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Computation of two classes of GA index of some nanostructures

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Let Σ be the class of finite graphs. A topological index is a function Top from Σ 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. In this paper we compute two classes of *GA* indices of nanostructures.

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1. Introduction

Throughout this paper graph means simple connected graph. Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. Suppose Graph denotes the class of all graphs. A map Top from Graphs into real numbers is called a topological index, if $G \cong H$ implies that $Top(G) = Top(H)$. Obviously, the maps Top_1 and Top_2 defined as the number of edges and vertices, respectively, are topological indices. The Wiener [6] 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. The eccentricity of vertex u is $\varepsilon(u) = \mathrm{Max}\{d(x,u) \mid x \in V(G)\}$. The maximum eccentricity over all vertices of G is called the diameter of G and denoted by $D(G)$ and the minimum eccentricity among the vertices of G is called radius of G and denoted by $R(G)$. Diudea [1-3] was the first scientist considered the problem of computing topological indices.

A class of geometric–arithmetic topological indices may be defined as $GA_{general} = \sum_{uv \in E} \frac{2\sqrt{Q_u Q_v}}{Q_u + Q_v}$, where Q_u is some quantity that in a unique manner can be associated with the vertex u of the graph G[4]. The first member of this class was considered by Vukicevic and Furtula [5], 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. [6] 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:

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

The third member of this class was considered by Bo Zhou et al. [7] 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:

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

The fourth member of this class was considered by M. Ghorbani et al.[8] by setting Q_u to be the number $\varepsilon(u)$ the eccentricity of vertex u:

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

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestic [9]. They are defined as:

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

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

Now we define a new version of Zagreb indices as follows [10]:

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

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

2. Results and discussion

In mathematics, groups are often used to describe symmetries of objects. This is formalized by the notion of a group action: every element of the group "acts" like a bijective map (or "symmetry") on some set. To clarify this notion, we assume that G is a group and X is a set. G is said to act on X when there is a map $\phi : G \times X \longrightarrow X$ such that all elements $x \in X$, (i) $\phi(e,x) = x$ where e is the identity element of G, and, (*ii*) $\phi(g, \phi(h,x)) = \phi(gh,x)$ for all $g,h \in G$. In this case, G is called a transformation group, X is called a G-set, and ϕ is called the group action. For simplicity we define $gx = \phi(g,x)$. In a group action, a group permutes the elements of X. The identity does nothing, while a composition of actions corresponds to the action of the composition. For a given X, the set $\{gx \mid g \in G\}$, where the group action moves x, is called the group orbit of x. The subgroup which fixes is the isotropy group of x.

An automorphism of the graph $G = (V, E)$ is a bijection σ 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, $\beta(e_1) = \beta(u)\beta(v)$.

Example 1. 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 [12,13] 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 2. 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 3. Let G be a graph in which, $Aut(G)$ acts both edge and vertex-transitively. Then $GA_4(G) = |E(G)|$.

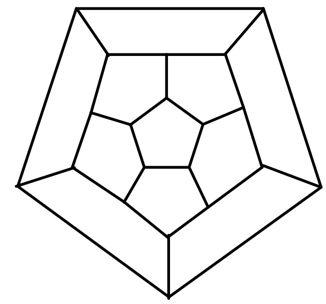

Fig. 1. The graph of fullerene C_{20}.

The fullerenes C_{20} and C_{60} are the only vertex 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 4. Let $G = (V, E)$ be a graph. If $Aut(G)$ on V has orbits E_i, $1 \le i \le s$, where $e_i = u_iv_i$ 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 $e_i = u_iv_i$ ($1 \le i \le s$).

A hypercube define as follows:

The vertex set of the hypercube H_n consist of all n-tuples $b_1b_2...b_n$ with $b_i \in \{0,1\}$. Two vertices are adjacent if the corresponding tuples differ in precisely one place. Darafsheh [11] proved H_n is vertex and edge transitive. We use of this result and we have the following theorems without proof:

Theorem 5. $M_2^*(H_n) = |E| = n^3.2^{n-1}$ and $GA_4(H_n) = |E| = n.2^{n-1}$.

