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A note on geometric – arithmetic index of fullerene

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The geometric-arithmetic index is another topological index was defined as $GA(G)=\sum_{uv\in E}\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$, in which degree of vertex *u* denoted by *d*(*u*). We now define a new version of *GA* index as $GA_4(G)=\sum_{e=uv\in E(G)}\frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)}$, where ε(*u*) is the eccentricity of vertex *u*. In this paper we compute these topological indices for fullerene graphs.

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1. Introduction

By a graph means 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. The fact that many interesting graphs are composed of simpler graphs that serve as their basic building blocks prompts and justifies interest in the type of relationship that exist between various graph-theoretical invariants of composite graphs and of their components. The composite graphs considered here arise from simpler graphs via several binary operations. Such operations are sometimes called graph products, and the resulting graphs are also known as product graphs.

Let *G* be a graph on *n* vertices. We denote the vertex and the edge set of *G* by *V*(*G*) and *E*(*G*), respectively. For two vertices *u* and *v* of *V*(*G*) we define their distance *d*(*u*, *v*) as the length of a shortest path connecting *u* and *v* in *G*. For a given vertex *u* of *V*(G) its eccentricity $\varepsilon(u)$ is the largest distance between *u* and any other vertex *v* of *G*. Hence, $\varepsilon(u)=\max_{v\in V(G)} d(u,v)$. The minimum and maximum eccentricity over all vertices of *G* are called the radius and diameter of *G* and denoted by *R*(*G*) and *D*(*G*), respectively. The eccentric connectivity index $\xi(G)$ of a graph *G* is defined as $\xi(G)=\sum_{u\in V(G)} d(u)\varepsilon(u)$, where *d*(*u*) denotes the degree of vertex *u* in *G*, *i*. *e*., the number of its neighbors in *G* [1-7]. The total eccentricity index of *G* is defined as $\theta(G)=\sum_{u\in V(G)}\varepsilon(u)$.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestic [8]. They are defined as:

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

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

Now we define a new version of Zagreb indices as follows [9]:

$$M_1^*(G)=\sum_{uv\in E(G)}\varepsilon(u)+\varepsilon(v) \text{ and } M_2^*(G)=\sum_{uv\in E(G)}\varepsilon(u)\varepsilon(v).$$

It is easy to see that for every connected graph *G*, $M_1^*(G)=\xi(G)$.

2. Geometric – arithmetic index

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* [10]. The first member of this class was considered by Vukicević and Furtula [11], by setting Q_u to be the

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

where degree of vertex *u* denoted by $d(u)$. The second member of this class was considered by Fath-Tabar et al. [12] by setting Q_u to be the number $n_u = n_u(e|G)$ 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 Zhou et al. [13] by setting Q_u to be the number $m_u = m_u$

$(e|G)$ of edges of G lying closer to the vertex u than to the vertex v for the edge uv of the graph G:

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

The fourth member of this class was defined by Ashrafi et al. [14] as follows:

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

where $\varepsilon(u)$ denotes to the eccentricity of vertex u.

A fullerene graph is a cubic 3-connected plane graph with pentagonal faces and hexagonal faces. Let F_n be a fullerene graph with n vertices. By the Euler formula one can see that F_n has 12 pentagonal and $n/2 - 10$ hexagonal faces [15,16]. By a Hamiltonian fullerene, means a fullerene with a Hamiltonian cycle.

Since every fullerene graph F is 3 regular, so $GA(F) = |E(F)|$. In other words, for two distinct isomers of a fullerene F of order $n \geq 26$, such as F_1 and F_2 $GA(F_1) = GA(F_2)$, while they have distinct GA_4. The similar conditions hold for Zagreb indices, *e. g* for two distinct isomer of fullerenes F_1 and F_2 with $|V(F_1)| = |V(F_2)|$, one can see $M_i(F_1) = M_i(F_2)$ while $M_i^*(F_1) \neq M_i^*(F_2)$, $i = 1, 2$.

Throughout this paper our notation is standard and mainly taken from standard books of graph theory such as [17, 18] and [19 – 46]. All graphs considered in this paper are simple and connected.

2. Main results and discussion

The aim of this section is to obtain some bounds of GA indices of fullerene graphs. At first, we must compute $GA_4(G)$, for some well-known class of graphs.

Example 1. Let K_n denotes the complete graph on n vertices. Then for every $v \in V(K_n)$, $d(v) = n-1$ and $\varepsilon(v) = 1$. This implies $GA_4(K_n) = \sum_{uv\in E(G)} \frac{2\sqrt{1}}{2} = \frac{n(n-1)}{2}$.

