MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **79** (2018) 467-475

ISSN 0340 - 6253

Maximum and Second Maximum of Geometric–Arithmetic Index of Tricyclic Graphs

Hanyuan Deng[a], Suresh Elumalai[b,*], Selvaraj Balachandran[c]

[a]*Key Laboratory of High Performance Computing and Stochastic Information Processing (HPCSIP) (Ministry of Education of China), College of Mathematics and Computer Science, Hunan Normal University, Changsha, Hunan 410081, P. R. China*
hydeng@hunnu.edu.cn

[b]*Department of Mathematics, Velammal Engineering College, Surapet, Chennai-66, Tamil Nadu, India*
sureshkako@gmail.com

[c]*Department of Mathematics, School of Humanities and Sciences, SASTRA University, Thanjavur, India*
bala_maths@rediffmail.com

(Received August 18, 2017)

Abstract

Geometric–arithmetic index is defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$, where d_u denotes the degree of a vertex u in G. In this paper, we obtain the first and second maximum values of geometric–arithmetic index for all tricyclic graphs on n vertices and the corresponding extremal graphs.

1 Introduction

We consider only simple, undirected and finite graphs. A graph is denoted by $G = G(V, E)$, where V is its vertex set and E its edge set. The order of G is the number $n = |V(G)|$ of its vertices and its size is the number $m = |E|$ of its edges. For two vertices u and v $(u, v \in V)$, if $uv \in E(G)$, we say u and v adjacent in G. The degree of a vertex

* Corresponding author

u, denoted d_u, is the number of vertices adjacent to it in G. The number of vertices of degree i in G will be denoted by $n_i = n_i(G)$. We denote the minimum and the maximum degree of vertices of G by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively.

During the last decades, a large number of topological indices were introduced and found some applications in chemistry, see e.g., [4, 5, 13]. The study of topological indices goes back to the seminal work by Wiener [15] in which he used the sum of all shortest-path distances, nowadays known as the Wiener index of a (molecular) graph for modeling physical properties of alkanes.

The geometric–arithmetic (GA) index is a newly proposed graph invariant in mathematical chemistry. Motivated by the definition of the Randić connectivity index, Vukičević and Furtula [14] proposed the geometric–arithmetic index. The geometric–arithmetic index $GA(G)$ of a graph G is defined as in [14] by

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \tag{1}$$

The reason for introducing a new index is to gain prediction of some property of molecules somewhat better than obtained by already indices. For physicochemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and acentric factor, it is noted in Rodriguez and Sigarreta [11] and Vukičević and Furtula [14] that the predictive power of GA index is somewhat better than the predictive power of other indices such as Randić index.

In [14] Vukičević and Furtula gave the lower and upper bounds for GA, and identified the trees with the minimum and the maximum GA indices, which are the star and the path respectively. In [1], Das and Trinajstić compared the GA and ABC indices for chemical trees and molecular graphs. In [16], Yuan, Zhou and Trinajstić gave the lower and upper bounds for the GA index for molecular graphs using the numbers of vertices and edges. They also determined the n-vertex molecular trees with the minimum, the second-minimum and the third-minimum, as well as the second-maximum and the third-maximum, GA indices. The details about mathematical properties of the GA indices and their applications in QSPR and QSAR can be found in the survey [2] reported by Das, Gutman and Furtula. For instance, see the recent papers [8–10, 12] and references cited therein.

Recently, Du et al. [3,7] determined the (molecular) trees, unicyclic and bicyclic graphs with maximum GA indices. In this paper, we will determine the first and second maximum graphs of GA indices for the tricyclic graphs.

2 Preliminaries

Let e be an edge of the graph G, connecting the vertices u and v. Then defining $GA\left(G\right)$ is by associating a weight $w\left(e\right)$ to the edge e:

$$w\left(e\right)=\frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

so that the geometric–arithmetic index is a sum of edge contributions:

$$GA\left(G\right)=\sum_{e\in E}w\left(e\right). \tag{2}$$

The weight $w\left(e\right)$ is positive-valued for all edges e.

