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ESTIMATING THE SECOND AND THIRD GEOMETRIC-ARITHMETIC INDICES

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Abstract

Arithmetic–geometric indices are graph invariants defined as the sum of terms $\sqrt{Q_u\,Q_v}/[(Q_u+Q_v)/2]$ over all edges uv of the graph, where Q_u is some quantity associated with the vertex u. If Q_u is the number of vertices (resp. edges) lying closer to u than to v, then one speaks of the second (resp. third) geometric–arithmetic index, GA_2 and GA_3. We obtain inequalities between GA_2 and GA_3 for trees, revealing that the main parameters determining their relation are the number of vertices and the number of pendent vertices.

Keywords: Distance (in graph), Distance between vertex and edge, Geometric-arithmetic index, Trees.

2000 AMS Classification: 05 C 12, 05 C 05.

1. Introduction

In this work we are concerned with simple graphs, that is graphs without multiple or directed edges, and without self–loops. Let $G = (\mathcal{V}(G), \mathcal{E}(G))$ be such a graph, with vertex set $\mathcal{V}(G)$ and edge set $\mathcal{E}(G)$. Let $n = |\mathcal{V}(G)|$ and $m = |\mathcal{E}(G)|$ be, respectively, the number of vertices and edges of G. In what follows it will be assumed that G is connected.

The distance between two vertices x and y in the graph G, denoted by $d(x, y)$, is the length (= number of edges) of a shortest path connecting x and y [1].

Let $e = uv$ be an edge of G connecting the vertices u and v. Motivated by a classical result of Wiener [16] (see also [9, pp. 126–127]), we define the numbers n_u and n_v as [7, 8, 3]

(1.1) $\quad n_u = |\{x \in \mathcal{V}(G) : d(x,u) < d(x,v)\}|,$

(1.2) $\quad n_v = |\{x \in \mathcal{V}(G) : d(x,u) > d(x,v)\}|.$

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In words: n_u is the number of vertices of G lying closer to vertex u than to vertex v of the edge uv, whereas n_v is the number of vertices of G lying closer to vertex v than to vertex u. It should be noted that n_u is not uniquely determined by the vertex $u \in \mathcal{V}(G)$, but also depends on the edge $uv \in \mathcal{E}(G)$ [7, 8].

Directly from (1.1) and (1.2) it follows that for (connected) bipartite graphs, and thus also in the case of trees, $n_u + n_v = n$ holds for any edge uv. Further, $n_u \geq 1$. In the case of trees, $n_u = 1$ if and only if u is a pendent vertex (a vertex of degree one).

Let $u, v, s, t \in \mathcal{V}(G)$. Let $e = uv$ and $f = st$ be two edges of G connecting, respectively, the vertices u and v and the vertices s and t. The distance between a vertex x and an edge $f = st$ of the graph G, denoted by $d(x, f)$, can be conveniently and consistently defined [11] as $\min\{d(x, s), d(x, t)\}$, recalling that this quantity does not satisfy the standard requirements that any "distance" should obey. Then, in analogy to n_u and n_v, we may introduce

$$m_u = |\{f \in \mathcal{E}(G) : d(f, u) < d(f, v)\}|, \tag{1.3}$$

$$m_v = |\{f \in \mathcal{E}(G) : d(f, u) > d(f, v)\}|. \tag{1.4}$$

In words: m_u is the number of edges of G lying closer to vertex u than to vertex v of the edge uv, whereas m_v is the number of edges of G lying closer to vertex v than to vertex u. Again, m_u is not uniquely determined by the vertex $u \in \mathcal{V}(G)$ but also depends on the edge $uv \in \mathcal{E}(G)$.

An immediate consequences of (1.3) and (1.4) is $m_u \geq 0$, with equality $m_u = 0$ if and only if u is a pendent vertex of G. In addition, $m_u + m_v \leq m - 1$ holds for any edge uv. In the case of trees, it is always the case that $m_u + m_v = m - 1 = n - 2$ and $m_u = n_u - 1$.