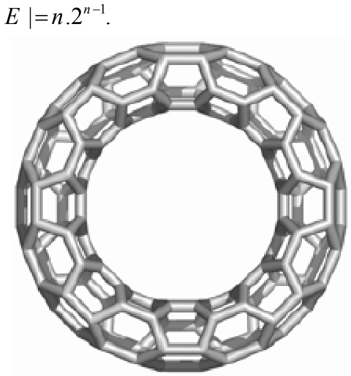

Fig. 2. The Zig-zag Polyhex Nanotube.

Apply our method on a toroidal fullerene R = R[p,q], in terms of its circumference (q) and its length (p), Fig. 1. To compute the eccentric connectivity index of this fullerene, we first prove its molecular graph is vertex transitive.

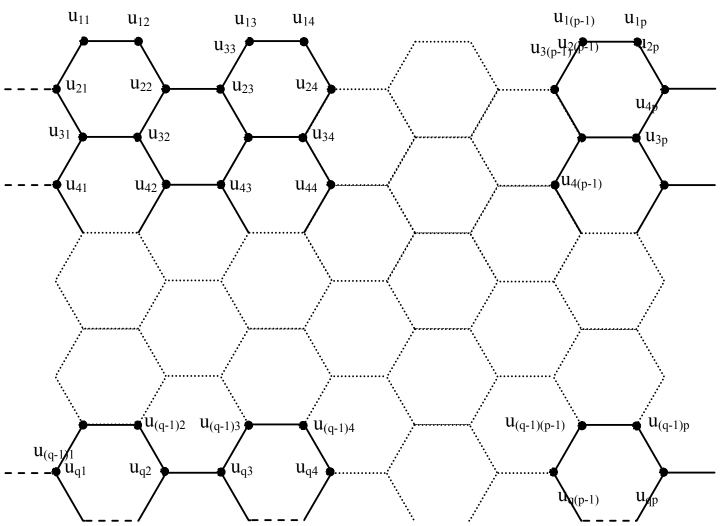

Fig. 3. A 2-Dimensional Lattice for T[p,q].

Lemma 6 — The molecular graph of a polyhex nanotorus is vertex transitive.

Proof — To prove this lemma, we first notice that p and q must be even. Consider the vertices u_{ij} and u_{rs} of the molecular graph of a polyhex nanotori T = T[p,q], Fig. 2. Suppose both of i and r are odd or even and σ is a horizontal symmetry plane which maps u_{it} to u_{rt}, $1 \le t \le p$ and π is a vertical symmetry which maps u_{tj} to u_{ts}, $1 \le t \le q$. Then σ and π are automorphisms of T and we have $\pi\sigma(u_{ij}) = \pi(u_{rj}) = u_{rs}$. Thus u_{ij} and u_{rs} are in the same orbit under the action of Aut(G) on V(G). On the other hand, the map θ defined by $\theta(u_{ij}) = \theta(u(p+1-i)j)$ is a graph automorphism of T and so if "i is odd and r is even" or "i is even and r is odd" then again u_{ij} and u_{rs} will be in the same orbit of Aut(G), proving the lemma.

Therem 7. $M_1^*(T[p,q]) = 2|E|D(T[p,q])$ and $M_2^*(T[p,q]) = |E|D^2(T[p,q])$.

Proof. By using Lemma 6 it is easy to see

$$M_1^*(T[p,q]) = \sum_{e=uv} \varepsilon(u)+\varepsilon(v) = 2|E|\varepsilon(u) = 2|E|D(T[p,q])$$

and

$$M_2^*(T[p,q]) = \sum_{e=uv} \varepsilon(u)^2 = |E|\varepsilon(u)^2 = 2|E|D(T[p,q]).$$

Corollary 8. $D(T[p,q]) = \dfrac{2M_2^*}{M_1^*}$.

Therem 9. $GA_2(T[p,q]) = |E|$.

Proof.

$$GA_2(T[p,q]) = \sum_{uv\in E(G)} \frac{2\sqrt{\deg(u)\deg(v)}}{\deg(u)+\deg(v)} = \sum_{uv\in E(G)} 1 = |E|.$$

Therem 10. $GA_4(T[p,q]) = |E|$.

Proof. Because Aut(T[p,q]) acts transitively on the set of vertices so, we have:

$$GA_4(T[p,q]) = \sum_{uv\in E(G)} \frac{2\sqrt{\varepsilon(u)\varepsilon(v)}}{\varepsilon(u)+\varepsilon(v)} = \sum_{uv\in E(G)} 1 = |E|.$$

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