Let G be a simple graph with $n\geq 2$ vertices and m edges. An edge of G connecting a vertex of degree i with a vertex of degree j will be called an (i,j)-edge. The number of (i,j)-edges will be denoted by e_{ij}. Clearly, $e_{ij}=e_{ji}$ and $\sum\limits_{1\leq i\leq j\leq n-1}e_{ij}=m$. Eq.(1) can now be rewritten as

$$\begin{aligned}GA\left(G\right)&=\sum_{1\leq i\leq j\leq n-1}\frac{2\sqrt{ij}}{i+j}e_{ij}=\sum_{1\leq i\leq j\leq n-1}\left[1-\frac{\left(\sqrt{i}-\sqrt{j}\right)^2}{i+j}\right]e_{ij}\\&=\sum_{1\leq i\leq j\leq n-1}e_{ij}-\sum_{1\leq i\leq j\leq n-1}\frac{\left(\sqrt{i}-\sqrt{j}\right)^2}{i+j}e_{ij}\end{aligned}$$

Let, as before, e be the edge of the graph G connecting the vertices u and v. Associate to the edge e a weight $w^*\left(e\right)$:

$$w^*\left(e\right)=\left[\frac{\left(\sqrt{d_u}-\sqrt{d_v}\right)^2}{d_u+d_v}\right]$$

For graphs without isolated vertices (in particular, for connected graphs),

$$GA\left(G\right)=m-\sum_{e\in E}w^*\left(e\right) \tag{3}$$

Lemma 2.1. *If G is a simple graph with m edges, then*

$$GA(G)=m-\sum_{uv\in E(G)}\frac{\left(\sqrt{d_u}-\sqrt{d_v}\right)^2}{d_u+d_v}. \tag{4}$$

For a connected graph G with m edges, from Eq.(3), we have $GA\left(G\right)=m-f\left(G\right)$, where $f\left(G\right)=\sum_{uv\in E(G)}\left[\frac{\left(\sqrt{d_u}-\sqrt{d_v}\right)^2}{d_u+d_v}\right]$. Thus, for a fixed m, $GA\left(G\right)$ is decreasing on $f\left(G\right)$. Using this fact, we will determine tricyclic graphs with large GA indices.

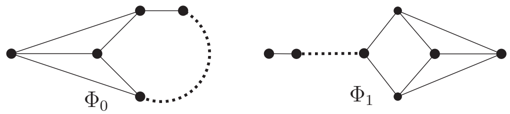

Figure 1. Tricyclic graphs Φ_0 and Φ_1 .

Let $\mathcal{G}_n$ be the set of all connected graphs with n vertices and $n+2$ edges. A graph $G \in \mathcal{G}_n$ is called a tricyclic graph. Let $\mathcal{G}_n^1 = \{G|G \in \mathcal{G}_n \text{ and } e_{33} = 5, e_{23} = 2, e_{22} = n-5\}$ and $\mathcal{G}_n^2 = \{G|G \in \mathcal{G}_n \text{ and } e_{12} = e_{23} = 1, e_{33} = 7, e_{22} = n-7\}$ with $\mathcal{G}_n^1 = \{\Phi_0\}$ and $\mathcal{G}_n^2 = \{\Phi_1\}$ are the unique tricyclic graphs with n vertices respectively (see Fig. 1). Table 1 lists the equivalence classes (Eq.cl.) of $\mathcal{G}_n$ with $n_1 = 0$ (i.e, each class pertaining to a particular degree sequence) that are of interest for the present considerations.

3 Main Results

In this section, we determine the first and second maximum of GA indices for tricyclic graphs.

Lemma 3.1. (See [6]) *There is a connected tricyclic graph G of order n with $n_1(G) = 0$ if and only if G satisfies Table 1.*

Table 1. Degree distributions of connected tricyclic graphs with $n_1 = 0$.

Eq.cl.	n_6	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 7)$
D_1	1	0	0	0	$n-1$	0	0
D_2	0	1	0	1	$n-2$	0	0
D_3	0	0	2	0	$n-2$	0	0
D_4	0	0	1	2	$n-3$	0	0
D_5	0	0	0	4	$n-4$	0	0

Lemma 3.2. *For the tricyclic graph Φ_0, we have $GA(\Phi_0) = n + \dfrac{4\sqrt{6}}{5}$.*

Lemma 3.3. *For the tricyclic graph Φ_1, we have $GA(\Phi_1) = n + \dfrac{6\sqrt{6}+10\sqrt{2}}{15}$.*

Theorem 3.4. *Let $G \in \mathcal{G}_n \backslash (\mathcal{G}_n^1 \cup \mathcal{G}_n^2)$ for $n \geq 6$, then*

$$GA(G) < n + \frac{6\sqrt{6}+10\sqrt{2}}{15} < n + \frac{4\sqrt{6}}{5}.$$

Proof. For $n = 5$ there exits exactly four non-isomorphic tricyclic graphs. So, it is enough to assume that $n \geq 6$. Two cases are considered as follows:

A) Tricyclic graphs without pendant vertices.

