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ORIGINAL PAPER

On geometric-arithmetic index

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Abstract The geometric-arithmetic (GA) index is a newly proposed graph invariant in mathematical chemistry. We give the lower and upper bounds for GA index of molecular graphs using the numbers of vertices and edges. We also determine the n-vertex molecular trees with the minimum, the second and the third minimum, as well as the second and the third maximum GA indices.

Keywords Geometric-arithmetic index · Molecular graphs · Molecular trees · Degree (of vertex)

1 Introduction

A topological index is a numerical descriptor of the molecular structure derived from the corresponding molecular graph. There are numerous topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [1].

Randić proposed a structural descriptor called the branching index [2] that later became the well-known Randić connectivity index, which is the most used molecular descriptor in QSPR and QSAR [e.g. 1,3–5].

Motivated by the definition of Randić connectivity index based on the end-vertex degrees of edges in a graph, Vukičević and Furtula [6] proposed a topological index

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named the geometric-arithmetic index. Let G be a simple graph with the vertex set $V(G)$ and the edge set $E(G)$. For $u \in V(G)$, d_u denotes the degree of the vertex u in G. The geometric-arithmetic index (GA index for short) of G is defined as [6].

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

For physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and acentric factor, it is noted in [6] that the predictive power of GA index is somewhat better than predictive power of the Randić connectivity index. In [6], Vukičević and Furtula gave the lower and upper bounds for the GA index, identified the trees with the minimum and the maximum GA indices, which are the star and the path respectively, and then the path is the unique molecular tree (tree with maximum degree at most four used to model carbon skeletons of acyclic hydrocarbons) with the maximum GA index.

In this paper, we establish further bounds for the GA index using other graph invariants, and determine the molecular trees with the minimum, the second and the third minimum, as well as the second and the third maximum GA indices.

2 Bounds for the GA index

Let G be a connected graph with n vertices. Then [6] $\mathrm{GA}(G) \geq \frac{2(n-1)^{3/2}}{n}$ with equality if and only if G is the star.

The upper bound in the following proposition has been noted in [6]. It is attained if and only if the degrees of the end vertices of any edge are equal, i.e. every component is regular.

Proposition 1 *Let G be a graph with m edges. Then*

$$\mathrm{GA}(G) \leq m$$

with equality if and only if every component of G is regular.

Proposition 2 *Let G be a graph with m edges and maximum degree Δ. Then*

$$\mathrm{GA}(G) \geq \frac{2m\sqrt{\Delta}}{1+\Delta}$$

with equality if and only if for every edge of G, its end vertices have degrees 1 *and* Δ.

Proof For any edge uv of G, assume that $d_u \leq d_v$. Then $\mathrm{GA}(G) = \sum_{uv \in E(G)} f\left(\frac{d_u}{d_v}\right)$, where $f(x) = \frac{2\sqrt{x}}{1+x}$, which is increasing for $\frac{1}{n-1} \leq x \leq 1$. Note that $f\left(\frac{d_u}{d_v}\right) \geq f\left(\frac{1}{\Delta}\right) = \frac{2\sqrt{\Delta}}{1+\Delta}$ with equality if and only if $d_u = 1$ and $d_v = \Delta$. The result follows. $\square$

By previous proposition, we have

Corollary 1 *Let G be a graph with n vertices and m edges. Then*

$$\mathrm{GA}(G) \geq \frac{2m\sqrt{n-1}}{n}$$

with equality if and only if G is the star.

By Corollary 1, among n-vertex trees, the star is the unique tree with the minimum GA index [6].

Nordhaus and Gaddum [7] gave bounds for the sum of the chromatic numbers of a graph and its complement. Nordhaus–Gaddum-type results for many graph invariants are known. Here we give Nordhaus–Gaddum-type result for the GA index. Let G be a graph with $n \geq 2$ vertices and let $\overline{G}$ be its complement. Then $(n-1)^{3/2} < \mathrm{GA}(G) + \mathrm{GA}(\overline{G}) \leq \frac{n(n-1)}{2}$ with right equality if and only if G is a regular graph. The lower bound follows from Corollary 1, and the upper bound follows from Proposition 1. Note that one of G or $\overline{G}$ is connected. Thus the upper bound is attained if and only if G is regular.

