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THE SECOND AND THIRD GEOMETRIC-ARITHMETIC INDICES OF UNICYCLIC GRAPHS[‡]

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Abstract

Recently, G. Fath-Tabar, B. Furtula and I. Gutman (*A new geometric-arithmetic index*, J. Math. Chem. **47**, 477–486, 2010) proposed the second geometric-arithmetic index GA_2 and B. Zhou, I. Gutman, B. Furtula and Z. Du (*On two types of geometric-arithmetic index*, Chem. Phys. Lett. **482**, 153–155, 2009) put forward the third geometric-arithmetic index GA_3, respectively. In (Gutman, I. and Furtula, B. *Estimating the second and third geometric-arithmetic indices*, Hacet. J. Math. Stat. **40** (1), 69–76, 2011), inequalities between GA_2 and GA_3 for trees, with the number of vertices and the number of pendent vertices, were obtained by I. Gutman and B. Furtula. In this paper, we obtain inequalities between the two indices for unicyclic graphs.

Keywords: Distance between vertex and edge, Geometric-arithmetic index, Unicyclic graph.

2000 AMS Classification: 05 C 12.

1. Introduction

Let $G = (V, E)$ be a connected simple graph with $|V| = n$ and $|E| = m$. The distance $d(u, v)$ of two vertices $u, v \in V(G)$ is the length of the shortest path connecting u and v in G. A *pendent vertex* of G is a vertex of degree one. An edge connecting a pendent vertex with its unique neighbor is called *a pendent edge*.

For any edge $e = uv \in E(G)$, we denote by $N_u = \{w \in V(G) : d(w, u) < d(w, v)\}$. Let $n_u = |N_u|$, i.e., n_u counts the number of vertices which are in positions closer to u than v of the edge uv.

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Let $w \in V(G)$ and $e = xy \in E(G)$. Define the distance $d(w,e)$ between w and e as $\min\{d(w,x), d(w,y)\}$. For an edge $uv \in E(G)$, let $M_u = \{e \in E(G) : d(e,u) < d(e,v)\}$. Then $m_u = |M_u|$ counts the number of edges of G lying closer to vertex u than to vertex v of the edge uv.

In [4], the *geometric-arithmetic index* GA was first defined as

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

where d_u stands for the degree of the vertex u.

Recently, G. Fath-Tabar *et al.* generalized GA to $GA_{general}(G)$, which was defined as [1] as

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

where Q_u is some quantity associated with the vertex u.

Replacing Q_u by n_u, G. Fath-Tabar *et al.* [1] defined it as the second geometric-arithmetic index, i.e.,

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

B. Zhou *et al.* [5] replaced Q_u by m_u, and then defined the third geometric-arithmetic index, i.e.,

$$(2) \qquad GA_3 = GA_3(G) = \sum_{uv \in E(G)} \frac{\sqrt{m_u m_v}}{\frac{1}{2}(m_u + m_v)}.$$

Geometric-arithmetic indices are a new class of topological descriptors, which are based on some properties of vertices of graphs. Details of their theory can be found in [2].

For unicyclic graphs with girth g, let $c_1, c_2, \ldots, c_g$ be the vertices on the cycle C, i.e., $V(C) = \{c_1, c_2, \ldots, c_g\}$.

Denote by $E(T)$ the set $\{e \in E(G) \mid e$ is a non-pendent edge and $e \notin E(C)\}$, by $E(P)$ the set of all pendent edges of G, and put $|E(P)| = p$.

For any edge $e = uv \in E(T)$, there must exist a path $P : v_0 v_1 v_2 \cdots v_k (= c_i)$ that contains the edge e, where v_i $(0 \le i \le k)$ are vertices in the same component of $G - E(C)$, v_0 is a pendent vertex and $c_i \in V(C)$.

Throughout this paper, for every edge $uv \notin E(C)$, let u be the vertex closer to v_0 than v. This means that u is more distant from C than v .

I. Gutman and B. Furtula [3] obtained inequalities between GA_2 and GA_3 for trees to estimate the second and third geometric-arithmetic indices. As a consequence, we continue to deduce inequalities for unicyclic graphs with even and odd girths, respectively.

