MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **65** (2011) 705-712

ISSN 0340 - 6253

Note on the Second Geometric–Arithmetic Index*

Zikai Tang, Yaoping Hou

Department of Mathematics, Hunan Normal University, Changsha, Hunan 410081, China
email: zikaitang@163.com (Z. Tang), yphou@hunnu.edu.cn (Y. Hou)

(Received May 13, 2010)

Abstract: Let $G = (V, E)$ be a simple graph and GA_2 is molecular-structure descriptor, belonging to the class of geometric-arithmetic indices. In this paper, the trees with second minimum and maximum GA_2 are characterized and the unicyclic graphs with minimum and maximum GA_2 are characterized.

1 Introduction

All graphs in this article are simple and finite. The vertex and edge sets of a graph G are $V(G)$ and $E(G)$, respectively. The degree of a vertex u in G is denoted by $\deg_G(u)$ or d_u. The number of vertices of G is denoted by $n(G)$ and it is called the order of G. The distance $d_G(u, v)$ between vertices u and $v \in V(G)$ is the number of edges on a shortest path connecting u and v in G. Molecular descriptors are playing a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [1]. There are numerous of topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [6–9] .

In [2, 4] the geometric-arithmetic index GA was conceived, defined as

$$GA = GA(G) = \sum_{uv\in E(G)} \frac{\sqrt{d_u\, d_v}}{\frac{1}{2}(d_u + d_v)} \tag{1.1}$$

*This research is supported by the Department of Education of Hunan Province (08C579) and National Natural Science Fund of China (10771061).

where uv is an edge of the graph G connecting the vertices u and v, d_u stands for the degree of the vertex u, and the summation goes over all edges of G.

Let $e = uv$ be an edge of G, connecting the vertices u and v. Define the sets

$$N(e, u, G) = \{x \in V(G) | d_G(x, u) < d_G(x, v)\}$$

$$N(e, v, G) = \{x \in V(G) | d_G(x, u) > d_G(x, v)\}$$

consisting of vertices of G lying closer to u than to v, and lying closer to v than to u, respectively. The number of such vertices is then

$$n_u(e) = n_u(e, G) = |N(e, u, G)| \text{ and } n_v(e) = n_v(e, G) = |N(e, v, G)|.$$

In [3] the second geometric-arithmetic index GA_2 was conceived by Fath-Tabar, Furtula and Gutman, defined as

$$GA_2 = GA_2(G) = \sum_{uv \in E(G)} \frac{\sqrt{n_u n_v}}{\frac{1}{2}(n_u + n_v)} \tag{1.2}$$

where the summation goes over all edges of G. In [3], they gave the lower and upper bounds for the GA_2 index, identified the trees with the minimum and the maximum GA_2 indices, which are the star and the path, respectively.

Lemma 1.1. *[3] Let G be a connected graph with n vertices and m edges. Then*

$$GA_2(G) \geq \frac{2m\sqrt{n-1}}{n} \tag{1.3}$$

with equality if and only if $G \cong S_n$, where S_n denotes the n-vertex star.

Lemma 1.2. *[3] Let G be a connected graph with n vertices and m edges. Then $GA_2(G) \leq m$, with equality if and only if all vertices of G are mutually equivalent.*

Lemma 1.3. *[3] Let G be a tree with n vertices. Then*

$$GA_2(S_n) \leq GA_2(G) \leq GA_2(P_n) \tag{1.4}$$

with the equality on the left if and only if $G \cong S_n$, where S_n denotes the n-vertex star and the equality on the right if and only if $G \cong P_n$, where P_n denotes the n-vertex path.

In this paper, we characterize the trees with the second minimum and second maximum GA_2 among all trees on n vertices and characterize the unicyclic graphs with minimum and maximum GA_2 among all unicyclic graphs on n vertices.

2 Tree with the second minimum and second maximum GA_2 index

First we consider the graph G_1 and graph G_2 depicted in Fig. 1. These two graphs differ only in the position of a terminal vertex: in G_2 this terminal vertex is moved from the b-branch to the a-branch. In what follows we assume that $a \geq b \geq 1$.

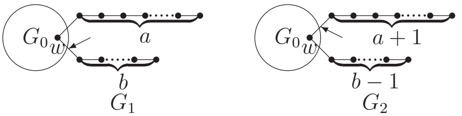

Fig. 1. The transformation $G_1 \longrightarrow G_2$ increases the GA_2 index if $a \geq b \geq 1$.