Proposition 3 *Let G be a triangle-free graph with n vertices and m edges. Then*

$$\mathrm{GA}(G) \geq \frac{4m^2}{n^2}$$

with equality if and only if G is the regular complete bipartite graph.

Proof For any $uv \in E(G)$, we have $d_u + d_v \leq n$. Then

$$\sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}} \leq \sum_{uv \in E(G)} \frac{n}{2\sqrt{d_u d_v}} = \frac{n}{2} R_{-1/2}(G),$$

where $R_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$ is the Randić index [8,9], for which we have $R_{-1/2}(G) \leq \frac{n}{2}$ with equality if and only if G has no isolated vertices and every component of G is regular. By the Cauchy–Schwarz inequality,

$$\mathrm{GA}(G) \geq m^2 \left(\sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}} \right)^{-1}$$

with equality if and only if $\frac{\sqrt{d_u d_v}}{d_u + d_v}$ is a constant for all $uv \in E(G)$. Thus

$$\mathrm{GA}(G) \geq m^2 \left(\frac{n}{2} \cdot \frac{n}{2} \right)^{-1} = \frac{4m^2}{n^2}.$$

If equality holds in the above inequality, then $d_u + d_v = n$ for any $uv \in E(G)$, G has no isolated vertices and every component of G is regular, and thus $d_u = \frac{n}{2}$ for any $u \in V(G)$, implying that G is the regular complete bipartite graph since G is triangle-free. Conversely, it is easily seen that the lower bound for $\mathrm{GA}(G)$ is attained for the regular complete bipartite graph. □

3 GA index of molecular graphs

A connected graph with the maximum degree at most four is a molecular graph representing hydrocarbons [10]. Let G be a molecular graph with $n \geq 3$ vertices and m edges, where $n-1 \leq m \leq 2n$. For integers i and j with $1 \leq i \leq j \leq 4$, an ij-edge means an edge that connects vertices of degree i and j, denote by m_{ij} the number of ij-edges of G. Then

$$\begin{aligned}\mathrm{GA}(G) &= \frac{2\sqrt{2}}{3}m_{12} + \frac{\sqrt{3}}{2}m_{13} + \frac{4}{5}m_{14} + m_{22} + \frac{2\sqrt{6}}{5}m_{23} + \frac{2\sqrt{2}}{3}m_{24} + m_{33}\\ &\quad + \frac{4\sqrt{3}}{7}m_{34} + m_{44}.\end{aligned}$$

Gutman and Miljković [11] deduced

$$\begin{aligned}m_{14} &= \frac{4n-2m}{3} - \frac{4}{3}m_{12} - \frac{10}{9}m_{13} - \frac{2}{3}m_{22} - \frac{4}{9}m_{23} - \frac{1}{3}m_{24} - \frac{2}{9}m_{33} - \frac{1}{9}m_{34}\\ m_{44} &= \frac{5m-4n}{3} + \frac{1}{3}m_{12} + \frac{1}{9}m_{13} - \frac{1}{3}m_{22} - \frac{5}{9}m_{23} - \frac{2}{3}m_{24} - \frac{7}{9}m_{33} - \frac{8}{9}m_{34}.\end{aligned}$$

Substituting these into the formula for $\mathrm{GA}(G)$, we have

$$\begin{aligned}\mathrm{GA}(G) = \frac{17}{15}m - \frac{4}{15}n + \left(\frac{2\sqrt{2}}{3} - \frac{11}{15}\right)m_{12} + \left(\frac{\sqrt{3}}{2} - \frac{7}{9}\right)m_{13} + \frac{2}{15}m_{22}\\ + \left(\frac{2\sqrt{6}}{5} - \frac{41}{45}\right)m_{23} + \left(\frac{2\sqrt{2}}{3} - \frac{14}{15}\right)m_{24}\\ + \frac{2}{45}m_{33} + \left(\frac{4\sqrt{3}}{7} - \frac{44}{45}\right)m_{34} \qquad (1)\end{aligned}$$

with positive coefficients for $m_{12}, m_{13}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}$. Also, Gutman and Miljković [11] deduced

