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Original Scientific Article

Comparison Between Geometric-arithmetic Indices

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Abstract. The concept of geometric–arithmetic indices (GA) was introduced in the chemical graph theory very recently. In this letter we compare the geometric–arithmetic indices for chemical trees, starlike trees and general trees. Moreover, we give a conjecture for general graphs. (doi: 10.5562/cca2005)

Keywords: Molecular Graph, Chemical Tree, Starlike Tree, Geometric-arithmetic Indices

INTRODUCTION

Let $G = (V, E)$ denote a simple graph with n vertices and m edges, $V(G) = \{1, 2, \ldots, n\}$ and $m = |E(G)|$.[1] Also, let d_i be the degree of the vertex i for $i = 1, 2,\ldots, n$. The maximum vertex degree is denoted by Δ in G. Recently, a new class of topological descriptors, based on some properties of vertices of graph is presented. These indices are named as "*geometric–arithmetic indices*" (GA_{general}) and their definition is as follows:

$$GA_{\text{general}} = GA_{\text{general}}(G) = \sum_{ij\in E(G)} \frac{\sqrt{Q_iQ_j}}{\frac{1}{2}(Q_i+Q_j)}, \qquad (1)$$

where Q_i is some quantity that in a unique manner can be associated with the vertex i of the graph G. The first member of this class was considered by Vukičević and Furtula[2] by setting Q_i to be the degree d_i of the vertex i of the graph G:

$$GA_1 = GA_1(G) = \sum_{ij\in E(G)} \frac{2\sqrt{d_id_j}}{d_i+d_j}.$$

For $i,j \in V(G)$, let $d(i,j|G)$ be the distance between the vertices i and j in G. For $ij \in E(G)$,

$$n_i = |\{x \in V(G) : d(x,i|G) < d(x,j|G)\}|$$

The second member of this class was considered by Fath-Tabar *et al.*[3] by setting Q_i to be the number n_i of vertices of G lying closer to the vertex i than to the vertex j for the edge ij of the graph G:

$$GA_2 = GA_2(G) = \sum_{ij\in E(G)} \frac{2\sqrt{n_in_j}}{n_i+n_j}.$$

Let x be a vertex and ij be an edge of the graph G. The distance between x and ij is defined as

$$d(x,ij|G) = \min\{d(x,i|G), d(x,j|G)\}.$$

For $ij \in E(G)$, let

$$m_i = |\{f \in E(G) : d(i,f|G) < d(j,f|G)\}|.$$

It should be noted that m_i is not a quantity that in a unique manner can be associated with the vertex i of the graph G, but that it depends on the edge ij. Yet, this restriction is not relevant for the definition of GA_3. Note that in all cases $m_i \ge 0$ and

$$m_i + m_j \le m-1.$$

Then, incorporating m_i as vertex quantity into Equation (1), the *third geometric–arithmetic index* is defined as,[4]

$$GA_3 = GA_3(G) = \sum_{ij\in E(G)} \frac{2\sqrt{m_im_j}}{m_i+m_j}.$$

It has been demonstrated, on the example of octane isomers, that GA index is well-correlated with a variety of physico-chemical properties.[2] Vukičević and Furtula[2] in order to study the predicive power of the GA index considered the following set of octane properties: boiling points, entropy, enthalpy of vaporization, stand-

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Table 1. Comparison of structure-property models based on the GA indices to models obtained by the connectivity index

Property	Correlation Coefficient	
	GA-index	Connectivity index
Boiling point	0.823	0.821
Entropy	0.912	0.906
Enthalpy of vaporization	0.941	0.936
Standard enthalpy of vaporization	0.966	0.958
Enthalpy of formation	0.858	0.850
Acentric factor	0.912	0.904

ard enthalpy of vaporization, enthalpy of formation and acentric factor. The structure-property models based on the GA indices were comparable (and in some cases even better than) to models obtained by the connectivity index.[5] This can be seen from data in Table 1, taken from the paper by Vukučević and Furtula.[2]

The mathematical properties and uses of geometric-arithmetic indices are studied by several groups.[2–4,6–13] A survey of mathematical properties of the GA indices and their uses in QSPR and QSAR is recently given by Das, Gutman and Furtula.[14] The above results indicate the potential of the GA molecular descriptors in the structure-property-activity modeling. In order to fully explore their potential, it is necessary to study the mathematical and computational properties and the range of applicability of the GA indices. The preliminary results are encouraging. We compare the first geometric–arithmetic index and the atom-bond connectivity index.[15] In this letter we compare the geometric–arithmetic indices for chemical trees, starlike trees and general trees. Moreover, we give a conjecture for general graphs. Finally, we give conclusion.