Proposition 2.1. *Let G_0 be a connected graph, $w \in V(G_0)$, $G_1 = G_0 + P_a + P_b$, and $G_2 = G_0 + P_{a+1} + P_{b-1}$ depicted in Fig. 1. Then $GA_2(G_1) \leq GA_2(G_2)$ with equality if and only if $|V(G_0)| = 1$.*

Proof. By the definition of GA_2, we have

$$\begin{aligned} GA_2(G_2) - GA_2(G_1) &= \sum_{u'v' \in E(G_2)} \frac{\sqrt{n_{u'}(e', G_2) n_{v'}(e', G_2)}}{\frac{1}{2}(n_{u'}(e', G_2) + n_{v'}(e', G_2))} \\ &- \sum_{uv \in E(G_1)} \frac{\sqrt{n_u(e, G_1) n_v(e, G_1)}}{\frac{1}{2}(n_u(e, G_1) + n_v(e, G_1))} . \end{aligned}$$

All terms cancel out except the terms pertaining to the edges indicated by arrows in Fig. 1, for which

$$\begin{aligned} \frac{\sqrt{n_{u'}(e', G_2) n_{v'}(e', G_2)}}{\frac{1}{2}(n_{u'}(e', G_2) + n_{v'}(e', G_2))} &= \frac{2\sqrt{(a+1)(n-a-1)}}{n} \\ \frac{\sqrt{n_u(e, G_1) n_v(e, G_1)}}{\frac{1}{2}(n_u(e, G_1) + n_v(e, G_1))} &= \frac{2\sqrt{b(n-b)}}{n} . \end{aligned}$$

We conclude that

$$GA_2(G_2) - GA_2(G_1) = \frac{2(\sqrt{(a+1)(n-a-1)} - \sqrt{b(n-b)})}{n} \geq 0$$

where the equality holds if and only if $a + b + 1 = n$, in other words, $|V(G_0)| = 1$. □

By Proposition 2.1 and Lemma 1.1, we obtain next proposition easily.

Proposition 2.2. *Let T be a tree with $n \geq 6$ and $T \ncong S_n, P_n, T_1, T_2$ (depicted in Fig. 2.). Then*

$$GA_2(S_n) < GA_2(T_2) < GA_2(T) < GA_2(T_1) < GA_2(P_n) \; .$$

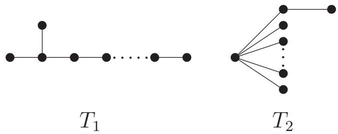

Fig. 2.

3 Unicyclic Graphs with minimum and maximum GA_2 index

Let $G = (V, E)$ be an unicyclic graph of order n with its circuit $C_m = v_1 v_2 \ldots v_m v_1$ of length m, $T_1, T_2, \ldots, T_k$ $(0 \leq k \leq m)$ are the all nontrivial components (they are all nontrivial trees) of $G - E(C_m)$, u_i is the common vertex of T_i and C_m, $i = 1, 2, \ldots, k$. Such an unicyclic graph is denoted by $C_m^{u_1, u_2, \ldots, u_k}(T_1, T_2, \ldots, T_k)$. Specially, $G = C_n$ for $k = 0$. And if $k = 1$, we write $C_m(T_1)$ for $C_m^{u_1}(T_1)$; and $C_3^{u_1}(S_{n-2}) = S_n + e$. Let $n(T_i) = l_i + 1$, $i = 1, 2, \ldots, k$, then $l = l_1 + l_2 + \cdots + l_k = n - m$. By Proposition 2.1, we have next lemma.

Lemma 3.1. *Let*

$$\begin{aligned} G_1 &= C_m^{u_1, u_2, \ldots, u_k}(S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1}) \\ G_2 &= C_m^{u_1, u_2, \ldots, u_k}(P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1}) \end{aligned}$$

where $u_1, u_2, \ldots, u_k$ are the centers of $S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1}$, respectively, in G_1; and $u_1, u_2, \ldots, u_k$ are the pendent of $P_{l_1+1}, P_{l_2+1}, \ldots, P_{l_k+1}$, respectively, in G_2. Then

$$GA_2(G_1) \leq GA_2(G) \leq GA_2(G_2)$$

for any unicyclic graph $G = C_m^{u_1, u_2, \ldots, u_k}(T_1, T_2, \ldots, T_k)$ of order n and $n(T_i) = l_i + 1$, $i = 1, 2, \ldots, k$, with the equality on the left (resp., on the right) if and only if $G \cong G_1$ (resp., $G \cong G_2$).