2. Inequalities of unicyclic graphs with even girth

From (1) and (2), for a unicyclic graph G with even girth, it is easy to obtain:

(I) if $e = uv \in E(T)$, then $n_u + n_v = n$, $m_u = n_u - 1$, $m_v = n_v$ and $m_u + m_v = n - 1$.

(II) if $e = uv \in E(C)$, then $n_u + n_v = n$, $m_u = n_u - 1$, $m_v = n_v - 1$ and $m_u + m_v = n - 2$.

Let s be the number of vertices of one of the maximal components of $G - V(C)$.

2.1. Theorem. *Let G be a unicyclic graph with even girth and p pendent edges. If $s \leq \frac{n}{2}$, then*

$$\begin{aligned} &\frac{n}{n-1}GA_2(G) - \left(\frac{2}{\sqrt{n-1}} - \frac{\sqrt{2}}{\sqrt{n-2}}\right)p - \frac{\sqrt{2}n}{\sqrt{n-2}} \\ &\quad < GA_3(G) \\ &\quad < \frac{n}{n-2}GA_2(G) - \left(\frac{2\sqrt{n-1}}{n-2} - \frac{n-1}{(n-2)\sqrt{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}}\right)p - \frac{(n-1)n}{(n-2)\sqrt{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}}. \end{aligned} \tag{3}$$

Proof. From above discussions, it follows that

$$GA_2 = \sum_{uv\in E(G)} \frac{\sqrt{n_u n_v}}{\frac{1}{2}(n_u+n_v)} = \sum_{uv\in E(G)} \frac{2\sqrt{n_u n_v}}{n}, \tag{4}$$

and

$$GA_3(G) = \sum_{uv\in E(T)} \frac{2\sqrt{(n_u-1)n_v}}{(n-1)} + \sum_{uv\in E(C)} \frac{2\sqrt{(n_u-1)(n_v-1)}}{(n-2)}.$$

Bearing in mind that $n_u + n_v = n$,

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

For any non-pendent edge $e = uv \in E(G)$, there is $0 < (n-1)/(n_u n_v) < 1$. Since for any real number $x \in (0,1)$,

$$1 - x < \sqrt{1-x} < 1 - \frac{x}{2},$$

we have

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

and

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

Proof of lower bound. Let e be a non-pendent edge uv, then $n_u n_v \geq 2(n-2)$ holds because of $n_u + n_v = n$. It is easy to see that

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

Then

$$
\begin{aligned}
GA_3(G) &> \sum_{uv\in E(T)} \frac{2\sqrt{(n_u-1)(n_v-1)}}{n-1} + \sum_{uv\in E(C)} \frac{2\sqrt{(n_u-1)(n_v-1)}}{n-2} \\
&> \sum_{uv\in E(T)\cup E(C)} \frac{2\sqrt{(n_u-1)(n_v-1)}}{n-1} \\
&= \sum_{uv\in E(T)\cup E(C)} \frac{2}{n-1}\sqrt{n_u n_v}\sqrt{1-\frac{n-1}{n_u n_v}} \\
&\geq \frac{2}{n-1}\sum_{uv\in E(T)\cup E(C)} \left(\sqrt{n_u n_v} - \frac{n-1}{\sqrt{2(n-2)}}\right). \qquad (5)
\end{aligned}
$$

From (4), we have

$$
\sum_{E(T)\cup E(C)} \sqrt{n_u n_v} = \frac{n}{2}GA_2(G) - p\sqrt{n-1},
$$

which substitutes back into (5) to yield

$$
GA_3 > \frac{n}{n-1}GA_2(G) - \left(\frac{2}{\sqrt{n-1}} - \frac{\sqrt{2}}{\sqrt{n-2}}\right)p - \frac{\sqrt{2}n}{\sqrt{n-2}}.
$$

Thus the lower bound of (3) is obtained.

