On the total version of geometric–arithmetic index

A. MAHMIANI[1] AND O. KHORMALI[2,•]

[1]*Department of Mathematics, Payame Noor University, P. O. Box: 19395–4697, Tehran, Iran*
[2]*Mathematics and Informatics Research Group, ACECR, Tarbiat Modares University, P.O.Box : 14115-343, Tehran, Iran*

(*Received March 9, 2013; Accepted March 14, 2013*)

ABSTRACT

The total version of geometric–arithmetic index of graphs is introduced based on the end-vertex degrees of edges of their total graphs. In this paper, beside of computing the total GA index for some graphs, its some properties especially lower and upper bounds are obtained.

Keywords: Geometric–arithmetic index, total graph, vertex degree.

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 [7]. The oldest topological index which introduced by Harold Wiener in 1947 is ordinary (vertex) version of Wiener index [9] 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 Randić [6] which is defined as the sum of certain bond contributions calculated from the vertex degree of the hydrogen suppressed molecular graphs.

•Corresponding Author (Tel/fax +98 21 82883493 E-mail: o_khormali@modares.ac.ir)

Motivated by the definition of Randić 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], Vukičević and Furtula [8] 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 [1,8,10].

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.

It is natural which we introduce the total version of geometric-arithmetic index 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 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 $T(G)$.

In this paper, we focus our attention to total version of GA index and its main results including lower and upper bounds.

2. PRIMARY RESULTS

Firstly, we compute the total GA index of some familiar graphs P_n, S_n, K_n, $K_{m,n}$ and C_n which are the path, star, complete graph, complete bipartite graph and cycle, respectively. Also, we compute it for $TUC_4C_8(S)$ nanotubes. Before computing, we mention to the relation between degree of vertices in graph G, Line graph $L(G)$ and total graph $T(G)$.

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

$$d_{T(G)}(e)=d_{L(G)}(e)+2=d_G(v)+d_G(z) \text{ and } d_{T(G)}(u)=2d_G(u)$$

Proof. Let G be a graph, $u \in V(G)$ and $e = vz \in E(G)$. Since $d_{L(G)}(e) = d_G(v) + d_G(z) - 2$ and e will be connected to v and z as vertices in $T(G)$, it is clear that $d_{T(G)}(e) = d_{L(G)}(e) + 2$. Also, Due to the definition of Total graph, we have $d_{T(G)}(u)=2d_G(u)$. □

Conclusion 2.2. The total GA index of some familiar graphs P_n, S_n, K_n, $K_{m,n}$ and C_n are as follows:

1. $GA_t(P_n) = (4n-13) + \frac{140\sqrt{2} + 240\sqrt{3} + 84\sqrt{6}}{105}$

2. $GA_t(S_n) = (n-1)(\frac{2\sqrt{n-1}}{n} + \frac{n-2}{2} + \frac{2\sqrt{2n}}{n+2} + \frac{2\sqrt{2n^2-2n}}{3n-2})$

3. $GA_t(K_n) = (n+1)\binom{n}{2}$

4. $GA_t(K_{m,n}) = mn(\frac{2\sqrt{mn}}{m+n} + \frac{m+n-2}{2} + \frac{2\sqrt{2n(m+n)}}{m+3n} + \frac{2\sqrt{2m(m+n)}}{3m+n})$

5. $GA_t(C_n) = 4n$

Now, we compute the total GA index of $TUC_4C_8(S)$ nanotubes. In Figure 1, the $TUC_4C_8(S)$ nanotube is depicted.

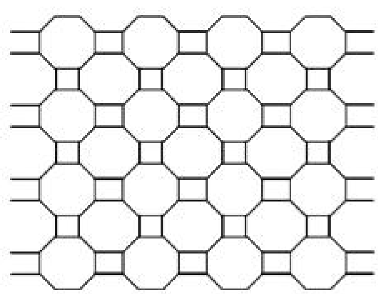

Figure 1. Two dimensional lattice of $TUC_4C_8(S)$ nanotube, p=4, q=4.

We denote the number of squares in one row of squares by p and the number of rows of squares by q. For example see the Figure 1. We show the molecular graph of $TUC_4C_8(S)$ nanotube with TUC in following computation.

Conclusion 3.2. The total GA index of TUC nanotube is

$$GA_t(TUC) = 60pq - 54p + 8p(\frac{\sqrt{6}}{5} + \frac{4\sqrt{30}}{11} + \frac{6\sqrt{5}}{9} + 1)$$

Proof. Consider the *TUC* nanotube. The number of edges of graph *TUC* line graph $L(TUC)$ and total graph $T(TUC)$ are $12pq-2p$, $24pq-8p$ and $60pq-14p$, respectively. If we consider to the edges of *TUC* in $T(TUC)$, there exist $4p$ edges with endpoints which have degrees 4 and 6, $2p$ edges with endpoints which have degrees 4 and 4 and $12pq-8p$ edges with endpoints which have degree 6.