Example 2. Let C_n denotes the cycle of length n. If n is even then for every i, then i-th row of distance matrix of C_n is $1,2,\ldots,\overset{i}{0},\ldots,(n-1)/2,\ n/2,\ (n-1)/2,\ldots,2,1$. When n is odd then the it is equal to $1,2,\ldots,\overset{i}{0},\ldots,(n-1)/2,\ (n-1)/2,\ldots,2,1$. Hence,

$$GA_4(C_n) = \begin{cases} \sum_{uv\in E(G)} \dfrac{2\sqrt{\frac{n}{2}\cdot\frac{n}{2}}}{\frac{n}{2}+\frac{n}{2}} = n & 2\,|\,n \\[2ex] \sum_{uv\in E(G)} \dfrac{2\sqrt{\frac{n-1}{2}\cdot\frac{n-1}{2}}}{\frac{n-1}{2}+\frac{n-1}{2}} = n & 2\nmid n \end{cases}.$$

Example 3. Let S_n be the star graph with $n + 1$ vertices. The central vertex is denoted by x and others vertices by $u_1, u_2, \ldots, u_n$. Then for every $1 \leq i, j \leq n$, we have $d(x, u_i) = 1$ and $d(u_i, u_j) = 2$. So, $GA_4(S_n) = \sum_{uv\in E(G)} \frac{2\sqrt{2}}{3} = \frac{2\sqrt{2}}{3} n$.

Example 4. Consider the fullerene graph C_{20} depicted in Fig. 1. By using distance matrix one can see, for every vertex x, $\varepsilon(x) = 5$. This implies $GA_4(C_{20}) = 30$. Since every fullerene graph F is 3 regular, then $\xi(F) = 3\theta(F)$. In other words, $\xi(C_{20}) = 3\theta(C_{20}) = 3\times 5\times 20 = 300$.

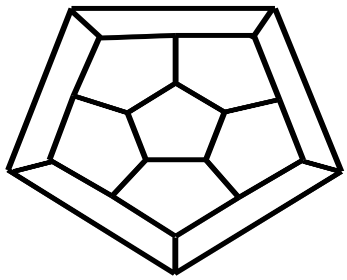

Fig. 1. The fullerene graph C_{20}.

Because C_{20} is *the* smallest fullerene, for every vertex x in fullerene graph F, $\varepsilon(x) \geq 5$ and so $\xi(F) \geq 45n/2$. On the other hand, $\xi(F) = 3\theta(F)$ if and only if $\xi^2(F) = 9\theta^2(F)$. This implies:

$$\theta^2(F) = [\sum_{u\in V(F)} \varepsilon(u)]^2 \geq \sum_{u\in V(F)} \varepsilon^2(u) + 2\sum_{u\neq v} \varepsilon(u)\varepsilon(v) \geq \theta(F) + 2M_2^*(F) \geq \theta(F) + 75n.$$

Let $t := \theta(F)$, then $t^2 - t - 75n \geq 0$. This non – equality hold if and only if $t \geq (1+\sqrt{300n+1})/2$. Thus $\xi(F) \geq 3(1+\sqrt{300n+1})/2$ and so, the following Theorem is proved:

Theorem 5. For a fullerene graph F with n vertices, an upper bound for eccentric connectivity index is as:

$$\xi(F) \geq 3(1+\sqrt{300n+1})/2.$$

In this section, we discuss about Hamiltonian fullerene graphs. It has been conjectured that every fullerene, is Hamiltonian [47].

Theorem 6. Let G be a Hamiltonian graph, then $M_2^*(G) \leq (\theta(G))^2$.

Proof. Without less of generality for every edge $e = uv$, let $\varepsilon(u) \leq \varepsilon(v)$. Thus

$$M_2^*(G) = \sum_{uv\in E(G)} \varepsilon(u)\varepsilon(v) \leq \sum_{u\in V(G)} \varepsilon(u)^2 \leq (\sum_{u\in V(G)} \varepsilon(u))^2 = (\theta(G))^2.$$

Lemma 7. Let G be a Hamiltonian graph. Then for every vertex $v \in V(G)$, $\varepsilon(v) \leq [n/2]$.

Proof. Suppose u be an arbitrary vertex of G. Since u and v are on a Hamiltonian cycle, then $d(u, v) \leq [n/2]$. This completes the proof.

As a result of Lemma 7, we can deduce the following Theorems:

Theorem 7. Let F be a Hamiltonian fullerene graph. Then

$$\xi(F) \le 9n[n/2]/2.$$

Theorem 8. Let F be a Hamiltonian fullerene graph. Then

$$\xi(F) \ge 2\theta(F).$$

Proof. A Hamiltonian graph has a Hamiltonian cycle. Thus for every vertex u in $V(G)$, $d(u) \ge 2$.

Theorem 9. Let F be a Hamiltonian fullerene graph. Then

$$M_1^*(F) \le 3n[n/2] \text{ and } M_2^*(F) \le 3n[n/2]^2/2.$$

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