PRELIMINARIES

A connected graph with maximum vertex degree at most 4 belongs to a family of molecular graphs depicting carbon compounds.[16] Its graphical representation may resemble a structural formula of some (usually organic) molecule. That was a primary reason for employing graph theory in chemistry. Nowadays this area of mathematical chemistry is called *chemical graph theory*.[16] A tree in which the maximum vertex degree does not exceed 4 is said to be a "*chemical tree*". A vertex of a graph is said to be pendent if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendent if one of its vertices is a pendent vertex. Denote, as usual, by $K_{1,n-1}$ and P_n, the star and the path on n vertices, respectively.

A tree is said to be starlike if exactly one of its vertices has degree greater than two. By $S(r_1, r_1, \ldots, r_k)$, we denote the starlike tree which has a vertex 1 of degree $k \geq 3$ and which has the property

$$S(r_1, r_2, \ldots, r_k) \setminus \{1\} = P_{r_1} \cup P_{r_2} \cup \ldots \cup P_{r_k}$$

This tree has $r_1 + r_2 + \ldots + r_k + 1 = n$ vertices and assumed that $r_1 \geq r_2 \geq \ldots \geq r_k \geq 1$. We say that the starlike tree $S(r_1, r_1, \ldots, r_k)$ has k branches, the lengths of which are $r_1, r_1, \ldots, r_k$, respectively.

COMPARISON BETWEEN GA_1 INDEX AND GA_2 INDEX

In this section we compare between GA_1 and GA_2 index for chemical trees and starlike trees. First we prove the following result:

Lemma. Let T be a chemical tree. Then the number of pendent vertices in T are $2a + b + 2$, where a is the number of four degree vertices and b is the number of three degree vertices in T.

Proof: If h_i is the number of vertices of degree i in T, then we have

$$h_1 + h_2 + h_3 + h_4 = n$$

and

$$h_1 + 2h_2 + 3h_3 + 4h_4 = 2(n-1).$$

From the two relations above we get

$$h_1 - h_3 - 2h_4 = 2, \text{ i.e. } h_1 = 2a + b + 2,$$

where $h_3 = b$ and $h_4 = a$. Hence the *Lemma*.

Now we compare between GA_1 index and GA_2 index for chemical tree T.

Theorem 1. Let T be a chemical tree of order n. Then,

$$GA_1(T) \geq GA_2(T)$$

with equality if and only if G is isomorphic to $K_{1,i}, i = 1, 2, 3, 4$.

Proof: If $T \cong K_{1,i}, i = 1, 2, 3, 4$; one can see easily that $GA_1(T) = GA_2(T)$. If $T \cong P_n$ ($n > 3$), then from the definition of GA indices, we have $GA_1(T) > GA_2(T)$.

Otherwise, $3 \leq \Delta \leq 4$, $n \geq 5$, and $T \cong K_{1,i}$, $i = 1, 2, 3, 4$. Since T is a chemical tree, we must have $1 \leq d_i \leq 4$ for all i. Thus we have the edges with possible degree pairs (4,1), (4,2), (4,3), (4,4), (3,1), (3,2), (3,3), (2,1), (2,2). In Table 2, we calculate the values of $\frac{2\sqrt{d_i d_j}}{d_i + d_j}$ for all above degree pairs. First we assume that $n \geq 10$. Let

Table 2. Calculated values of $\frac{2\sqrt{d_i d_j}}{d_i + d_j}$ for possible degree pairs