B) Tricyclic graphs containing at least one pendant vertex.

Case (A): Lemma 3.1 and Table 2 gives us the result.

Table 2. The connected tricyclic graphs with $n_1 = 0$ and their GA.

Eq.cl.	e_{23}	e_{24}	e_{25}	e_{26}	e_{33}	e_{34}	e_{35}	e_{44}	e_{22}	GA
D_1	0	0	0	6	0	0	0	0	$n-4$	$n+3\sqrt{3}-4$
D_2	2	0	4	0	0	0	1	0	$n-5$	$n+\frac{35\sqrt{15}+160\sqrt{10}+112\sqrt{6}-700}{140}$
D_2	3	0	5	0	0	0	0	0	$n-6$	$n+\frac{50\sqrt{10}+42\sqrt{6}-210}{35}$
D_3	0	6	0	0	0	0	0	1	$n-5$	$n+4\sqrt{2}-4$
D_3	0	8	0	0	0	0	0	0	$n-6$	$n+\frac{16\sqrt{2}-18}{3}$
D_4	4	4	0	0	1	0	0	0	$n-7$	$n+\frac{24\sqrt{6}+40\sqrt{2}-90}{15}$
D_4	6	4	0	0	0	0	0	0	$n-8$	$n+\frac{36\sqrt{6}+40\sqrt{2}-120}{15}$
D_4	5	3	0	0	0	1	0	0	$n-7$	$n+\frac{14\sqrt{6}+4\sqrt{3}+14\sqrt{2}-49}{7}$
D_4	3	3	0	0	1	1	0	0	$n-6$	$n+\frac{42\sqrt{6}+20\sqrt{3}+70\sqrt{2}-175}{35}$
D_4	4	2	0	0	0	2	0	0	$n-6$	$n+\frac{168\sqrt{6}+120\sqrt{3}+140\sqrt{2}-630}{105}$
D_4	2	2	0	0	1	2	0	0	$n-5$	$n+\frac{84\sqrt{6}+120\sqrt{3}+140\sqrt{2}-420}{105}$
D_5	12	0	0	0	0	0	0	0	$n-10$	$n+\frac{24\sqrt{6}-50}{5}$
D_5	10	0	0	0	1	0	0	0	$n-9$	$n+4\sqrt{6}-8$
D_5	8	0	0	0	2	0	0	0	$n-8$	$n+\frac{16\sqrt{6}-30}{5}$
D_5	6	0	0	0	3	0	0	0	$n-7$	$n+\frac{12\sqrt{6}-20}{5}$
D_5	4	0	0	0	4	0	0	0	$n-6$	$n+\frac{8\sqrt{6}-10}{5}$
D_5	2	0	0	0	5	0	0	0	$n-5$	$n+\frac{4\sqrt{6}}{5}$

Case (B): If G is a tricyclic graph containing at least one pendant vertex, then we characterize the following subcases.

Subcase (1): G has at least two pendant vertices.

Let x_1 and x_2 be two pendant vertices and adjacent to vertices y_1 and y_2, respectively, and $d_{y_1} = r_1 \geq d_{y_2} = r_2$, then $r_1 \geq r_2 \geq 2$.

(1) If $r_1 \geq r_2 \geq 3$, then

$$f(G) = \sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\right)^2}{d_u + d_v} \geq \frac{\left(\sqrt{1} - \sqrt{r_1}\right)^2}{1 + r_1} + \frac{\left(\sqrt{1} - \sqrt{r_2}\right)^2}{1 + r_2}$$
$$\geq 2 \times \frac{\left(\sqrt{1} - \sqrt{3}\right)^2}{1 + 3} = 2 - \sqrt{3}.$$

From Lemma 2.1, we have $GA(G) = m - f(G) \leq n + \sqrt{3}$ and the equality holds for the unique graph depicted in Fig. 2.