Proof of upper bound. Now it can be seen that

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

For any edge uv of G, $n_u n_v \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ holds. It follows that

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

Since $s \leq \frac{n}{2}$ and $n_u + n_v = n$, we get $n_u \leq n_v$ for each $e \in E(T)$. Suppose that

$$
f(x) = \frac{cx}{(c+x)^2},
$$

where c is a constant. By calculating the derivative of $f(x)$:

$$
f'(x) = \frac{c(c+x)(c-x)}{(c+x)^4},
$$

one can see easily that $f(x)$ decreases with increasing of x for $x \geq c$. Let $c = n_u - 1$. If $n_u \leq n_v = x$, then $n_u - 1 \leq n_v - 1 = x - 1$ and $f(n_v - 1) > f(n_v)$ hold, which implies that

$$
\sum_{uv\in E(T)} \frac{2\sqrt{(n_u-1)n_v}}{(n-1)} < \sum_{uv\in E(T)} \frac{2\sqrt{(n_u-1)(n_v-1)}}{(n-2)}. \qquad (6)
$$

Therefore,

$$\begin{aligned}
GA_3(G) &< \sum_{uv\in E(T)\cup E(C)} \frac{2\sqrt{(n_u-1)(n_v-1)}}{n-2} \\
&= \sum_{uv\in E(T)\cup E(C)} \frac{2}{n-2}\sqrt{n_u n_v}\sqrt{1-\frac{n-1}{n_u n_v}} \\
&< \sum_{uv\in E(T)\cup E(C)} \frac{2}{n-2}\left(\sqrt{n_u n_v}-\frac{n-1}{2\sqrt{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}}\right) \\
&< \frac{2}{n-2}\sum_{uv\in E(T)\cup E(C)} \sqrt{n_u n_v}-\frac{(n-1)(n-p)}{(n-2)\sqrt{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}} \\
&< \frac{n}{n-2}GA_2(G)-\left(\frac{2\sqrt{n-1}}{n-2}-\frac{n-1}{(n-2)\sqrt{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}}\right)p \\
&\qquad -\frac{(n-1)n}{(n-2)\sqrt{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}}. \qquad \square
\end{aligned}$$

Now, we discuss the case when a graph G with even girth does not satisfy $s \le \frac{n}{2}$.

2.2. Theorem. *Let G be a unicyclic graph with even girth and p pendent edges. Then*

$$\begin{aligned}
&\frac{n}{n-1}GA_2(G)-\left(\frac{2}{\sqrt{n-1}}-\frac{\sqrt{2}}{\sqrt{n-2}}\right)p-\frac{\sqrt{2}n}{\sqrt{n-2}} \\
&\qquad < GA_3(G) \\
&\qquad < GA_2(G)-\frac{2p\sqrt{n-1}}{n}+\frac{(3n-8)(n-6)}{4}.
\end{aligned}$$

Proof. Note that $n_u+n_v=n$, and $4n_u n_v \le n^2$. It is easy to obtain that:

$$\frac{n_u n_v}{n^2} > \frac{(n_u-1)(n_v-1)}{(n-2)^2}.$$

That is

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

Suppose $e=uv\in E(T)$. Since $n_u \le n_v$, similarly to the proof of (6), there is

$$\frac{n_u n_v}{n^2} > \frac{(n_u-1)n_v}{(n-1)^2}.$$

That is

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

It follows that

$$
\begin{aligned}
GA_3(G) &= \sum_{uv\in E(T)} \frac{2\sqrt{(n_u-1)n_v}}{(n-1)} + \sum_{uv\in E(C)} \frac{2\sqrt{(n_u-1)(n_v-1)}}{(n-2)} \\
&< \sum_{\substack{uv\,\in\,E(T)\\ n_u\,\le\,n_v}} \frac{2\sqrt{(n_u-1)n_v}}{(n-1)} + \sum_{\substack{uv\,\in\,E(T)\\ n_u\,>\,n_v}} \frac{2\sqrt{(n_u-1)n_v}}{n-1} \\
&\qquad + \sum_{uv\in E(C)} \frac{2\sqrt{n_u n_v}}{n} \\
&< \sum_{\substack{uv\,\in\,E(T)\\ n_u\,>\,n_v}} \frac{2\sqrt{(n_u-1)n_v}}{n-1} + \sum_{\{uv\,\in\,E(T)|n_u\,\le\,n_v\}\,\cup\,E(C)} \frac{2\sqrt{n_u n_v}}{n}.
\end{aligned}
$$