(d_i,d_j)	(4,1)	(4,2)	(4,3)	(4,4)	(3,1)	(3,2)	(3,3)	(2,1)	(2,2)
$\frac{2\sqrt{d_i d_j}}{d_i + d_j}$	0.8	$\sqrt{\frac{8}{9}}$	$\sqrt{\frac{48}{49}}$	1	$\sqrt{\frac{3}{4}}$	$\sqrt{\frac{24}{25}}$	1	$\sqrt{\frac{8}{9}}$	1

a be the number of vertices of degree four and also let b be the number of vertices of degree three in T. Then there are at most $4a + 3b$ non-pendent edges ij with not $d_i = d_j = 2$. By *Lemma*, the number of pendent vertices are $2a + b + 2$ in T. From Table 2, we have

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} \geq 0.8$$

for each pendent edge $ij \in E(T)$ and

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} \geq \sqrt{\frac{8}{9}}$$

for each non-pendent edge $ij \in E(T)$.
Since $n \geq 10$, we have

$$\frac{2\sqrt{n_i n_j}}{n_i + n_j} \leq 0.6$$

for each pendent edge $ij \in E(T)$ and

$$\frac{2\sqrt{n_i n_j}}{n_i + n_j} \leq 1$$

for each non-pendent edg $ij \in E(T)$.
Using above results, we get

$$\begin{aligned} GA_1(T) - GA_2(T) &= \sum_{ij \in E(T), d_j = 1} \left(\frac{2\sqrt{d_i d_j}}{d_i + d_j} - \frac{2\sqrt{n_i n_j}}{n_i + n_j} \right) \\ &+ \sum_{ij \in E(T), d_i = d_j = 2} \left(\frac{2\sqrt{d_i d_j}}{d_i + d_j} - \frac{2\sqrt{n_i n_j}}{n_i + n_j} \right) \\ &+ \sum_{ij \in E(T), d_j > 2} \left(\frac{2\sqrt{d_i d_j}}{d_i + d_j} - \frac{2\sqrt{n_i n_j}}{n_i + n_j} \right) \\ &\geq 0.2\big(2a + b + 2\big) - 0.06\big(4a + 3b\big) > 0, \end{aligned}$$

as

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} = 1 \geq \frac{2\sqrt{n_i n_j}}{n_i + n_j} \quad \text{for } d_i = d_j = 2.$$

Next we have to show that $GA_1(T) > GA_2(T)$ for $5 \leq n \leq 9$. If $n = 5$, then $T \cong T_1$ (Figure 1) as $T \ncong K_{1,4}, P_5$. For $T = T_1$, we have $GA_1(T) > GA_2(T)$. Otherwise, $6 \leq n \leq 9$. Now we consider two cases (a) $\Delta = 3$, (b) $\Delta = 4$.

Case (a): $\Delta = 3$. Using Table 2, we have

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} - \frac{2\sqrt{n_i n_j}}{n_i + n_j} > 0.866 - 0.746 = 0.12$$

for each pendent edge $ij \in E(T)$, as $n \geq 6$ and

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} - \frac{2\sqrt{n_i n_j}}{n_i + n_j} > 0.97 - 1 = -0.03$$

for each non-pendent edge $ij \in E(T)$.

In this case there are at least three pendent edges in T. Using above results, we get $GA_1(T) > GA_2(T)$ as $n \leq 9$.

Case (b): $\Delta = 4$. If $T \cong T_2$ (Figure 1), then one can see easily that $GA_1(T) > GA_2(T)$. Otherwise, $7 \leq n \leq 9$. In this case there are at least four pendent edges and at most four non-pendent edges in T as $n \leq 9$. Using Table 2, we have

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} - \frac{2\sqrt{n_i n_j}}{n_i + n_j} > 0.8 - 0.7 = 0.1$$

for each pendent edge $ij \in E(T)$, as $n \geq 7$ and

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} - \frac{2\sqrt{n_i n_j}}{n_i + n_j} > 0.94 - 1 = -0.06$$

for each non-pendent edge $ij \in E(T)$. Thus we get $GA_1(T) > GA_2(T)$. This completes the proof.