By Lemma 1.2, we can get next proposition.

Proposition 3.2. *$G = C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$ be an unicyclic graph of order $n \geq 4$. Then*

$$GA_2(G) \leq GA_2(C_n),$$

with the equality if and only if $G \cong C_n$

Let $G_1 = C_m^{w_1,w_2,\dots,w_k}(S_{l_1+1}, S_{l_2+1}, \dots, S_{l_k+1})$ be an unicyclic graphs, $u, v \in C_m$, $deg_{G_1}(w_1) \geq 3$, $deg_{G_1}(w_i) \geq 3$, $w_1u_1, \dots, w_1u_p$ $(p \geq 1)$ are pendent edges incident with w_1 and $w_iv_1, \dots, w_iv_q$, $(q \geq 1)$ are pendent edges incident with w_i(depicted in Fig. 3). G_1' obtained by removing edges $w_iv_1, \dots, w_iv_q$ and replacing edges $w_1v_1, \dots, w_1v_q$. We say that G_1' is a Tr_1-**transform** of G_1(depicted in Fig. 3, left). G_1'' obtained by removing edges $w_1u_1, \dots, w_1u_p$ and replacing edges $w_iu_1, \dots, w_iu_p$. We say that G_1'' is a Tr_2-**transform** of G_1 (depicted in Fig. 3, right).

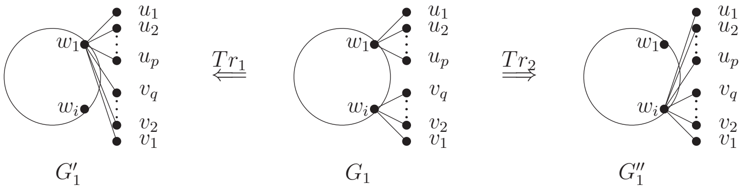

Fig. 3. The transformations Tr_1, Tr_2

Lemma 3.3. *Let $G_1 = C_m^{w_1,w_2,\dots,w_k}(S_{l_1+1}, S_{l_2+1}, \dots, S_{l_k+1})$ be an unicyclic graphs and $deg_{G_1}(w_1) = l_1 + 2$, $deg_{G_1}(w_i) = l_i + 2$. G_1' be a Tr_1-**transform** of G_1, G_1'' be a Tr_2-**transform** of G_1 depicted in Fig. 3. Then $GA_2(G_1') \leq GA_2(G_1)$ or $GA_2(G_1'') \leq GA_2(G_1)$.*

Proof. We divide $E(G_1)$ into the following five groups: (i) $E_1 = \{e = uv \in G_1 | deg_{G_1}(v) = 1$ and $deg_{G_1}(u) \geq 3\}$; (ii) $E_2 = \{e = uv \in C_m | d(u, w_1) \leq d(v, w_1)$ and $d(u, w_i) \leq d(v, w_i)\}$; (iii) $E_3 = \{e = uv \in C_m | d(u, w_1) \geq d(v, w_1)$ and $d(u, w_i) \geq d(v, w_i)\}$; (iv) $E_4 = \{e = uv \in C_m | d(u, w_1) < d(v, w_1)$ and $d(u, w_i) > d(v, w_i)\}$; (v) $E_5 = \{e = uv \in C_m | d(u, w_1) > d(v, w_1)$ and $d(u, w_i) < d(v, w_i)\}$.

By the definition of GA_2, we have

$$GA_2(G_1) = \sum_{i=1}^{5} \sum_{uv \in E_i} \frac{\sqrt{n_u(e, G_1) n_v(e, G_1)}}{\frac{1}{2}(n_u(e, G_1) + n_v(e, G_1))}.$$

For G_1' be a Tr_1-**transform** of G_1, G_1'' be a Tr_2-**transform** of G_1 depicted in Fig. 3. We easily have that if $uv \in E_i$ $(1 \le i \le 3)$, then

$$\frac{\sqrt{n_u(e,G_1)n_v(e,G_1)}}{\frac{1}{2}(n_u(e,G_1)+n_v(e,G_1))} = \frac{\sqrt{n_{u'}(e',G_1')n_{v'}(e',G_1')}}{\frac{1}{2}(n_{u'}(e',G_1')+n_{v'}(e',G_1'))} = \frac{\sqrt{n_{u''}(e'',G_1'')n_{v''}(e'',G_1'')}}{\frac{1}{2}(n_{u''}(e'',G_1'')+n_{v''}(e'',G_1''))}.$$

