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On the edge and total GA indices of some graphs

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Abstract

The edge and total versions of geometric-arithmetic (GA) index of graphs are introduced based on the end-vertex degrees of edges of their line and total graphs, respectively. In this paper, the edge and total GA indices are computed for some graphs by using some results on GA index and graphs.

Keywords : Geometric–arithmetic index; Line graph; Total Graph; Degree (of a vertex).

1   Introduction

A single number that can be used to characterize some property of the graph of a molecule is called a topological index for that graph. There are numerous topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [8]. The oldest topological index which introduced by Harold Wiener in 1947 is ordinary (vertex) version of Wiener index [10] which is the sum of all distances between vertices of a graph. Also, the edge versions of Wiener index which were based on distance between edges introduced by Iranmanesh et al. in 2008 [3].

One of the most important topological indices is the well-known branching index introduced by Randic [7] which is defined as the sum of certain bond contributions calculated from the vertex degree of the hydrogen suppressed molecular graphs.

Motivated by the definition of Randic connectivity index based on the end-vertex degrees of edges

in a graph connected G with the vertex set $V(G)$ and the edge set $E(G)$ [2, 4], Vukicevic and Furtula [9] proposed a topological index named the geometric-arithmetic index (shortly GA) as

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

where $d_G(u)$ denotes the degree of the vertex u in G. The reader can find more information about geometric-arithmetic index in [1, 9, 12].

In [5], the edge version of geometric-arithmetic index introduced based on the end-vertex degrees of edges in a line graph of G which is a graph such that each vertex of $L(G)$ represents an edge of G; and two vertices of $L(G)$ are adjacent if and only if their corresponding edges share a common endpoint in G, as follows

$$GA_e(G) = \sum_{ef \in E(L(G))} \frac{2\sqrt{d_{L(G)}(e)d_{L(G)}(f)}}{d_{L(G)}(e) + d_{L(G)}(f)}$$

where $d_{L(G)}(e)$ denotes the degree of the edge e in G.

The total version of geometric-arithmetic index is introduced based on the end-vertex degrees of edges in a total graph of G which is a graph such that the vertex set of $T(G)$ corresponds to the

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vertices and edges of G and two vertices are adjacent in $T(G)$ if and only if their corresponding elements are either adjacent or incident in G as follows

$$GA_t(G) = \sum_{xy \in E(T(G))} \frac{2\sqrt{d_{T(G)}(x)d_{T(G)}(y)}}{d_{T(G)}(x) + d_{T(G)}(y)}$$

where $d_{T(G)}(x)$ denotes the degree of the vertex x in $T(G)$, [6].

In this paper, the edge and total GA index is computed for $TUC_4C_8(R)$ and TUAC$_6$[p',q'] nanotubes. Also, we compute edge GA index for subdivision graph $S(G)$.

2   The edge and total GA for $TUC_4C_8(R)$ and TUAC$_6$[p',q'] nanotubes

We use the notations q and p for the number of rows of squares and number of squares in a row, respectively in the $TUC_4C_8(R)$ nanotubes which is mentioned in Figure 1 with $q = 4$ and $p = 8$. We denote $TUC_4C_8(R)$nanotube with $T(p,q)$. A
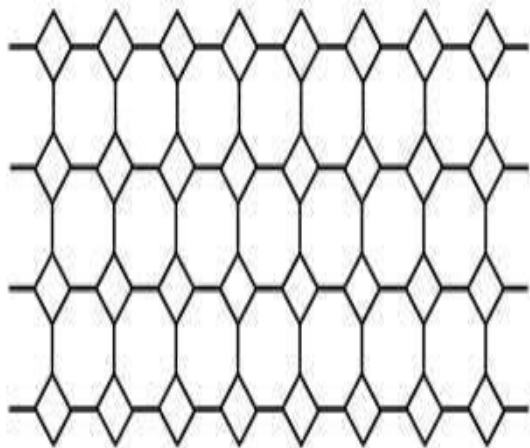

