J Math Chem (2010) 47:477–486
DOI 10.1007/s10910-009-9584-7

ORIGINAL PAPER

A new geometric–arithmetic index

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Received: 28 April 2009 / Accepted: 27 July 2009 / Published online: 13 August 2009

Abstract A new molecular-structure descriptor GA_2, belonging to the class of geometric–arithmetic indices, is considered. It is closely related to the Szeged and vertex PI indices. The main properties of GA_2 are established, including lower and upper bounds. The trees with minimum and maximum GA_2 are characterized.

Keywords Geometric–arithmetic index · Szeged index · PI index · Distance (in graph) · Molecular-structure descriptor

1 Introduction

In a recent paper [1] the so-called *geometric–arithmetic index* GA was conceived, defined as

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

where uv is an edge of the (molecular) graph G connecting the vertices u and v, where d_u stands for the degree of the vertex u, and where the summation goes over

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all edges of G. It is easy to recognize that GA is just the first representative of a class of topological indices of the form

$$GA_{\text{general}} = GA_{\text{general}}(G) = \sum_{uv \in E(G)} \frac{\sqrt{Q_u\, Q_v}}{\frac{1}{2}(Q_u + Q_v)} \tag{1}$$

where Q_u is some quantity that in a unique manner can be associated with the vertex u of the graph G.

In this work we focus our attention to another member of this class, which we denote by GA_2 and which—tentatively—may be referred to as the *second geometric–arithmetic index*. Whereas GA is defined so as to be related to the famous Randić index [2–4], GA_2 is constructed in such a manner that it is related with Szeged and PI indices (see below).

Let G be a connected graph with n vertices and m edges, with vertex set $V(G)$ and edge set $E(G)$. As usual [5], the distance $d(x, y|G)$ between two vertices $x, y \in V(G)$ is defined as the length (= number of edges) of the shortest path that connects x and y.

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

$$\mathbf{N}(e, u, G) = \{\, x \in V(G) \,|\, d(x, u|G) < d(x, v|G) \,\}$$
$$\mathbf{N}(e, v, G) = \{\, x \in V(G) \,|\, d(x, u|G) > d(x, v|G) \,\}.$$

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

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

Note that vertices equidistant to u and v are not included into either $\mathbf{N}(e, u, G)$ or $\mathbf{N}(e, v, G)$. Such vertices exist only if the edge uv belongs to an odd-membered cycle. Hence, in the case of bipartite graphs, $\mathbf{N}(e, u, G) \cup \mathbf{N}(e, v, G) = V(G)$ and, consequently,

$$n_u(e, G) + n_v(e, G) = n \tag{2}$$

for all edges of the graph G.

It it also worth noting that $u \in \mathbf{N}(e, u, G)$ and $v \in \mathbf{N}(e, v, G)$, which implies that $n_u(e) \geq 1$ and $n_v(e) \geq 1$.

A previously much studied molecular-structure descriptor is the *Szeged index*:

$$Sz = Sz(G) = \sum_{uv \in E(G)} n_u(e) \cdot n_v(e). \tag{3}$$

Its main mathematical properties are outlined in the review [6] whereas data on its numerous chemical and pharmacological applications can be found in the book [7] and the references cited therein.

Another recently conceived structure descriptor [8–12], based on the numbers $n_u(e)$ and $n_v(e)$, is the so-called *vertex PI index*:

$$PI_v = PI_v(G) = \sum_{uv \in E(G)} [n_u(e) + n_v(e)]. \tag{4}$$

Recall that the abbreviation PI comes from "*Padmakar–Ivan*" where "*Padmakar*" is the first name of Khadikar, the inventor of the PI index [7,13–15], whereas "*Ivan*" is the first name of Gutman, who did not at all contribute to the development of this structure descriptor.

Because of (2), the vertex PI index of a bipartite graph with n vertices and m edges satisfies the simple identity

$$PI_v(G) = m\,n. \tag{5}$$

Now, motivated by the expressions occurring on the right-hand sides of Eqs. (3) and (4), and in view of the general formula (1), we define the *second geometric–arithmetic index* as

$$GA_2 = GA_2(G) = \sum_{uv \in E(G)} \frac{\sqrt{n_u(e) \cdot n_v(e)}}{\frac{1}{2}[n_u(e) + n_v(e)]}. \tag{6}$$

2 Bounds for the second geometric–arithmetic index

We say that the vertices x and y of a graph G are equivalent if the subgraphs $G - x$ and $G - y$ are isomorphic, $G - x \cong G - y$.