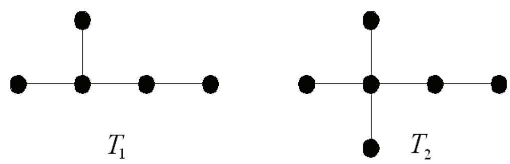

Figure 1. Two trees T1 and T2.

Now we compare between $GA_1(T)$ index and $GA_2(T)$ index for starlike trees.

Theorem 2. Let $S(r_1, r_1, \ldots, r_k)$ be a starlike tree of order n. Then

$$GA_1(S) \geq GA_2(S)$$

with equality if and only if S is isomorphic to star $K_{1,n-1}$.

Proof: When $r_1 = r_2 = \ldots = r_k = 1$, we have

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} = \frac{2\sqrt{n-1}}{n} = \frac{2\sqrt{n_i n_j}}{n_i + n_j}$$

for any edge $ij \in E(S)$. Thus we have $GA_1(K_{1,n-1}) = GA_2(K_{1,n-1})$. Otherwise, $r_1 \geq 2$.

First we assume that $r_k \geq 2$. Then $r_1 \geq r_2 \geq \ldots \geq r_k \geq 2$ and $n \geq 7$. Thus we have the edges with possible degree pairs $(k,1)$, $(k,2)$, $(2,1)$, $(2,2)$. For each edge ij we have

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} \geq \frac{2\sqrt{n_i n_j}}{n_i + n_j}$$

except possibly edges ij with degree pair $(k,2)$. Now we have

$$\frac{\sqrt{2k}}{k+2} > \frac{\sqrt{n-1}}{n}, \tag{2}$$

that is,

$$2(n-1) - k + \frac{2}{n-1} > \frac{4}{k}$$

which, evidently, is always obeyed. Also we have

$$\frac{\sqrt{2}}{3} > \frac{\sqrt{2(n-2)}}{n}, \tag{3}$$

that is,

$$n + \frac{4}{n-2} > 7$$

which, evidently, is always obeyed. Moreover, we have

$$r_i(n - r_i) \leq \frac{n^2}{4} \text{ for } 1 \leq i \leq k. \tag{4}$$

Now,

$$GA_1(S) = \frac{2\sqrt{2k}}{k+2}k + \sum_{i=1}^{k}(r_i - 2) + \frac{2\sqrt{2}}{3}k$$

and

$$GA_2(S) = \sum_{i=1}^{k}\sum_{j=2}^{r_i} \frac{2\sqrt{j(n-j)}}{n} + \frac{2\sqrt{n-1}}{n}k$$

$$\leq \sum_{i=1}^{k}(r_i - 2) + \frac{2\sqrt{2(n-2)}}{n}k + \frac{2\sqrt{n-1}}{n}k$$

by (4) and $r_k \geq 2$

$$< \sum_{i=1}^{k}(r_i - 2) + \frac{2\sqrt{2}}{3}k + \frac{2\sqrt{2k}}{k+2}k \quad \text{by (2) and (3)}$$

$$= GA_1(S).$$

Next we assume that some of r_i are equal to 1. Let $r_1 \geq r_2 \geq \ldots \geq r_q \geq 2$, $r_{q+1} = r_{q+2} = \ldots = r_k = 1$. Similarly, we can easily show that

$$\sum_{i=1}^{q}\sum_{j=1}^{r_i} \frac{2\sqrt{j(n-j)}}{n} < \frac{2\sqrt{2k}}{k+2}q + \sum_{i=1}^{q}(r_i - 2) + \frac{2\sqrt{2}}{3}q$$

and

$$\frac{\sqrt{k}}{k+1} \geq \frac{\sqrt{n-1}}{n}.$$

From above results we have

$$GA_1(S) > GA_2(S).$$

This completes the proof.

COMPARISON BETWEEN GA_2 INDEX AND GA_3 INDEX

In this section we compare between GA_2 index and GA_3 index for any tree T.

Theorem 3. For any tree T,

$$GA_2(T) > GA_3(T).$$

Proof: For any tree T,

$$n_i = m_i + 1,\ n_j = m_j + 1$$

for any edge $ij \in E(T)$.