Next for $uv \in E_4$, by induction on the size of E_4 we prove that

$$\frac{\sqrt{n_u(e,G_1)n_v(e,G_1)}}{\frac{1}{2}(n_u(e,G_1)+n_v(e,G_1))} \ge \frac{\sqrt{n_{u'}(e',G_1')n_{v'}(e',G_1')}}{\frac{1}{2}(n_{u'}(e',G_1')+n_{v'}(e',G_1'))},$$

or

$$\frac{\sqrt{n_u(e,G_1)n_v(e,G_1)}}{\frac{1}{2}(n_u(e,G_1)+n_v(e,G_1))} \ge \frac{\sqrt{n_{u''}(e'',G_1'')n_{v''}(e'',G_1'')}}{\frac{1}{2}(n_{u''}(e'',G_1'')+n_{v''}(e'',G_1''))}.$$

Denote t be the size of E_4. When $t=1$, we have $e = w_1w_i \in E_4, n_{w_1}(e) \ge n_{w_i}(e)$ or $n_{w_1}(e) \le n_{w_i}(e)$. If $n_e(w_1) \le n_e(w_i)$, by Tr_2-**transform** of G_1, we have

$$n_{w_1''}(e'') = n_{w_1}(e) - l_1, n_{w_i''}(e'') = n_{w_i}(e) + l_i$$

So when $t=1$, we have

$$\frac{\sqrt{n_{w_1}(e,G_1)n_{w_i}(e,G_1)}}{\frac{1}{2}(n_{w_1}(e,G_1)+n_{w_i}(e,G_1))} \ge \frac{\sqrt{n_{w_1''}(e'',G_1'')n_{w_i''}(e'',G_1'')}}{\frac{1}{2}(n_{w_1''}(e'',G_1'')+n_{w_i''}(e'',G_1''))}.$$

Suppose the above result holds when $t=d$. Let $d(w_1,w_i) = d+1$, $P = w_1x_1\ldots x_dw_i$ be a path. By induction hypothesis, we have $deg_{G_1}(x_i) = 2(1 \le i \le d)$ and $n_{w_1}(e_1) \ge n_{x_1}(e_1), n_{w_i}(e_d) \le n_{x_d}(e_d)$ or $n_{w_1}(e_1) \le n_{x_1}(e_1), n_{w_i}(e_d) \ge n_{x_d}(e_d)$.

If $n_{w_1}(e_1) \le n_{x_1}(e_1), n_{w_i}(e_d) \ge n_{x_d}(e_d)$, we have $n_{x_{i-1}}(e_i) \le n_{x_i}(e_i)(2 \le i \le d)$. By Tr_2-**transform** of G_1, we get G_1''.

$$n_{x_{i-1}''}(e_i'') = n_{x_{i-1}}(e_i) - l_1, n_{x_i''}(e_i'') = n_{x_i}(e_i) + l_i.$$

So when $t = d+1$ $e_i \in E_4$ $(1 \le i \le d)$, we have that

$$\frac{\sqrt{n_{x_{i-1}}(e_i,G_1)n_{x_i}(e_i,G_1)}}{\frac{1}{2}(n_{x_{i-1}}(e_i,G_1)+n_{x_i}(e_i,G_1))} \ge \frac{\sqrt{n_{x_{i-1}''}(e_i'',G_1'')n_{x_i''}(e_i'',G_1'')}}{\frac{1}{2}(n_{x_{i-1}''}(e_i'',G_1'')+n_{x_i''}(e_i'',G_1''))}.$$

If $uv \in E_5$ we can similarly prove that

$$\frac{\sqrt{n_u(e,G_1)n_v(e,G_1)}}{\frac{1}{2}(n_u(e,G_1)+n_v(e,G_1))} \le \frac{\sqrt{n_{u'}(e',G_1')n_{v'}(e',G_1')}}{\frac{1}{2}(n_{u'}(e',G_1')+n_{v'}(e',G_1'))}$$

or

$$\frac{\sqrt{n_u(e,G_1)n_v(e,G_1)}}{\frac{1}{2}(n_u(e,G_1)+n_v(e,G_1))} \ge \frac{\sqrt{n_{u''}(e'',G_1'')n_{v''}(e'',G_1'')}}{\frac{1}{2}(n_{u''}(e'',G_1'')+n_{v''}(e'',G_1''))}.$$