Figure 1: Two dimensional lattice of $TUC_4C_8(R)$ nanotube, $q = 4, p = 8$..

single-wall carbon nanotube can be imagined as graphene sheet rolled at a certain "chiral" angle with respect to a plane perpendicular to the tube's long axis. Tubes having chiral angle = 30° are called "armchair". Armchair polyhex nanotube graph, that denoted by TUAC$_6$ [p',q'] , is a nanotube that p' and q' are the number of hexagons in length and width of molecular graph, respectively. Also, it has j rows which $1 \le j \le q'$ as shown in Figure 2. In addition we denote

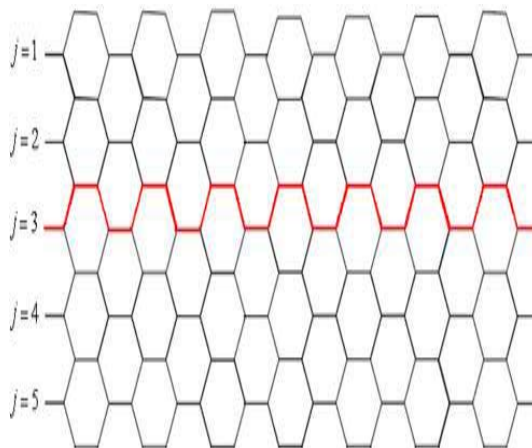TUAC$_6$ [p',q'] nanotube with T'(p',q'). Also, due to these notations, $|E(T'(p',q'))| = 6p'q' + p'$.

Figure 2: Armchair polyhex nanotube ,TUAC6[7,5], with $1 \le j \le 5$ rows.

Lemma 2.1 *Let Gbe a graph, $u \in V(G)$ and $e = vz \in E(G)$. Then we have:*

$$d_{L(G)}(e) = d_G(v) + d_G(z) - 2$$

Due to the definition of line graph, we have clearly this result.

The edge GA index of $T(p,q)$ nanotube is

$$GA_e(T(p,q)) = 12pq + p(\frac{32\sqrt{3} - 84}{5})$$

Consider the $T(p,q)$ nanotube. The number of edges of graph $T(p,q)$ and line graph $L(T(p,q))$ are $6pq - p$ and$12pq - 4p$, respectively. If we consider to the edges of $L(T(p,q))$, there exist $2p$ edges with endpoints which have degrees 3 and 3, $8p$ edges with endpoints which have degrees 4 and 3 and $12pq - 14p$ edges with endpoints which have degree 4.

Therefore, with using the edge GA index formula and number of edges with their degrees in $L(G)$, the desire result can be obtained.

The edge GA index of T'(p',q') nanotube is

$$GA_e(T'(p',q')) = 12p'q' + p'(\frac{8\sqrt{6}}{5} + \frac{32\sqrt{3}}{7} + \frac{6\sqrt{5}}{9} - 14)$$

Consider the T'(p',q') nanotube. The number of edges of graph T'(p',q') and line graph $L(T'(p',q'))$ are $6p'q' + p'$ and$12p'q' - 2p'$, respectively. If we consider to the edges of $L(T(p,q))$, there exist $4p'$ edges with endpoints which have degrees 2 and 3, $8p'$ edges with endpoints which have degrees 4 and 3 and $12p'q' - 14p'$ edges with endpoints which have degree 4.

Therefore, with using the edge GA index formula and number of edges with their degrees in $L(T'(p',q'))$, the desire result can be obtained.

Lemma 2.2 (6) *Let G be a graph, $u \in V(G)$ and $e = vz \in E(G)$. Then we have:*
$d_{T(G)}(e) = d_{L(G)}(e) + 2 = d_G(v) + d_G(z)$ *and*
$d_{T(G)}(u) = 2d_G(u)$.