Recently, a new class of graph invariants, the so-called *geometric-arithmetic indices*, has been conceived [15], whose general definition is the following [18]

$$\mathrm{GA} = \mathrm{GA}(G) = \sum_{uv \in \mathcal{E}(G)} \frac{\sqrt{Q_u\,Q_v}}{\frac{1}{2}\,(Q_u + Q_v)},$$

where Q_u is some quantity associated with the vertex u. Eventually, it could be demonstrated [15, 5] that these graph invariants are useful molecular structure descriptors, and can be applied in chemistry. Details on GA-indices and their applications can be found in the review [5]; for some most recent works along these lines see [2, 10, 17, 4]. In [4] the choices $Q_u \equiv n_u$ and $Q_u \equiv m_u$ were put forward, resulting in the so-called *second geometric-arithmetic index*,

$$\mathrm{GA}_2 = \mathrm{GA}_2(G) = \sum_{uv \in \mathcal{E}(G)} \frac{\sqrt{n_u\,n_v}}{\frac{1}{2}\,(n_u + n_v)}, \tag{1.5}$$

and the *third geometric-arithmetic index*,

$$\mathrm{GA}_3 = \mathrm{GA}_3(G) = \sum_{uv \in \mathcal{E}(G)} \frac{\sqrt{m_u\,m_v}}{\frac{1}{2}\,(m_u + m_v)}. \tag{1.6}$$

At this point it is worth mentioning that the numbers n_u and m_u are used also within several other graph invariants of importance in current chemical researches; for more details see the recent papers [12, 13, 14] and the references cited therein.

2. Second and third geometric-arithmetic indices of trees

If T is an n-vertex tree, then because of $n_u+n_v = n$, $m_u+m_v = n-2$ and $m_u = n_u-1$, Equations (1.5) and (1.6) are simplified as

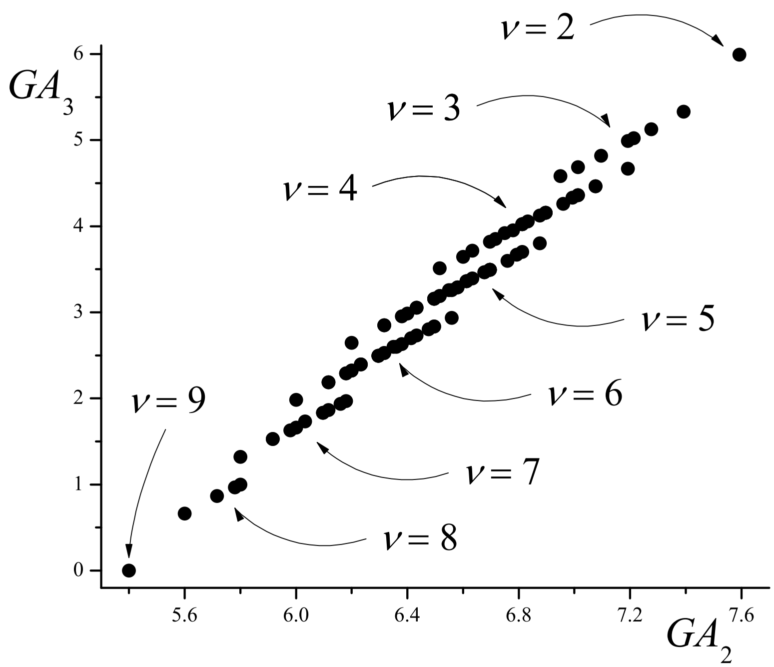
$$\text{GA}_2(T) = \frac{2}{n} \sum_{uv\in\mathcal{E}(T)} \sqrt{n_u\, n_v} \tag{2.1}$$

and

$$\text{GA}_3(T) = \frac{2}{n-2} \sum_{uv\in\mathcal{E}(T)} \sqrt{(n_u-1)(n_v-1)}. \tag{2.2}$$

The forms of the right-hand sides of (2.1) and (2.2) suggest that in the case of trees there must exist some relation between the two GA-indices. That this indeed is the case was established by a exhaustive numerical study [6]. In Figure 1 we show a typical correlation of this kind.

Figure 1. Correlation between the GA_2 and GA_3 indices of trees with 10 vertices (106 data points).



The data points form several nearly parallel lines. The factor determining to which line each data point belongs is the number ν of pendent vertices. For more details see [6].

3. Inequalities involving the second and third geometric-arithmetic indices of trees

A vertex u having just one first neighbor is said to be a *pendent vertex*. An edge connecting a pendent vertex with its unique neighbor is referred to as a *pendent edge*. If

$n \geq 3$ then an n-vertex tree has an equal number of pendent vertices and pendent edges, which will be denoted by ν. It is easy to see that $2 \leq \nu \leq n-1$.

We first prove an auxiliary identity.

Denote by $\sum\limits_{uv\in\mathcal{E}(T)}^{*}$ the summation over non-pendent edges of the tree T.