(2) If $r_2 = 2$ and $r_1 \geq 3$, then $e_{12} \geq 1$ and G has at least one $(2,t)$-edge for some $t \geq 3$. Since $\frac{(\sqrt{1}-\sqrt{r_1})^2}{1+r_1} \geq \frac{(\sqrt{1}-\sqrt{3})^2}{1+3}$ and $\frac{(\sqrt{2}-\sqrt{t})^2}{2+t} \geq \frac{(\sqrt{2}-\sqrt{3})^2}{2+3}$, we have

$$f(G) = \sum_{uv \in E(G)} \frac{\left(\sqrt{d_u}-\sqrt{d_v}\right)^2}{d_u+d_v} \geq \frac{(\sqrt{1}-\sqrt{2})^2}{1+2} + \frac{(\sqrt{1}-\sqrt{3})^2}{1+3} + \frac{(\sqrt{2}-\sqrt{3})^2}{2+3}$$
$$= \frac{90-12\sqrt{6}-15\sqrt{3}-20\sqrt{2}}{30}.$$

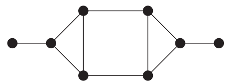

Figure 2. The unique tricyclic graph G with two pendant vertices and $GA(G) = 8+\sqrt{3}$.

From Lemma 2.1, we get

$$GA(G) = m - f(G) \leq n + \frac{12\sqrt{6}+15\sqrt{3}+20\sqrt{2}-30}{30} \approx n + 1.7886$$

equality holds if and only if $G \in \mathcal{G}_n^3$, where $\mathcal{G}_n^3 = \{G | G \in \mathcal{G}_n$ and $e_{33} = 8, e_{23} = e_{13} = e_{12} = 1, e_{22} = n-11\}$

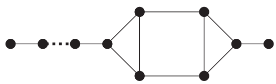

Figure 3. A tricyclic graph $G \in \mathcal{G}_n^3$ with $GA(G) = n + 1.7886$.

(3) If $r_1 = r_2 = 2$, then G has at least two $(2,t)$-edges, where $t \geq 3$ and

$$f(G) = \sum_{uv \in E(G)} \frac{\left(\sqrt{d_u}-\sqrt{d_v}\right)^2}{d_u+d_v} \geq 2 \times \frac{(\sqrt{1}-\sqrt{2})^2}{1+2} + 2 \times \frac{(\sqrt{2}-\sqrt{3})^2}{2+3}$$
$$= \frac{60-12\sqrt{6}-20\sqrt{2}}{15}.$$

From Lemma 2.1, we have

$$GA(G) = m - f(G) \leq n + \frac{12\sqrt{6}+20\sqrt{2}-30}{15} \approx n + 1.8452$$

equality holds if and only if $G \in \mathcal{G}_n^3$, where $\mathcal{G}_n^3 = \{G | G \in \mathcal{G}_n$ and $e_{33} = 8, e_{23} = e_{12} = 2, e_{22} = n-12\}$. Thus, for any tricyclic graph G with $n \geq 10$ and at least two pendant vertices, the maximum value of GA index is $n + \frac{12\sqrt{6}+20\sqrt{2}-30}{15}$.

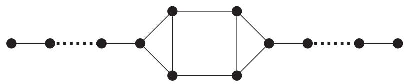

Figure 4. A tricyclic graph $G \in \mathcal{G}_n^3$ with $GA(G) = n + 1.8452$.

Subcase (2): G has exactly one pendant vertex.

Let x be the pendant vertex and adjacent to vertex y, then $d_y = r \geq 2$.

(1) If $r \geq 3$, then

$$f(G) = \sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\right)^2}{d_u + d_v} \geq \frac{(\sqrt{1} - \sqrt{r})^2}{1 + \sqrt{r}} \geq \frac{(\sqrt{1} - \sqrt{3})^2}{1 + \sqrt{3}} = \frac{2 - \sqrt{3}}{2}.$$

From Lemma 2.1, we have $GA(G) = m - f(G) \leq n + \dfrac{2 + \sqrt{3}}{2} \approx n + 1.8660$ and the equality holds for the unique graph depicted in Fig. 5.

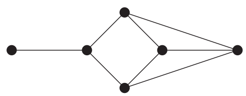

Figure 5. The unique tricyclic graph G with one pendant vertex with $GA(G) = 6 + 1.8660$.