As usual, by K_n we denote the complete graph on n vertices. Among connected graphs K_n is the only graph for which $n_u(e) = n_v(e) = 1$ holds for all edges $e = uv$.

In view of the well-known fact that the geometric mean is less than or equal to the arithmetic mean, we have for any geometric–arithmetic index of a graph G with m edges,

$$GA_{\text{general}}(G) \leq m.$$

The special case of this is:

Proposition 1 *Let G be a connected graph. Then $GA_2(G) \leq m$, with equality if and only if all vertices of G are mutually equivalent.*

Only a few molecular graphs have the property $GA_2 = m$: the cycle and K_2.

Since for any edge $e = uv$ we have $n_u(e) + n_v(e) \geq 2$ and $\sqrt{n_u(e) \cdot n_v(e)} \leq [n_u(e) + n_v(e)]/2$, directly from Eqs. 4 and 6 we get:

Proposition 2 *For any connected graph G,*

$$GA_2(G) \leq \frac{1}{2}\, PI_v(G)$$

with equality if and only if $n_u(e) = n_v(e) = 1$ holds for all edges $e = uv$, i. e., if and only if $G \cong K_n$.

Recall that in the case of bipartite graphs (that is, in the case of almost all molecular graphs), $PI_v = m\,n$.

Proposition 3 *For any connected graph with m edges,*

$$GA_2(G) \le \sqrt{m\,Sz(G)} \tag{7}$$

with equality if and only if $G \cong K_n$.

Proof Because of $n_u(e)\,,\; n_v(e) \ge 1$,

$$GA_2(G) \le \sum_{uv \in E(G)} \sqrt{n_u(e) \cdot n_v(e)}. \tag{8}$$

Applying the Cauchy–Schwarz inequality,

$$\begin{aligned} \sum_{uv \in E(G)} \sqrt{n_u(e) \cdot n_v(e)} &= \sum_{uv \in E(G)} 1 \cdot \sqrt{n_u(e) \cdot n_v(e)} \\ &\le \sqrt{\left(\sum_{uv \in E(G)} 1^2\right)\left(\sum_{uv \in (EG)} n_u(e) \cdot n_v(e)\right)} \\ &= \sqrt{m \cdot Sz(G)}. \end{aligned} \tag{9}$$

Equality in (9) occurs if and only if $n_u(e) = n_v(e)$ holds for all e. For equality in (8), in addition it must be $n_u(e) = n_v(e) = 1$, which implies $G \cong K_n$. □

Proposition 4 *For any connected graph with m edges,*

$$GA_2(G) \le \sqrt{Sz(G) + m(m-1)} \tag{10}$$

with equality if and only if $G \cong K_n$.

Proof

$$\begin{aligned} [GA_2(G)]^2 &= \sum_{uv} \frac{4\,n_u(e) \cdot n_v(e)}{[n_u(e) + n_v(e)]^2} \\ &\quad + 2 \sum_{uv \ne u'v'} \frac{2\sqrt{n_u(e) \cdot n_v(e)}}{n_u(e) + n_v(e)} \cdot \frac{2\sqrt{n_{u'}(e') \cdot n_{v'}(e')}}{n_{u'}(e') + n_{v'}(e')} \\ &\le \sum_{uv} [n_u(e) \cdot n_v(e)] + 2 \sum_{uv \ne u'v'} (1) \cdot (1) \\ &= \sum_{uv} [n_u(e) \cdot n_v(e)] + 2\,\frac{m(m-1)}{2} \end{aligned} \tag{11}$$

and inequality (10) follows from (3). The case of equality is analyzed in the same manner as in the previous propositions. □

Proposition 5 *For the complete graph inequalities* (7) *and* (10) *are equivalent. For all other connected graphs the upper bound* (10) *is better than* (7).