3.1. Lemma. *If T is an n-vertex tree, $n \geq 3$ with ν pendent vertices, then*

$$\sum_{uv\in\mathcal{E}(T)}^{*} \sqrt{n_u\, n_v} = \frac{n}{2}\, GA_2(T) - \nu\sqrt{n-1}. \tag{3.1}$$

Proof. There are ν pendent edges for which $n_u = 1,\ n_v = n-1$ or $n_u = n-1,\ n_v = 1$. Therefore

$$\sum_{uv\in\mathcal{E}(T)} \sqrt{n_u\, n_v} = \sum_{uv\in\mathcal{E}(T)}^{*} \sqrt{n_u\, n_v} + \nu\sqrt{n-1}.$$

Formula (3.1) is then obtained by taking into account Equation (2.1). □

The star S_n is the n-vertex tree in which $n-1$ vertices are pendent. Therefore, by Equation (2.1), $\mathrm{GA}_2(S_n) = \frac{2}{n}\,(n-1)^{3/2}$, and by Equation (2.2), $GA_3(S_n) = 0$.

3.2. Theorem. *Let T be an n-vertex tree, $n \geq 4$ different from the star, having ν pendent vertices. Then*

$$\begin{aligned} &\frac{n}{n-2}\left(1 - \frac{n-1}{2(n-2)}\right)\mathrm{GA}_2(T) - \frac{2\sqrt{n-1}}{n-2}\left(1 - \frac{n-1}{2(n-2)}\right)\nu \\ &\qquad < GA_3(T) < \frac{n}{n-2}\left(1 - \frac{n-1}{2\lceil n/2\rceil\lfloor n/2\rfloor}\right)\mathrm{GA}_2(T) \\ &\qquad\qquad - \frac{2\sqrt{n-1}}{n-2}\left(1 - \frac{n-1}{2\lceil n/2\rceil\lfloor n/2\rfloor}\right)\nu. \end{aligned} \tag{3.2}$$

Proof. If the edge uv is pendent, then $(n_u-1)(n_v-1) = 0$. Therefore, Equation (2.2) can be rewritten as

$$GA_3(T) = \frac{2}{n-2} \sum_{uv\in\mathcal{E}(T)}^{*} \sqrt{(n_u-1)(n_v-1)}. \tag{3.3}$$

Now, bearing in mind that $n_u + n_v = n$,

$$\sqrt{(n_u-1)(n_v-1)} = \sqrt{n_u\, n_v}\,\sqrt{1 - \frac{n-1}{n_u\, n_v}}. \tag{3.4}$$

For any non-pendent edge $uv \in \mathcal{E}(G)$ we have $0 < (n-1)/(n_u\, n_v) < 1$. Since for any real number $x \in (0,1)$

$$1 - x < \sqrt{1-x} < 1 - \frac{x}{2} \tag{3.5}$$

we get

$$\sqrt{1 - \frac{n-1}{n_u\, n_v}} > 1 - \frac{n-1}{n_u\, n_v} \tag{3.6}$$

and

$$\sqrt{1 - \frac{n-1}{n_u\, n_v}} < 1 - \frac{n-1}{2n_u\, n_v}. \tag{3.7}$$

For a non-pendent edge uv both inequalities (3.6) and (3.7) are strict.

Proof of the lower bound. Since $n_u + n_v = n$ for a non-pendent edge uv, $n_u\, n_v \geq 2(n-2)$. Therefore, from (3.6),

$$\sqrt{1 - \frac{n-1}{n_u\, n_v}} > 1 - \frac{n-1}{2(n-2)},$$

which substituted back into (3.4) and then back into (3.3) yields

$$\mathrm{GA}_3(T) > \frac{2}{n-2} \left(1 - \frac{n-1}{2(n-2)}\right) \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v}.$$

The lower bound in Theorem 2.2 follows now by using the identity (3.1).

Proof of the upper bound is analogous: For any edge uv of the tree T, $n_u\, n_v \leq \lceil n/2 \rceil \lfloor n/2 \rfloor$. Therefore, from (3.7),

$$\sqrt{1 - \frac{n-1}{n_u\, n_v}} < 1 - \frac{n-1}{2\lceil n/2 \rceil \lfloor n/2 \rfloor},$$

which substituted back into (3.4) and then back into (3.3) yields

$$\mathrm{GA}_3(T) < \frac{2}{n-2} \left(1 - \frac{n-1}{2\lceil n/2 \rceil \lfloor n/2 \rfloor}\right) \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v}.$$