Summarizing above, let $G_1 = C_m^{w_1,w_2,\ldots,w_k}(S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1})$ be an unicyclic graph and $deg_{G_1}(w_1) = l_1 + 2, deg_{G_1}(w_i) = l_i + 2$. G_1' be a Tr_1-**transform** of G_1, G_1'' be a Tr_2-**transform** of G_1 depicted in Fig.3. Then $GA_2(G_1') \leq GA_2(G_1)$ or $GA_2(G_1'') \leq GA_2(G_1)$. □

Proposition 3.4. *Let $G = C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$ be an unicyclic graph of order $n \geq 4$. Then*

$$GA_2(G) \geq GA_2(C_4^{u_1}(S_{n-3}))$$

with the equality if and only if $G \cong C_4^{u_1}(S_{n-3})$.

Proof. First, by Lemma 3.1, we have

$$GA_2(C_m^{u_1,u_2,\ldots,u_k}(S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1})) \leq GA_2(C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)).$$

Let $G_0 = C_m^{u_1,u_2,\ldots,u_k}(S_{l_1+1}, S_{l_2+1}, \ldots, S_{l_k+1})$ $(k \geq 1)$. By Lemma 3.3, we can obtain a series graphs G_i, $0 \leq i \leq k-1$, G_i obtained by Tr_1-**transform** or Tr_2-**transform** G_{i-1} and $GA_2(C_m(S_{n-m+1})) \leq \cdots \leq GA_2(G_{i+1}) \leq GA_2(G_i) \leq \cdots \leq GA_2(G_0)$.

By calculating,

$$GA_2(C_m(S_{n-m+1})) = \frac{2(n-m)\sqrt{n-1}}{n} + \frac{4k\sqrt{k(k+n-m)}}{n+2k-m} + d\ .$$

where $k = [m/2]$, $d = 2(m-2k)$.

When $m = 2k$ $(k \geq 3)$, we have

$$GA_2(C_m(S_{n-m+1})) - GA_2(C_{m-2}(S_{n-m+3}))$$
$$= \frac{2(n-2k)\sqrt{n-1}}{n} + \frac{4k\sqrt{k(n-k)}}{n} - \left(\frac{2(n-2k+2)\sqrt{n-1}}{n} + \frac{4(k-1)\sqrt{(k-1)(n-k+1)}}{n}\right) > 0\ .$$

When $m = 2k+1$ $(k \geq 2)$, we have

$$GA_2(C_m(S_{n-m+1})) - GA_2(C_{m-2}(S_{n-m+3}))$$
$$= \frac{2(n-2k-1)\sqrt{n-1}}{n} + \frac{4k\sqrt{k(n-k-1)}}{n-1} - \frac{2(n-2k+1)\sqrt{n-1}}{n} - \frac{4(k-1)\sqrt{(k-1)(n-k)}}{n-1}$$
$$= \frac{4k\sqrt{k(n-k-1)} - 4k\sqrt{(k-1)(n-k)}}{n-1} + \frac{4n\sqrt{(k-1)(n-k)} - 4(n-1)\sqrt{n-1}}{n(n-1)} > 0\ .$$

When $m = 4, m = 3$, we have

$$GA_2(C_4(S_{n-3})) - GA_2(C_3(S_{n-2}))$$
$$= \frac{2(n-4)\sqrt{n-1}}{n} + \frac{8\sqrt{2(n-2)}}{n} - \left(\frac{2(n-3)\sqrt{n-1}}{n} + \frac{4\sqrt{n-2}}{n-1} + 2\right) < 0\ .$$

Summarizing above, $C_4^{u_1}(S_{n-3})$ have the minimum GA_2 index among all unicyclic graphs of order $n \geq 4$. □

References

[1] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[2] 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.

[3] G. Fath–Tabar, B. Furtula, I. Gutman, A new geometric–arithmetic index, *J. Math. Chem.* **47** (2010) 477–486.

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

[5] F. Buckley, F. Harary, *Distance in Graphs*, Addison–Wesley, Redwood, 1990.

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

[7] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* **4** (1971) 2332–2339.

[8] K. C. Das, I. Gutman, Estimating the Szeged index, *Appl. Math. Lett.* **16** (2009) 1680–1684.

[9] B. Liu, I. Gutman, On a conjecture on Randić indices, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 143–154.