Proof The inequality $\sqrt{m\, Sz} \geq \sqrt{Sz + m(m-1)}$ is easily transformed into $Sz \geq m$, which because of $n_u(e) \cdot n_v(e) \geq 1$ is obeyed by all graphs with m edges. Equality happens if and only if $n_u(e) = n_v(e) = 1$ for all edges. □

Proposition 6 *Let G be a connected graph with n vertices and $m \geq 1$ edges. Then*

$$GA_2(G) \geq \frac{2}{n}\sqrt{Sz + m(m-1)}. \tag{12}$$

Equality in (12) *is attained if and only if $G \cong K_2$.*

Inequality (12) should be compared with (10).

Proof Start with Eq. 11 and use the facts that $n_u(e)+n_v(e) \leq n$ and $n_u(e)\cdot n_v(e) \geq 1$. Then

$$\begin{aligned}[GA_2(G)]^2 &\geq \frac{4}{n^2}\sum_{uv}[n_u(e)\cdot n_v(e)] + 2\sum_{uv\neq u'v'}\left(\frac{2}{n}\right)\left(\frac{2}{n}\right)\\ &= \frac{4}{n^2}\, Sz(G) + \frac{4}{n^2}\binom{m}{2}\end{aligned}$$

from which (12) follows straightforwardly.

Requirement $n_u(e) \cdot n_v(e) = 1$ is satisfied for all edges if G is a complete graph, whereas $n_u(e)+n_v(e) = n$ is satisfied for all edges if G is bipartite. Therefore equality in (12) happens only if G is a bipartite complete graph, i. e., $G \cong K_2$. □

Proposition 7 *Let G be a connected graph with n vertices and m edges. Then*

$$GA_2(G) \geq \frac{2m\sqrt{n-1}}{n} \tag{13}$$

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

Proof Without loss of generality we may choose the vertices of the edge $e = uv$ so that $n_u(e) \geq n_v(e)$. Then, by denoting $n_u(e)/n_v(e)$ by x, we get

$$\frac{\sqrt{n_u(e)\cdot n_v(e)}}{\frac{1}{2}[n_u(e)+n_v(e)]} = \frac{2\sqrt{x}}{x+1}.$$

The variable x assumes values between 1 and $n-1$. In that interval the function $2\sqrt{x}/(x+1)$ monotonically decreases. Therefore,

$$\frac{2\sqrt{x}}{x+1} \geq \frac{2\sqrt{n-1}}{(n-1)+1} = \frac{2\sqrt{n-1}}{n}$$

with equality if and only if e is a pendent edge. The inequality (13) follows.

Note that the star S_n is the only n-vertex graph whose all edges are pendent. □

Proposition 8 *For the complete graph with two vertices, inequalities* (12) *and* (13) *are equivalent. For all other connected graphs the lower bound* (13) *is better than* (12).

Proof The right-hand sides of (12) and (13) are equal for $G \cong K_2$, when $n = 2$, $m = 1$, and $Sz = 1$. The inequality $(2m/n)\sqrt{n-1} \geq (2/n)\sqrt{Sz + m(m-1)}$ is easily transformed into $Sz \leq m[m(n-2)+1]$. For connected graphs, $m(n-2)+1 \geq (n-1)(n-2)+1 = n^2 - 3n + 3$, which for $n > 2$ exceeds the maximal value of the product $n_u(e) \cdot n_v(e)$, namely $\lfloor n/2 \rfloor \lceil n/2 \rceil$. Therefore $Sz \leq m[m(n-2)+1]$ holds for all connected graphs with $n > 2$ vertices. □

3 Trees with extremal second geometric–arithmetic index

Trees are connected bipartite graphs with $n-1$ edges. For them Eq. (2) holds, and GA_2 is simplified as

$$GA_2 = \frac{2}{n-1} \sum_{uv} \sqrt{n_u(e) \cdot n_v(e)}.$$

Note that the summation on the right-hand side of the above formula goes over $n-1$ terms.

Proposition 9 *The star* S_n *is the* n*-vertex tree with minimum second geometric–arithmetic index.*

Proof Since $n_u(e) + n_v(e) = n$, the minimum value of the product $n_u(e) \cdot n_v(e)$ is $1 \times (n-1) = n-1$, which happens if e is a pendent edge. The star is the only tree in which all edges are pendent. □

In order to determine the tree with maximum GA_2-value we need an auxiliary result. Consider the trees T_1 and T_2 depicted in Fig. 1. These two trees differ only in the position of a terminal vertex: in tree T_2 this terminal vertex is moved from the b-branch to the a-branch. In what follows we assume that $a \geq b$.