(2) If $r = 2$, then G has at least one $(2, t)$-edge, where $t \geq 3$.

(a) If $t \geq 4$, then

$$\begin{aligned} f(G) &= \sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\right)^2}{d_u + d_v} > \frac{(\sqrt{1} - \sqrt{2})^2}{1 + 2} + \frac{(\sqrt{2} - \sqrt{t})^2}{2 + t} \\ &\geq \frac{(\sqrt{1} - \sqrt{2})^2}{1 + 2} + \frac{(\sqrt{2} - \sqrt{4})^2}{2 + 4} = \frac{6 - 4\sqrt{2}}{3}. \end{aligned}$$

From Lemma 2.1, we have

$$GA(G) = m - f(G) < n + \frac{4\sqrt{2}}{3} \approx n + 1.8856.$$

(b) If $t = 3$, then

$$\begin{aligned} f(G) &= \sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\right)^2}{d_u + d_v} \geq \frac{(\sqrt{1} - \sqrt{2})^2}{1 + 2} + \frac{(\sqrt{2} - \sqrt{t})^2}{2 + t} \\ &= \frac{(\sqrt{1} - \sqrt{2})^2}{1 + 2} + \frac{(\sqrt{2} - \sqrt{3})^2}{2 + 3} = \frac{30 - 6\sqrt{6} - 10\sqrt{2}}{15}. \end{aligned}$$

From Lemma 2.1, we have

$$GA(G) = m - f(G) \leq n + \frac{6\sqrt{6} + 10\sqrt{2}}{15} \approx n + 1.9226$$

equality holds if and only if $G \in \mathcal{G}_n^2$.

Thus, from the above arguments and calculations. If G is a tricyclic graph with $\delta = 1$, then $GA(G) \leq GA(\Phi_1)$ and if G is a tricyclic graph with $\delta \geq 2$, then $GA(G) < GA(\Phi_1) < GA(\Phi_0)$. This completes the proof. ■

Acknowledgment: The authors would like to express their sincere gratitude to the anonymous referees for a very careful reading of this paper and for all their insightful comments, which lead to a number of improvements to this paper. The first author is supported by the Hunan Provincial Innovation Foundation for Postgraduate (CX2017B170) and the Construct Program of the Key Discipline in Hunan Province.

References

[1] K. C Das, Trinajstić, Comparison between first geometric–arithmetic index and atom–bond connectivity index, *Chem. Phys. Lett.* **497** (2010) 149–151.

[2] K. C Das, I. Gutman, B. Furtula, Survey on geometric–arithmetic indices of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 595–644.

[3] Z. Du, B. Zhou, N. Trinajstić, On geometric–arithmetic indices of (molecular) trees, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 681–697.

[4] I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications I*, Univ. Kragujevac, Kragujevac, 2010.

[5] I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications II*, Univ. Kragujevac, Kragujevac, 2010.

[6] I. Gutman, A. Ghalavand, T. Dehghan–Zadeh, A. R. Ashrafi, Graphs with smallest forgotten index, *Iranian J. Math. Chem.* **8** (2017) 259–273.

[7] N. H. M. Husin, R. Hasni, Z. Du, On extremum geometric–arithmetic indices of (molecular) trees, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 375–386.

[8] T. Mansour, M. A. Rostami, S. Elumalai, G. B. A. Xavier, Correcting a paper on Randić and geometric–arithmetic indices, *Turk. J. Math.* **41** (2017) 27–32.

[9] J. M. Rodríguez, J. M. Sigarreta, On the geometric–arithmetic index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 103–120.

[10] J. M. Rodríguez, J. M. Sigarreta, Spectral study of the geometric–arithmetic index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 121–135.

[11] J. M. Rodríguez, J. M. Sigarreta, Spectral properties of geometric–arithmetic index, *Appl. Math. Comput.* **277** (2016) 142–153.

[12] J. M. Sigarreta, Bounds for the geometric–arithmetic index of a graph, *Miskolc Mathematical Notes,* **16** (2015) 1199–1212.

[13] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009.

[14] D. Vukičević, 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.

[15] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[16] Y. Yuan, B. Zhou, N. Trinajstić, On geometric–arithmetic index, *J. Math. Chem.* **47** (2) (2010) 833–841.