The upper bound follows now by Lemma 2.1. □

3.3. Theorem. *Let T be the same tree as in Theorem 2.2. Then,*

$$\begin{aligned}
&\frac{n}{n-2}\, GA_2(T) - \left(\frac{2\sqrt{n-1}}{n-2} - \frac{\sqrt{2}\,(n-1)}{(n-2)^{3/2}}\right)\nu - \frac{\sqrt{2}\,(n-1)^2}{(n-2)^{3/2}} \\
&\quad < \mathrm{GA}_3(T) < \frac{n}{n-2}\, \mathrm{GA}_2(T) - \left(\frac{2\sqrt{n-1}}{n-2} - \frac{n-1}{(n-2)\sqrt{\lceil n/2 \rceil \lfloor n/2 \rfloor}}\right)\nu \\
&\qquad - \frac{(n-1)^2}{(n-2)\sqrt{\lceil n/2 \rceil \lfloor n/2 \rfloor}}.
\end{aligned} \tag{3.8}$$

Proof. **Proof of lower bound.** Start with (3.4) and use (3.5). This gives

$$\begin{aligned}
\sqrt{n_u\, n_v}\, \sqrt{1 - \frac{n-1}{n_u\, n_v}} &> \sqrt{n_u\, n_v} \left(1 - \frac{n-1}{n_u\, n_v}\right) = \sqrt{n_u\, n_v} - \frac{n-1}{\sqrt{n_u\, n_v}} \\
&\geq \sqrt{n_u\, n_v} - \frac{n-1}{\sqrt{2(n-2)}},
\end{aligned} \tag{3.9}$$

which substituted back into (3.3), and bearing in mind that the tree T has $n-1-\nu$ non-pendent edges, results in

$$\mathrm{GA}_3(T) > \frac{2}{n-2} \left[\sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v} - \frac{n-1}{\sqrt{2(n-2)}}(n-1-\nu)\right].$$

The lower bound in (3.8) is now obtained by using Lemma 2.1.

Proof of the upper bound. This time, instead of (3.9) we have

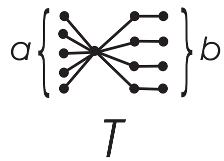
$$\begin{aligned}
\sqrt{n_u\, n_v}\, \sqrt{1 - \frac{n-1}{n_u\, n_v}} &< \sqrt{n_u\, n_v} \left(1 - \frac{n-1}{2\, n_u\, n_v}\right) = \sqrt{n_u\, n_v} - \frac{n-1}{2\sqrt{n_u\, n_v}} \\
&\leq \sqrt{n_u\, n_v} - \frac{n-1}{2\sqrt{\lceil n/2 \rceil \lfloor n/2 \rfloor}},
\end{aligned}$$

and then we have to proceed in a fully analogous manner as in the previous part of the proof. □

3.4. Theorem.

(a) *The lower bound in* (3.8) *is greater than or equal to the lower bound in* (3.2).
(b) *The two lower bounds are equal if and only if the tree T is of the form shown in Figure 2.*

Figure 2. Trees in which for all non-pendent edges uv, $n_u = 2$ or $n_v = 2$ or both; $a \geq 0$, $b \geq 1$



For such trees (and only for them) the lower bounds in Theorems 2.2 and 2.3 are equal.

Proof. The tree T specified in Theorems 2.2 and 2.3 necessarily possesses non-pendent edges. Let uv be such an edge. Then because of $n_u + n_v = n$ and $n_u, n_v \geq 2$ it must be

(3.10) $\quad n_u\, n_v \geq 2(n-2).$

This implies

$$\frac{\sqrt{n_u\, n_v}}{2(n-2)} \geq \frac{1}{\sqrt{2(n-2)}}$$

and

$$\sqrt{n_u\, n_v} - \frac{n-1}{2(n-2)} \sqrt{n_u\, n_v} \leq \sqrt{n_u\, n_v} - \frac{n-1}{\sqrt{2(n-2)}},$$

and finally

$$\frac{2}{n-2}\left[\sqrt{n_u\, n_v} - \frac{n-1}{2(n-2)} \sqrt{n_u\, n_v}\right] \leq \frac{2}{n-2}\left[\sqrt{n_u\, n_v} - \frac{n-1}{\sqrt{2(n-2)}}\right].$$

Summation of the above expression over all non-pendent edges of T yields

$$\frac{2}{n-2}\left(1 - \frac{n-1}{2(n-2)}\right) \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v} \leq \frac{2}{n-2} \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v} - \frac{\sqrt{2}\,(n-1)}{(n-2)^{3/2}}\,(n-1-\nu).$$