In the difference of the GA_2-values of T_1 and T_2, namely in

$$\frac{2}{n-1} \sum_{uv \in E(T_1)} \sqrt{n_u(e, T_1) \cdot n_v(e, T_1)} - \frac{2}{n-1} \sum_{u'v' \in E(T_2)} \sqrt{n_{u'}(e', T_2) \cdot n_{v'}(e', T_2)}$$

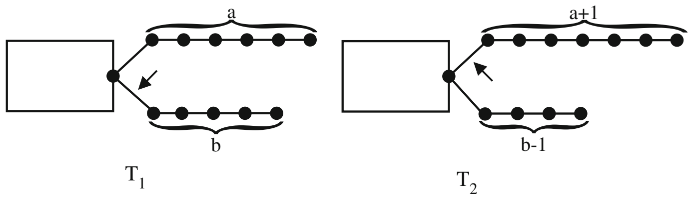

Fig. 1 The transformation $T_1 \rightarrow T_2$ increases the GA_2 index provided $a \geq b$

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

$$n_u(e, T_1) \cdot n_v(e, T_1) = b(n - b)$$
$$n_{u'}(e', T_2) \cdot n_{v'}(e', T_2) = (a + 1)(n - a - 1).$$

From

$$b(n - b) - (a + 1)(n - a - 1) = -(a + 1 - b)(n - a - b - 1)$$

we conclude that

$$\frac{2}{n - 1} \left[\sqrt{b(n - b)} - \sqrt{(a + 1)(n - a - 1)}\right]$$

is negative-valued for $a \geq b$, implying that

$$GA_2(T_2) > GA_2(T_1).$$

In other words, the transformation $T_1 \rightarrow T_2$, in which a vertex from a shorter branch is moved to a longer branch, increases the second geometric–arithmetic index.

We are now ready to state and prove:

Proposition 10 *The path P_n is the n-vertex tree with maximum second geometric–arithmetic index.*

Proof By continuing the above described transformation $T_1 \rightarrow T_2$ we can move all vertices from the shorter branch to the longer branch, always increasing the GA_2-value. Repeating the transformation sufficiently many times, we necessarily arrive at the path P_n. □

At this point it is natural to attempt to characterize the general n-vertex graphs having minimum and maximum GA_2. One answer is simple:

Proposition 11 *The star S_n is the connected n-vertex graph with minimum second geometric–arithmetic index.*

Proof The index GA_2 will certainly be minimal if the following three conditions are simultaneously satisfied:

(a) for all edges e, the denominator $n_u(e) + n_v(e)$ in Eq. 6 is as large as possible, namely equal to n;
(b) for all edges e, the numerator $\sqrt{n_u(e) \cdot n_v(e)}$ in Eq. 6 is as small as possible, which was shown above to be equal to $\sqrt{n-1}$;
(c) the number of summands in Eq. 6 is as small as possible, which in case of connected graphs is equal to $n - 1$.

It is easy to verify that the star, and only the star, satisfies all these three conditions. □

Dobrynin [16] proved that among connected n-vertex graphs the complete bipartite graph $K_{n/2,n/2}$ (for even n) or $K_{(n-1)/2,(n+1)/2}$ (for odd n) has maximum Szeged index. We conjecture that the same graph has also maximal GA_2 index.

4 Numerical examples and discussion

In Table 1 are given the GA, GA_2, PI, and Sz indices of the octane isomers. Note that by Eq. 5, all PI-values are mutually equal. The correlation between GA and GA_2 is shown in Fig. 2.