Thus we conclude that

$$
\begin{aligned}
GA_3(G) - GA_2(G) &< \sum_{\substack{uv\,\in\,E(T)\\ n_u\,>\,n_v}} \left(\frac{2\sqrt{(n_u-1)n_v}}{n-1} - \frac{2\sqrt{n_u n_v}}{n}\right) - \frac{2p}{n}\sqrt{n-1} \\
&< \sum_{\substack{uv\,\in\,E(T)\\ n_u\,>\,n_v}} \left(\frac{2\sqrt{n_u n_v}}{n-1} - \frac{2\sqrt{n_u n_v}}{n}\right) - \frac{2p}{n}\sqrt{n-1} \\
&= \frac{2}{n(n-1)} \sum_{\substack{uv\,\in\,E(T)\\ n_u\,>\,n_v}} \sqrt{n_u n_v} - \frac{2p}{n}\sqrt{n-1} \\
&< \frac{2}{n(n-1)} \sum_{\substack{uv\,\in\,E(T)\\ n_u\,>\,n_v}} n_u - \frac{2p}{n}\sqrt{n-1}. \qquad (7)
\end{aligned}
$$

Now let us estimate the maximum value of

$$
M := max\{\sum_{\substack{uv\,\in\,E(T)\\ n_u\,>\,n_v}} n_u\}.
$$

First we notice that there must be only one component of $G-E(C)$ that contains edges satisfying $n_u > n_v$, which implies $n_u > \frac{n}{2}$. Denote this component by $G(T_0)$. Let P_1 be the longest path in $G(T_0)$ with length l_1, put $P_1 := c_i v_1 v_2 \dots v_{l_1}, where c_i \in V(C)$ and v_{l_1} is a pendent vertex. Let P^* be the set of pendent vertices that are in $G(T_0)$.

For a non-pendent edge $e \in E(T_0)\backslash E(P^*)$, by the operation of dividing the edge $c_i v_1$ into $c_i v_e$ and $v_e v_1$, and then contracting e (deleting the edge e and then identifying the two ends of e), we get a new graph which we denote by $G(T_1)$. Denote the value of n_u for the edge e by $n_u(e)$.

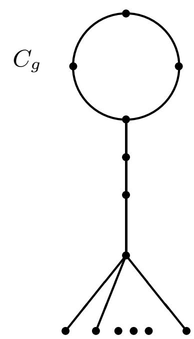
Note that $n_u(v_e v_1 \in G(T_1)) \ge n_u(e \in G(T_0)) + \mathrm{dist}(v_1, v_{l_1}) - 1$. For the other edges f, for edges f on the path from v_1 to $v \in G(T_0)$, it holds that $n_u(f \in G(T_1)) = n_u(f \in G(T_0)) - 1$; and for all other edges f, it holds that $n_u(f \in G(T_1)) = n_u(f \in G(T_0))$, thus we have $\sum_{e\in G(T_1)} n_u > \sum_{e\in G(T_0)} n_u$, i.e., $M(G(T_0)) < M(G(T_1))$. By repeating this process until there exist only pendent edges and the edges on the longest path, we have

$$
M(G(T_0)) < M(G(T_1)) < \cdots < M(G(T_k)).
$$

If $e = xy$ is a pendent edge with y as its pendent vertex, and v_{l_k} is the pendent vertex of the longest path $P_k = c_i v_1 v_2 \dots v_{l_k}$ in $G(T_k)$, let $G'(T_1) = G(T_k) - e + x v_{l_k - 1}$.

Then $n_u(f \in G'(T_1)) \geq n_u(f \in G'(T_0))$, and $M(G'(T_1)) < M(G(T_k))$. Repeating this operation until all non-pendent edges are incident with v_{l_k-1}, we get a new graph, denoted by $G'(T_r)$. Now we can get the maximum value of M with p pendent edges of the graph in Figure 1.