If we consider to the edges of $L(TUC)$ in $T(TUC)$, there exist $8p$ edges with endpoints which have degrees 5 and 6, $4p$ edges with endpoints which have degrees 4 and 5 and $24pq-20p$ edges with endpoints which have degree 6.

If we consider to the edges of $T(TUC)$ that are not the edges of *TUC* and $L(TUC)$, there exist $8p$ edges with endpoints which have degrees 4 and 4, $8p$ edges with endpoints which have degrees 4 and 5, $8p$ edges with endpoints which have degrees 6 and 5 and $24pq-28p$ edges with endpoints which have degree 6. Therefore, the desire result can be obtained. □

3. BOUNDS FOR TOTAL GA INDEX

In following, we will find some bounds for total GA index.

Proposition 3.1. Let G be a connected graph with n vertices and m edges. Therefore, we have

$$GA_t(G) \le \left(\sum_{u\in V(G)} d_G{}^2(u) \right) + m$$

where $d_G(u)$ is the degree of vertex $u \in V(G)$.

Proof. Consider a connected graph G with n vertices and m edges. Due to the fact that the geometric mean is less than or equal to the arithmetic mean, we have for total GA index of graph G,

$$GA_t(G) \le |E(T(G))| = |E(G)| + |E(L(G))| + |E(T(G)) \setminus E(G) \cup E(L(G))| =$$
$$m + \left(\left(\sum_{u\in V(G)} d_G{}^2(u) \right) - m \right) + 2m = \left(\sum_{u\in V(G)} d_G{}^2(u) \right) + m.$$

□

Theorem 3.2. Let G be a simple graph with n vertices and m edges, then

$$0 \le GA_t(G) \le \binom{n}{2}(n+1)$$

Lower bound is achieved if and only if G is an empty graph, and upper bound is achieved if and only if G is a complete graph.

Proof. Since $\frac{2\sqrt{d_{T(G)}(x)d_{T(G)}(y)}}{d_{T(G)}(x)+d_{T(G)}(xy)}$ is positive for each edge of total graph of G. Then, $GA_t(G) \geq 0$ and if G is empty, $GA_t(G) = 0$. Also, Due to the fact that the geometric mean is less than or equal to the arithmetic mean, we have

$$GA_t(G) \leq 1.|E(T(G))| \leq 1.\binom{n}{2}(n+1).$$

And if G is complete graph K_n, $GA_t(K_n) = |E(T(K_n))| = \binom{n}{2}(n+1)$. □

Theorem 3.3. Let *G* be a nonempty simple graph with *n* vertices and *m* edges, then

$$(4n-13)+\frac{140\sqrt{2}+240\sqrt{3}+84\sqrt{6}}{105} \leq GA_t(G) \leq \binom{n}{2}(n+1)$$

Lower bound is achieved if and only if *G* is a path P_n and upper bound is achieved if and only if *G* is a complete graph K_n.

Proof. The upper bound follows from Theorem 3.2. Now, we prove the lower bound. As we know from vertex version of GA index, the acyclic graphs have the least vertex GA index. Therefore, the only graph which its line graph is acyclic is path. Then, the edge GA index has its least value for paths. In addition, paths have the minimum edges among all nonempty simple connected graphs. Hence,

$$GA_t(G) \geq GA_t(P_n) = (4n-13)+\frac{140\sqrt{2}+240\sqrt{3}+84\sqrt{6}}{105}$$ □

REFERENCES

1. G. H. Fath-Tabar, B. Furtula and I. Gutman, A new geometric-arithmetic index, *J. Math. Chem.*, **47** (2010) 477–486.
2. I. Gutman and B. Furtula, *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008.
3. A. Iranmanesh, I. Gutman, O. Khormali and A. Mahmiani, The edge versions of Wiener index, *MATCH Commun. Math. Comput. Chem.*, **61:3** (2009) 663–672.
4. X. Li and I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors*, Univ. Kragujevac, Kragujevac, 2006.
5. A. Mahimiani, O. Khormali and A. Iranmanesh, On the edge version of geometric-arithmetic index, *Dig. J. Nanomat. Bios.*, **7 :2** (2012) 411 – 414.
6. M. Randic, On the characterization of molecular branching, *J. Amer. Chem. Soc.*, **97** (1975) 6609 – 6615.

7. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Weinheim, Wiley-VCH, 2000.
8. D. Vukicevic and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.*, **46** (2009) 1369–1376.
9. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.*, **69** (1947) 17–20.
10. Y. Yuan, B. Zhou and N. Trinajsti, On geometric-arithmetic index, *J. Math. Chem.*, **47** (2010) 833–841.