By inspection of Fig. 2, some peculiar relations between the two geometric–arithmetic indices can be envisaged. At the first glance there exists a (nearly linear, but very weak) correlation between GA and GA_2. The data points **15**, **13**, **5**, **9**, **2**, and **1**

Table 1 The GA, GA_2, PI, and Sz indices of the octane isomers; for details see text and Fig. 2

#	Octanes	GA	GA_2	PI	Sz
1	n-Octane	6.88562	5.99142	56	84
2	2-Methyl heptane	6.65466	5.78683	56	79
3	3-Methyl heptane	6.71124	5.68461	56	76
4	4-Methyl heptane	6.71124	5.65286	56	75
5	2,2-Dimethyl hexane	6.28562	5.48002	56	71
6	3,3-Dimethyl hexane	6.37124	5.34605	56	67
7	2,3-Dimethyl hexane	6.52068	5.44827	56	70
8	2,4-Dimethyl hexane	6.48027	5.48002	56	71
9	2,5-Dimethyl hexane	6.42369	5.58224	56	74
10	3,4-Dimethyl hexane	6.57726	5.37780	56	68
11	2,3,4-Trimethyl pentane	6.33013	5.24368	56	65
12	2,2,3-Trimethyl pentane	6.17837	5.17321	56	63
13	2,2,4-Trimethyl pentane	6.05466	5.27543	56	66
14	2,3,3-Trimethyl pentane	6.20741	5.14146	56	62
15	2,2,3,3-Tetramethyl butane	5.80000	4.96863	56	58
16	3-Ethyl-2-methyl pentane	6.57726	5.34605	56	67
17	3-Ethyl-3-methyl pentane	6.45685	5.24383	56	64
18	3-Ethyl hexane	6.76781	5.55064	56	72

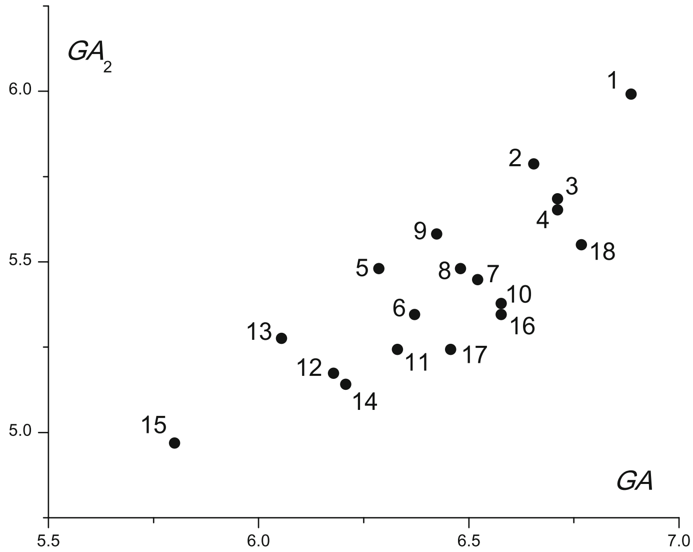

Fig. 2 The first geometric–arithmetic index (GA) of the octane isomers vs. their second geometric–arithmetic index (GA_2). The numbering is same as in Table 1

form an almost perfect straight line with increasing slope. If we denote the number of quaternary and tertiary carbon atoms by n_4 and n_3, we may immediately check that for these isomers (n_4, n_3) is equal to (2, 0), (1, 1), (1, 0), (0, 2), (0, 1), and (0, 0), respectively. This shows that both GA and GA_2 are increasing functions of the extent of branching of the molecular skeleton. It is worth noting that the molecules **15**, **13**, **5**, **9**, and **2** are all branched at the very end of their carbon-atom chains.

From Fig. 2 it is seen that the data points are grouped into several clusters. By direct checking we verified that each cluster corresponds to a particular choice of (n_4, n_3). Note that the apparent outlier **11** pertains to 2,3,4-trimethyl pentane, the only octane isomer for which $(n_4, n_3) = (0, 3)$.

Thus, the isomers belonging to the same cluster are those similarly branched. Within each such cluster (provided that there are two or more data points), the proportionality between GA and GA_2 is inverse. For instance, the data points **7**, **8**, **9**, **10**, and **16**, all pertaining to $(n_4, n_3) = (0, 2)$, lie nearly on a straight line with decreasing slope.

The above described relations between GA and GA_2, which hold not only for octanes, but for all chemical trees, indicate that these indices depend in the same way on one structural feature (namely, on branching), but have a different dependence on some other details of molecular structure. This gives hope that GA and GA_2 will both be simultaneously applicable in QSPR and QSAR studies.

Acknowledgments B. F. and I. G. thank the Serbian Ministry of Science for support, through Grant no. 144015G.

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