The total GA index of $T(p,q)$ nanotube is

$$GA_t(T(p,q)) =$$

$$30pq - 27p + 8p(\frac{\sqrt{6}}{5} + \frac{2\sqrt{5}}{9} + \frac{3\sqrt{30}}{11})$$

Consider the $T(p,q)$ nanotube. The number of edges of graph $T(p,q)$, line graph $L(T(p,q))$ and total graph $T(T(p,q))$ are $6pq - p$, $12pq - 4p$ and $30pq - 7p$, respectively. If we consider to the edges of $T(p,q)$ in $T(T(p,q))$, there exist $4p$ edges with endpoints which have degrees 4 and 6, and $6pq - 5p$ edges with endpoints which have degree 6.

If we consider to the edges of $L(T(p,q))$ in $T(T(p,q))$, there exist $8p$ edges with endpoints which have degrees 5 and 6, $2p$ edges with endpoints which have degrees 5 and 5 and $12pq - 14p$ edges with endpoints which have degree 6.

If we consider to the edges of $T(T(p,q))$ that are not the edges of $T(p,q)$ and $L(T(p,q))$, there exist $4p$ edges with endpoints which have degrees 4 and 5, $4p$ edges with endpoints which have degrees 5 and 6, $8p$ edges with endpoints which have degrees 6 and 5 and $12pq - 10p$ edges with endpoints which have degree 6. Therefore, the desire result can be obtained. The total GA index of $T'(p',q')$ nanotube is

$$GA_t(T'(p',q')) = 30p'q' - 23p' + 8p'(\frac{\sqrt{6}}{5} + \frac{4\sqrt{5}}{9} + \frac{3\sqrt{30}}{11})$$

Consider the $T'(p',q')$ nanotube. The number of edges of graph $T'(p',q')$, line graph $L(T'(p',q'))$ and total graph $T(T'(p',q'))$ are $6p'q' + p'$, $12p'q' - 2p'$ and $30p'q' + p'$, respectively. If we consider to the edges of $T'(p',q')$ in $T(T'(p',q'))$, there exist $2p'$ edges with endpoints which have degrees 4 and 4, $4p'$ edges with endpoints which have degrees 4 and 6, and $6p'q' - 5p'$ edges with endpoints which have degree 6.

If we consider to the edges of $L(T'(p',q'))$ in $T(T'(p',q'))$, there exist $4p'$ edges with endpoints which have degrees 4 and 5, $8p'$ edges with endpoints which have degrees 5 and 6 and $12p'q' - 14p'$ edges with endpoints which have degree 6.

If we consider to the edges of $T(T'(p',q'))$ that are not the edges of $T'(p',q')$ and $L(T'(p',q'))$, there exist $4p'$ edges with endpoints which have degrees 4 and 4, $4p'$ edges with endpoints which have degrees 4 and 5, $4p'$ edges with endpoints which have degrees 6 and 5 and $12p'q' - 10p'$ edges with endpoints which have degree 6. Therefore, the desire result can be obtained.

3 The edge GA for subdivision graphs

Firstly, we restate the subdivision graph which constructed from a graph G.

Suppose $G = (V, E)$ is a connected graph with the vertex set $V(G)$ and the edge set $E(G)$. Give an edge $e = (u, v)$, let $V(e) = \{u, v\}$. The subdivision graph $S(G)$ which is related graphs to graph G have been defined as follows (See [11]):

Subdivision Graph: $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length two, or equivalently, by inserting an additional vertex into each edge of G. See Figure 3 (c).