$$\begin{aligned}m_{12} &= 2(n-m) - \frac{2}{3}m_{13} - \frac{1}{2}m_{14} + \frac{1}{3}m_{23} + \frac{1}{2}m_{24} + \frac{2}{3}m_{33} + \frac{5}{6}m_{34} + m_{44}\\ m_{22} &= 3m - 2n - \frac{1}{3}m_{13} - \frac{1}{2}m_{14} - \frac{4}{3}m_{23} - \frac{3}{2}m_{24} - \frac{5}{3}m_{33} - \frac{11}{6}m_{34} - 2m_{44},\end{aligned}$$

and then we have

$$\begin{aligned}\mathrm{GA}(G) = &\left(\frac{4\sqrt{2}}{3} - 2\right)n + \left(3 - \frac{4\sqrt{2}}{3}\right)m + \left(\frac{\sqrt{3}}{2} - \frac{1}{3} - \frac{4\sqrt{2}}{9}\right)m_{13}\\ &+ \left(\frac{3}{10} - \frac{\sqrt{2}}{3}\right)m_{14} + \left(\frac{2\sqrt{2}}{9} - \frac{4}{3} + \frac{2\sqrt{6}}{5}\right)m_{23} + \left(\sqrt{2} - \frac{3}{2}\right)m_{24}\\ &+ \left(\frac{4\sqrt{2}}{9} - \frac{2}{3}\right)m_{33} + \left(\frac{5\sqrt{2}}{9} - \frac{11}{6} + \frac{4\sqrt{3}}{7}\right)m_{34} + \left(\frac{2\sqrt{2}}{3} - 1\right)m_{44}\end{aligned} \tag{2}$$

with negative coefficients for $m_{13}, m_{14}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}$. From Eqs. (1) and (2), we have:

Proposition 4 *Let G be a molecular graph with $n \geq 4$ vertices and m edges with $n - 1 \leq m \leq 2n$. Then*

$$\frac{17}{15}m - \frac{4}{15}n \leq \mathrm{GA}(G) \leq \left(3 - \frac{4\sqrt{2}}{3}\right)m - \left(2 - \frac{4\sqrt{2}}{3}\right)n$$

with left equality if and only if G has only vertices of degree one and four, and with right equality if and only if G is either a path or a cycle.

In the following, we consider molecular trees, for which $m = n - 1$. We use the techniques from [12].

4 Molecular trees with small GA indices

In [6], a lower bound for the GA index of a molecular tree was given, which is attained if and only if it contains only vertices of degree one and four. There exists an n-vertex tree containing only vertices of degree one and four if and only if $n \equiv 2 \pmod 3$. We now determine the n-vertex molecular trees with the minimum, the second and third minimum GA indices.

Let G be an n-vertex molecular tree. Let $F = \mathrm{GA}(G) - \frac{13}{15}n + \frac{17}{15}$. Then from Eq. (1),

$$\begin{aligned}F = &\ 0.20947571m_{12} + 0.088247626m_{13} + 0.13333333m_{22} + 0.068684786m_{23}\\ &+ 0.0094757082m_{24} + 0.044444444m_{33} + 0.011965541m_{34}.\end{aligned}$$

Let n_i be the number of vertices of degree i, $i = 1, 2, 3, 4$. Then $2n_2 = m_{12} + 2m_{22} + m_{23} + m_{24}$, $3n_3 = m_{13} + m_{23} + 2m_{33} + m_{34}$. Consider $n_2 + n_3$. If $n_2 + n_3 \geq 5$, then comparing the coefficients of $m_{12}, m_{13}, m_{22}, m_{23}, m_{33}$ and m_{34} with the coefficient 0.0094757082 of m_{24} in the expression for F, we find that $F \geq 0.0094757082(2n_2 + 3n_3)$ and thus

$$F \geq 0.0094757082 \times 10 = 0.094757082 > 0.0908,$$

if $n_2 + n_3 = 4$ and $n_3 > 0$, then

$$F \geq 0.0094757082 \times 6 + 0.011965541 \times 3 = 0.092750872 > 0.0908,$$

and if $n_2 = 0$ and $n_3 = 3$, then

$$F \geq 0.011965541 \times 9 = 0.10768987 > 0.0908.$$

The left cases are $(n_2, n_3) = (4, 0)$, and $n_2+n_3 = 0, 1, 2, 3$ with $n_2+n_3 \neq (0, 3)$, and the graphical feasible combinations of $m_{12}, m_{13}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}$, for which $F \leq 0.0908$ are listed below, where $n \equiv k \pmod 3$:

n_2	n_3	Non-zero m_{ij}	F	k	n
0	0		0	2	$n \geq 5$
1	1	$m_{24} = 2, m_{34} = 3$	0.054848	2	$n \geq 17$
3	0	$m_{24} = 6$	0.056854	2	$n \geq 17$
0	1	$m_{34} = 3$	0.035897	1	$n \geq 13$
2	0	$m_{24} = 4$	0.037903	1	$n \geq 13$
1	2	$m_{24} = 2, m_{34} = 6$	0.090745	1	$n \geq 25$
1	0	$m_{24} = 2$	0.018951	0	$n \geq 9$
0	2	$m_{34} = 6$	0.071793	0	$n \geq 21$
2	1	$m_{24} = 4, m_{34} = 3$	0.073799	0	$n \geq 21$
4	0	$m_{24} = 8$	0.075806	0	$n \geq 21$

Obviously, the smaller F is, the smaller value of the GA index is. From the results above, we have:

Proposition 5 *(i) If $n \equiv 2 \pmod 3$, then among the n-vertex molecular trees,*

(a) for $n \geq 5$, the ones with only degrees one and four are the unique trees with the minimum GA index, which is equal to $\frac{13}{15}n - \frac{17}{15}$;

(b) for $n \geq 17$, the ones with a single vertex of degree two adjacent to two vertices of degree four, and a single vertex of degree three adjacent to three vertices of degree four are the unique trees with the second minimum GA index, which is equal to $\frac{13}{15}n + \frac{12\sqrt{3}}{7} + \frac{4\sqrt{2}}{3} - \frac{89}{15}$;

(c) for $n \geq 17$, the ones with three vertices of degree two, each adjacent to two vertices of degree four, and without vertices of degree three are the unique trees with the third minimum GA index, which is equal to $\frac{13}{15}n + 4\sqrt{2} - \frac{101}{15}$.

(ii) If $n \equiv 1 \pmod 3$, then among n-vertex molecular trees,

(a) for $n \geq 13$, the ones with a single vertex of degree three adjacent to three vertices of degree four, and without vertices of degree two are the unique trees with the minimum GA index, which is equal to $\frac{13}{15}n + \frac{12\sqrt{3}}{7} - \frac{61}{15}$;

(b) for $n \geq 13$, the ones with two vertices of degree two adjacent to four vertices of degree four, and without vertices of degree three are the unique trees with the second minimum GA index, which is equal to $\frac{13}{15}n + \frac{8\sqrt{2}}{3} - \frac{73}{15}$;

(c) *for $n \geq 25$, the ones with a single vertex of degree two adjacent to two vertices of degree four, and two vertices of degree three, each adjacent to three vertices of degree four are the unique trees with the third minimum GA index, which is equal to* $\frac{13}{15}n + \frac{4\sqrt{2}}{3} + \frac{24\sqrt{3}}{7} - \frac{133}{15}$.

(iii) *If* $n \equiv 0 \pmod 3$, *then among the n-vertex molecular trees,*

(a) *for $n \geq 9$, the ones with a single vertex of degree two adjacent to two vertices of degree four, and without vertices of degree three are the unique trees with the minimum GA index, which is equal to* $\frac{13}{15}n + \frac{4\sqrt{2}}{3} - 3$;

(b) *for $n \geq 21$, the ones with two vertices of degree three, each adjacent to three vertices of degree four, and without vertices of degree two are the unique trees with the second minimum GA index, which is equal to* $\frac{13}{15}n + \frac{24\sqrt{3}}{7} - 7$;

(c) *for $n \geq 21$, the ones with two vertices of degree two, each adjacent to two vertices of degree four, and a single vertex of degree three adjacent to three vertices of degree four are the unique trees with the third minimum GA index, which is equal to* $\frac{13}{15}n + \frac{8\sqrt{2}}{3} + \frac{12\sqrt{3}}{7} - \frac{39}{5}$.

By comparing previous proposition and the results in [12], we find that the molecular trees with the minimum GA index, and for $n \equiv 0, 2 \pmod 3$, the molecular trees with the second minimum GA index are just those with the minimum and the second minimum Randić connectivity indices, respectively, however, the molecular trees with the second minimum GA index are different from those with the second minimum Randić connectivity index when $n \equiv 1 \pmod 3$, and the molecular trees with the third minimum GA index are different from those with the third minimum Randić connectivity index.