Now, by substituting Equation (3.1) into

$$\frac{2}{n-2}\left(1 - \frac{n-1}{2(n-2)}\right) \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v}$$

and

$$\frac{2}{n-2} \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v} - \frac{\sqrt{2}\,(n-1)}{(n-2)^{3/2}}\,(n-1-\nu),$$

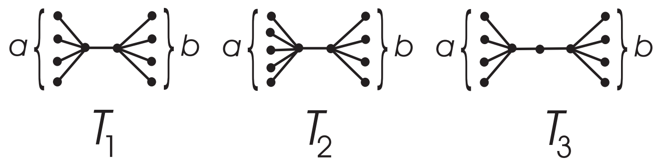
we arrive at the lower bounds in Theorems 2.2 and 2.3, respectively. This proves part (a) of Theorem 2.4.

Equality between the two lower bounds will happen if and only if for all non-pendent edges of T equality holds in (3.10). Thus we must have either $n_u = 2$ or $n_v = 2$, or both. Thus either the vertex u or the vertex v or both have a unique pendent neighbor. Therefore, the respective trees are of the form depicted in Figure 2. □

3.5. Theorem.

(a) *The upper bound in* (3.8) *is less than or equal to the upper bound in* (3.2).
(b) *The two upper bounds are equal if and only if the tree T is of the form shown in Figure 3.*

Figure 3. Trees in which for all non-pendent edges uv, $n_u = \lceil n/2 \rceil$ or $n_u = \lfloor n/2 \rfloor$



The tree T_1 has an even number of vertices, $a = b = (n-2)/2$. The trees T_2 and T_3 have an odd number of vertices. For T_2, $a = (n-1)/2$, $b = (n-3)/2$. For T_3, $a = b = (n-3)/2$. For these trees (and only for them) the upper bounds in Theorems 2.2 and 2.3 are equal.

Proof. This time we start with

$$n_u\, n_v \leq \lceil n/2 \rceil \, \lfloor n/2 \rfloor, \tag{3.11}$$

and proceed in the same way as in the proof of Theorem 2.4. We then get

$$\frac{2}{n-2}\left(1 - \frac{n-1}{2\lceil n/2 \rceil \, \lfloor n/2 \rfloor}\right) \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v}$$
$$\geq \frac{2}{n-2} \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v} - \frac{(n-1)}{(n-2)\sqrt{\lceil n/2 \rceil \, \lfloor n/2 \rfloor}}\,(n-1-\nu)\ .$$

Substituting Equation (3.1) into

$$\frac{2}{n-2}\left(1 - \frac{n-1}{2\lceil n/2 \rceil \, \lfloor n/2 \rfloor}\right) \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v}$$

and

$$\frac{2}{n-2} \sum_{uv \in \mathcal{E}(T)}^{*} \sqrt{n_u\, n_v} - \frac{(n-1)}{(n-2)\sqrt{\lceil n/2 \rceil \, \lfloor n/2 \rfloor}}\,(n-1-\nu),$$

we arrive at the upper bounds in Theorems 2.2 and 2.3, respectively. This proves part (a) of Theorem 2.5.

Equality between the two upper bounds will happen if and only if for all non-pendent edges of T equality holds in (3.11). A simple combinatorial argument shows that the trees having this property are those depicted in Figure 3. □

4. Concluding remarks

The motivation for the research whose results are communicated in the present paper are the peculiar features seen from Figure 1. Namely, although the right-hand sides of the expressions (2.1) and (2.2) are similar, from these formulas one cannot immediately conclude that the correlation between GA_2 and GA_3 is linear, that the data points lie on several mutually parallel and almost equidistant straight lines, and that the number ν of pendent vertices determines to which line a particular data point belongs. Theorems 2.2 and 2.3 are aimed at providing an explanation for the mentioned empirical findings. The lower and upper bounds stated in Theorem 2.3 appear to be especially satisfactory: both the lower and the upper bounds for GA_3 are linear functions of GA_2 with equal slopes (equal to $n/(n-2)$), and both linearly decrease with increasing values of ν.

Unfortunately, the true slopes of the $\mathrm{GA}_3/\mathrm{GA}_2$-lines were found [6] to be significantly different from $n/(n-2)$. Therefore, the present results cannot be considered as a complete solution of the problem, and more work along these lines would be necessary. Yet, the present results shed a lot of light on the relations between the GA_2- and GA_3-indices (especially of saturated hydrocarbons), and thus could be directly used in chemical applications [5].

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