Figure 1. Unicyclic graphs $G'(T_r)$ with even girth, p pendent edges and maximum value of M



$G'(T_r)$

Then it follows that

$$\begin{aligned}\max \sum_{\substack{uv \in E(T) \\ n_u > n_v}} n_u &= \left(\frac{n}{2}\right) + \left(\frac{n}{2}+1\right) + \cdots + (n-c) \\ &< \left(\frac{n}{2}\right) + \left(\frac{n}{2}+1\right) + \cdots + (n-4) \\ &= \frac{(3n-8)(n-6)}{4}.\end{aligned}$$

Substituting the above result into (7) and by the lower bound in Theorem 2.1, we complete the proof. □

3. Inequalities of unicyclic graphs with odd girth

3.1. Theorem. *If G is a unicyclic graph with odd girth l and p pendent edges, then*

$$\begin{aligned}& GA_2(G) - (n-l-p)\sqrt{n-2} - \frac{2p\sqrt{n-1}}{n} \\ &\quad < GA_3(G) \\ &\quad < GA_2(G) - \frac{(n-l-p)}{n(n-1)}\sqrt{2(n-2)} - \frac{2p\sqrt{n-1}}{n}.\end{aligned}$$

Proof. For a unicyclic graph G with odd girth l, if edge $e = uv \in E(G) \backslash E(C)$, then $n_u + n_v = n$, $m_u = n_u - 1$, $m_v = n_v$, and $m_u + m_v = n - 1$ hold. Let a_i be the number of vertices of the component that contains the vertex c_i in $G - E(C)$. Then for any edge $e = uv \in E(C)$, there exists a number a_i such that $n_u + n_v = n - a_i$, $m_u = n_u$, $m_v = n_v$, and $m_u + m_v = n - a_i$. Thus

$$GA_2(G) = \sum_{E(T)} \frac{2\sqrt{n_u n_v}}{n} + \sum_{E(C)} \frac{2\sqrt{n_u n_v}}{n - a_i} + \frac{2p\sqrt{n-1}}{n}, \tag{8}$$

and

$$GA_3(G) = \sum_{E(T)} \frac{2\sqrt{(n_u - 1)n_v}}{n-1} + \sum_{E(C)} \frac{2\sqrt{n_u n_v}}{n - a_i}. \tag{9}$$

From (8) and (9), we can get

$$\begin{aligned} GA_2(G) - GA_3(G) &= \sum_{E(T)} \left(\frac{2\sqrt{n_u n_v}}{n} - \frac{2\sqrt{(n_u-1)n_v}}{n-1} \right) + \frac{2p\sqrt{n-1}}{n} \\ &< \sum_{E(T)} \left(\frac{2\sqrt{n_u n_v}}{n-1} - \frac{2\sqrt{(n_u-1)n_v}}{n-1} \right) + \frac{2p\sqrt{n-1}}{n} \\ &= \frac{2}{n-1} \sum_{E(T)} (\sqrt{n_u n_v} - \sqrt{(n_u-1)n_v}) + \frac{2p\sqrt{n-1}}{n} \\ &< \frac{2}{n-1} \sum_{E(T)} \frac{n_v}{2\sqrt{(n_u-1)n_v}} + \frac{2p\sqrt{n-1}}{n} \\ &= \frac{1}{n-1} \sum_{E(T)} \sqrt{\frac{n_v}{n_u - 1}} + \frac{2p\sqrt{n-1}}{n} \\ &\leq (n-l-p)\sqrt{n-2} + \frac{2p\sqrt{n-1}}{n}, \end{aligned}$$

and

$$\begin{aligned} GA_2(G) - GA_3(G) &> \sum_{E(T)} \sqrt{n_u n_v} \left(\frac{1}{n} - \frac{1}{n-1} \right) + \frac{2p\sqrt{n-1}}{n} \\ &\geq \frac{(n-l-p)}{n(n-1)} \sqrt{2(n-2)} + \frac{2p\sqrt{n-1}}{n}. \end{aligned}$$

The proof is completed. □

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