5 Molecular trees with large GA indices

It has been shown in [6] that among the n-vertex (molecular) trees, the path is the unique tree with the maximum GA index. We now determine the n-vertex molecular trees with the second and the third maximum GA indices.

Let G be an n-vertex molecular tree. Let $J = n - 3 + \frac{4\sqrt{2}}{3} - \mathrm{GA}(G)$. Then from Eq. (2),

$$\begin{aligned} J &= 0.095847291 m_{13} + 0.17140452 m_{14} + 0.039267756 m_{23} + 0.085786438 m_{24} \\ &\quad + 0.11900753 m_{33} + 0.057915813 m_{34} + 0.057190958 m_{44}. \end{aligned}$$

As in previous section, let n_i be the number of vertices of degree i, where $i = 1, 2, 3, 4$. Then $3n_3 = m_{13} + m_{23} + 2m_{33} + m_{34}$ and $4n_4 = m_{14} + m_{24} + m_{34} + 2m_{44}$. For $n_3 + n_4 \geq 3$, if $n_4 \geq 1$, then comparing the coefficients of m_{14}, m_{24}, m_{44} with $0.057915813 - 0.039267756 = 0.018648057$ in the expression for J, where 0.039267756 is the coefficient of m_{23} and 0.057915813 is the coefficient of m_{34}, we have

$$\begin{aligned} J &\geq 0.039267756 \times (m_{13} + m_{23} + 2m_{33} + m_{34}) \\ &\quad + 0.018648057 \times (m_{14} + m_{24} + m_{34} + 2m_{44}) \\ &\geq 0.018648057 \times (3n_3 + 4n_4) \geq 0.018648057 \times 10 > 0.1744, \end{aligned}$$

and if $n_3 \geq 3$ and $n_4 = 0$, then

$$J \geq 0.039267756 \times (m_{13} + m_{23} + 2m_{33}) \geq 0.039267756 \times 9 > 0.1744.$$

For $n_3 + n_4 = 2$, if $n_3 = 2$ and $n_4 = 0$, then $m_{13} + m_{23} + 2m_{33} = 6$, and thus

$$J \geq 0.039267756 \times 6 > 0.1744,$$

if $n_3 = n_4 = 1$, then $m_{13} + m_{23} + m_{34} = 3$, $m_{14} + m_{24} + m_{34} = 4$, and thus

$$\begin{aligned} J &\geq 0.039267756 \times 3 + (0.057915813 - 0.039267756) \times 4 \\ &= 0.19239550 > 0.1744, \end{aligned}$$

and if $n_3 = 0$ and $n_4 = 2$, then

$$J \geq 0.057190958 \times 4 > 0.1744.$$

If $n_3 = 0$ and $n_4 = 1$, then

$$J \geq 0.085786438 \times 4 > 0.1744.$$

The left cases are $n_3 + n_4 = 0, 1$ with $(n_3, n_4) \neq (0, 1)$, and the graphical feasible combinations of $m_{13}, m_{14}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}$, for which $J \leq 0.1744$ are listed below:

n_3	n_4	Non-zero m_{ij}	J	n
0	0		0	$n \geq 3$
1	0	$m_{23} = 3$	0.11780	$n \geq 7$
1	0	$m_{13} = 1, m_{23} = 2$	0.17438	$n \geq 6$

Obviously, the smaller J is, the greater value of the GA index is. Thus, we have:

Proposition 6 *Among the n-vertex molecular trees, the path is the unique tree with the maximum* GA *index, which is equal to* $n - 3 + \frac{4\sqrt{2}}{3}$, *and for* $n \geq 7$, *the trees with a single vertex of degree three adjacent to three vertices of degree two and without vertices of degree four are the unique trees with the second maximum* GA *index, which is equal to* $n - 7 + 2\sqrt{2} + \frac{6\sqrt{6}}{5}$, *and the trees with a single vertex of degree three adjacent to two vertices of degree two and one vertex of degree one and without vertices of degree four are the unique trees with the third maximum GA index, which is equal to* $n - 6 + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$.

By comparing previous proposition and the results in [12], we note that the molecular trees with the maximum, the second and the third maximum GA indices are just those with the maximum, the second and the third maximum Randić connectivity indices, respectively.

6 Comment

Recently, a new formulation of geometric-arithmetic index was proposed in [13].

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