Given $G = (V, E)$, where $|E(G)| \subset \begin{pmatrix} V(G) \\ 2 \end{pmatrix}$, we may define another set that we use:
$EV(G) := \{\{e, v\} | e \in E(G), V(G) \ni v \in V(e)\}$

We can write the subdivision operator above as follows:
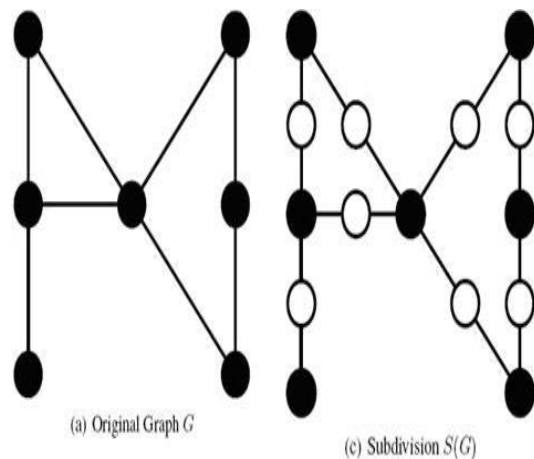$$S(G) := \left(V(G) \bigcup E(G), EV(G) \right)$$

Figure 3: The subdivision operator S(G).

Theorem 3.1 *Let G be a graph with n vertices and m edges. Then we have:*

$$GA(S(G)) = 2\sqrt{2} \sum_{u \in V(G)} \frac{(d_G(u))^{\frac{3}{2}}}{2 + d_G(u)}$$

According to the formula of GA index and the structure of *S(G)*, we have

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

$$\sum_{uv \in E(S(G))} \frac{2\sqrt{d_G(u)2}}{2 + d_G(u)}$$

Also $|E(S(G))| = \sum_{u \in V(G)} d_G(u)$, then

$$GA(S(G)) = \sum_{uv \in E(S(G))} \frac{2\sqrt{d_G(u)2}}{2 + d_G(u)} =$$

$$2\sqrt{2} \sum_{u \in V(G)} \frac{(d_G(u))^{\frac{3}{2}}}{2 + d_G(u)}$$

Theorem 3.2 *Let G be a graph with n vertices and m edges. Then we have:*

$$GA_e(S(G)) = \sum_{u \in V(G)} \binom{d_G(u)}{2} + GA(G)$$

Due to the structure of *S(G)*, the number of edges of *L(S(G))* is $\frac{1}{2} \sum_{u \in V(G)} (d_G(u))^2$.

If we take two adjacent edges $e = uv$ and $f = wz$ in *S(G)* as the vertices of an edge in *L(S(G))* that two disjoint vertices u and w are in $V(G)$, the quantity $\frac{2\sqrt{d_{L(G)}(e)d_{L(G)}(f)}}{d_{L(G)}(e) + d_{L(G)}(f)}$ will be $\frac{2\sqrt{d_G(u)d_G(w)}}{d_G(u) + d_G(w)}$. In addition, the number of these pair of edges in *S(G)* is equal to $|E(G)|$. Then if we name the set of these pair of edges with A then we have

$$\sum_{(e,f) \in A} \frac{2\sqrt{d_{L(G)}(e)d_{L(G)}(f)}}{d_{L(G)}(e) + d_{L(G)}(f)} =$$

$$\sum_{uw \in E(G)} \frac{2\sqrt{d_G(u)d_G(w)}}{d_G(u) + d_G(w)} = GA(G)$$

For remaining pair of edges $e' = u'v'$ and $f' = u'z'$ in *S(G)* as the endpoints of edges in *L(S(G))* that only the vertex u' is in $V(G)$, we have

$$\sum_{(e,f) \in B} \frac{2\sqrt{d_{L(G)}(e)d_{L(G)}(f)}}{d_{L(G)}(e) + d_{L(G)}(f)} =$$

$$\sum_{(e,f) \in B} \frac{2\sqrt{d_G(u)d_G(u)}}{d_G(u) + d_G(u)} = |B|$$

which B is the set of pair of edges (e', f') in *L(S(G))*.

If we look an vertex v of G in *S(G)*, the number of elements of B which is common in v is $\binom{d_G(v)}{2}$.

Therefore $|B| = \sum_{u \in V(G)} \binom{d_G(u)}{2}$.

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