

$$[GA_4(G)]^2 = \sum_{uv\in E}\frac{4\varepsilon(u)\varepsilon(v)}{(\varepsilon(u)+\varepsilon(v))^2} + 4\sum_{uv\ne u'v'}\frac{\sqrt{\varepsilon(u)\varepsilon(v)}\sqrt{\varepsilon(u')\varepsilon(v')}}{(\varepsilon(u)+\varepsilon(v))(\varepsilon(u')+\varepsilon(v'))}$$
$$\ge \sum_{uv\in E}\frac{4\varepsilon(u)\varepsilon(v)}{(\varepsilon(u)+\varepsilon(v))^2} = \frac{M_2^*(G)}{[M_1^*(G)]^2}.$$

An automorphism of the graph $G = (V, E)$ is a bijection $\sigma$ on $V$ which preserves the edge set $e$, i. e., if $e = uv$ is an edge, then $\sigma(e)=\sigma(u)\sigma(v)$ is an edge of $E$. Here the image of vertex $u$ is denoted by $\sigma(u)$. The set of all automorphisms of $G$ under the composition of mappings forms a group which is denoted by $Aut(G)$. $Aut(G)$ acts transitively on $V$ if for any vertices $u$ and $v$ in $V$ there is $\alpha\in Aut(G)$ such that $\alpha(u)=v$. Similarly $G = (V, E)$ is called edge-transitive graph if for any two edges $e_1 = uv$ and $e_2 = xy$ in $E$ there is an element $\beta\in Aut(G)$ such that $\beta(e_1)=e_2$ where $\beta(e_1)=\beta(u)\beta(v)$. Let $G = (V, E)$ be a graph. If $Aut(G)$ acts edge-transitively on $V$, then we have the following lemma:

**Lemma 3.** $GA_4(G) = 2|E|\frac{\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$, for every $e = uv \in E(G)$.

**Lemma 4.** $M_2^*(G) = |E|\,\varepsilon(u)\varepsilon(v).$, for every $e = uv\in E(G)$.

**Example 5.** Let $S_n$ be the star graph with $n + 1$ vertices. It is easy to see that $S_n$ is edge- transitive. So we have:

$$GA_4(S_n) = 2n \times \sqrt{\frac{2}{3}}.$$

Fullerenes are molecules in the form of polyhedral closed cages made up entirely of $n$ three coordinate carbon atoms and having 12 pentagonal and (n/2 - 10) hexagonal faces, where $n$ is equal or greater than 20. Hence, the smallest fullerene, $C_{20}$, (n = 20) has 12 pentagons and its point groups, is well known to be $C_i$. In the following example we compute the $GA_4$ index of $C_{20}$.

**Example 6.** Consider the fullerene graph $C_{20}$ shown in Fig. 1. It is easy to see $C_{20}$ is edge transitive. Furthermore, because $C_{20}$ is vertex transitive so by computing values of $\varepsilon(u)$ and $\varepsilon(v)$ we have, $\varepsilon(u) = \varepsilon(v) = 5$. In the other word |E| = 30 and $GA_4(C_{20}) = 30$.

In the general we have the following theorem without proof:

**Theorem 7.** Let $G$ be a graph in which, $Aut(G)$ acts both edge and vertex-transitively on $V$. Then $GA_4(G) = |E(G)|$.

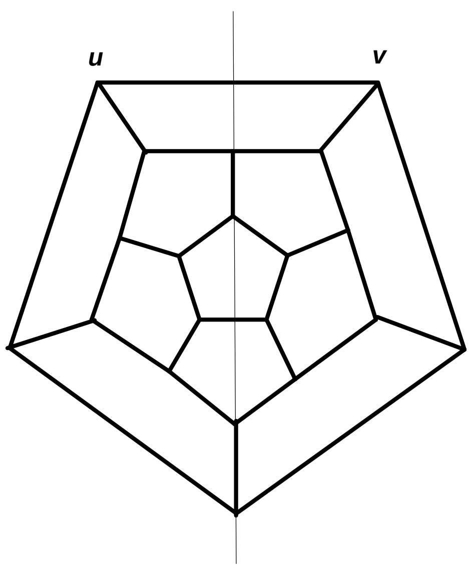


*Fig. 1. The graph of fullerene $C_{20}$.*

The fullerene $C_{20}$ is the only edge transitive fullerene. So it is important how to compute $GA_4$ index for the case which $G$ is not transitive graph. One can apply the following Lemma for this case:

**Lemma 8.** Let $G = (V, E)$ be a graph. If $Aut(G)$ on $V$ has orbits $E_i$, $1 \le i \le s$, where $e_i = u_i v_i$ is an edge of $G$. then:

$$M_2^*(G) = \sum_{i=1}^{s} |E_i| \, \varepsilon(u_i)\varepsilon(v_i) \text{ and}$$

$$GA_4(G) = 2\sum_{i=1}^{s} |E_i| \sqrt{\frac{\varepsilon(u_i)\varepsilon(v_i)}{\varepsilon(u_i)+\varepsilon(v_i)}}.$$

**Proof.** The values of $\varepsilon(u)$ and $\varepsilon(v)$ for every $e \in E_i$ are equal. So,. it is enough to compute $\varepsilon(u_i)$ and $\varepsilon(v_i)$ for $e_i = u_i v_i$ $(1 \le i \le s)$.

A hypercube define as follows:

The vertex set of the hypercube $H_n$ consist of all n-tuples $b_1 b_2 \ldots b_n$ with $b_i \in \{0,1\}$. Two vertices are adjacent if the corresponding tuples differ in precisely one place. Darafsheh[20] proved $H_n$ is vertex and edge transitive. We use of this result and we have the following theorems without proof:

**Theorem 9.** $M_2^*(H_n) = |E| = n^3.2^{n-1}$.

**Theorem 10.** $GA_4(H_n) = |E| = n.2^{n-1}$.

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