Without loss of generality, we can assume that $n_i \geq n_j$ for any non-pendent edge $ij \in E(T)$, that is, we have

$$\frac{n_i}{n_j} = \frac{m_i + 1}{m_j + 1} \leq \frac{m_i}{m_j}$$

and

$$\frac{n_j}{n_i} \geq \frac{m_j}{m_i}.$$

From above results we have

$$\left(\frac{n_i}{n_j}\right)^{\frac{1}{4}} - \left(\frac{n_j}{n_i}\right)^{\frac{1}{4}} \leq \left(\frac{m_i}{m_j}\right)^{\frac{1}{4}} - \left(\frac{m_j}{m_i}\right)^{\frac{1}{4}}$$

Squaring both sides and simplifying, we get

$$\sqrt{\frac{n_i}{n_j}}+\sqrt{\frac{n_j}{n_i}}\leq\sqrt{\frac{m_i}{m_j}}+\sqrt{\frac{m_j}{m_i}}$$

that is,

$$\frac{\sqrt{n_i n_j}}{n_i+n_j}\geq\frac{\sqrt{m_i m_j}}{m_i+m_j}$$

for any non-pendent edge $ij\in E(T)$. But for any pendent edge $ij\in E(T)$,

$$\frac{\sqrt{n_i n_j}}{n_i+n_j}>0=\frac{\sqrt{m_i m_j}}{m_i+m_j}.$$

Thus we have $GA_2(T) > GA_3(T)$. This completes the proof.

Corollary. Let T be a chemical tree or starlike tree of order n. Then

$$GA_1(T)>GA_3(T).$$

Proof: By Theorem 1, Theorem 2, and Theorem 3, we get the required result.

Finally, the following conjecture holds.

Conjecture. For any connected graph G,

$$GA_1(T)\geq GA_2(T)\geq GA_3(T).$$

CONCLUSION

In this report we discuss the comparison between first and second geometric-arithmetic indices for chemical trees and starlike trees. Besides these, it has been shown that second geometric-arithmetic index is greater than to the third geometric-arithmetic index for any tree. Comparison between these indices, in the case of general graphs, remains an open problem.

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REFERENCES

1. R. J. Wilson, *Introduction to Graph Theory*, Oliver & Boyd, Edinburgh, 1974, 2nd printing.
2. D. Vukičević and B. Furtula, *J. Math. Chem.* **46** (2009) 1369–1376.
3. G. Fath-Tabar, B. Furtula, and I. Gutman, *J. Math. Chem.* **47** (2010) 477–486.
4. B. Zhou, I. Gutman, B. Furtula, and Z. Du, *Chem. Phys. Lett.* **482** (2009) 153–155.
5. (a) R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000; (b) R. Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009, Vol. I and II.
6. Y. Yuan, B. Zhou, and N. Trinajstić, *J. Math. Chem.* **47** (2010) 833–841.
7. K. C. Das, *MATCH Commun. Math. Comput. Chem.* **64** (3) (2010) 619–630.
8. K. C. Das, I. Gutman, and B. Furtula, *Discrete Appl. Math.* **159** (2011) 2030–2037.
9. K. C. Das, I. Gutman, and B. Furtula, *Iranian J. Math. Chem.* **1** (2) (2010) 17–28.
10. K. C. Das, I. Gutman, and B. Furtula, *Iranian J. Math. Chem.* **1** (2) (2010) 29–36.
11. M. Mogharrab and G. H. Fath-Tabar, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 33–38.
12. I. Gutman and B. Furtula (Eds.), *Novel Molecular Structure Descriptors - Theory and Applications I*, University of Kragujevac, Kragujevac, Serbia, 2010 pp. 137–172.
13. B. Furtula amd I. Gutman, *J. Chemometrics* **25** (2011) 87–91.
14. K. C. Das, I. Gutman, and B. Furtula, *MATCH Commun. Math. Comput. Chem.* **65** (3) (2011) 595–644.
15. K. C. Das and N. Trinajstić, *Chem. Phys. Lett.* **497** (2010) 149–151.
16. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1983; 2nd revised ed. 1992.