# The Second Geometric-Arithmetic Index for Trees and Unicyclic Graphs 

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#### Abstract

Let $G$ be a finite and simple graph with edge set $E(G)$. The second geometric-arithmetic Index is defined as $$
G A_{2}(G)=\sum_{u v \in E(G)} \frac{2 \sqrt{n_{u} n_{v}}}{n_{u}+n_{v}},
$$ where $n_{u}$ denotes the number of vertices in $G$ lying closer to $u$ than to $v$. In this paper we find a sharp upper bound for $G A_{2}(T)$, where $T$ is tree, in terms of the order and maximum degree of the tree. We also find a sharp upper bound for $G A_{2}(G)$, where $G$ is a unicyclic graph, in terms of the order, maximum degree and girth of $G$. In addition, we characterize the trees and unicyclic graphs which achieve the upper bounds.


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## 1 Introduction

Let $G$ be a simple connected graph with vertex set $V=V(G)$ and edge set $E=E(G)$. The integers $n=n(G)=|V(G)|$ and $m=m(G)=|E(G)|$ are the order and the size of the $\operatorname{graph} G$, respectively. We write $\operatorname{deg}_{G}(v)=\operatorname{deg}(v)$ for the degree of a vertex $v$ and $\Delta=\Delta(G)$ for the maximum degree of $G$. Let $u, v \in V(G)$, then the distance $d_{G}(u, v)$ between $u$ and $v$ is defined as the length of a shortest path in $G$ connecting $u$ and $v$.

[^0]In [5], a new class of topological descriptors, based on some properties of the vertices of a graph is presented. These descriptors are named as geometric-arithmetic indices, $G A_{\text {general }}$, and defined as:

$$
G A_{\text {general }}(G)=\sum_{u v \in E(G)} \frac{2 \sqrt{Q_{u} Q_{v}}}{Q_{u}+Q_{v}}
$$

where $Q_{u}$ is some quantity that in a unique manner can be associated with the vertex $u$ of the graph $G$. The geometric-arithmetic index $G A$ is defined in [6] as:

$$
G A(G)=\sum_{u v \in E(G)} \frac{2 \sqrt{\operatorname{deg}(u) \operatorname{deg}(v)}}{\operatorname{deg}(u)+\operatorname{deg}(v)} .
$$

The geometric-arithmetic index is well studied in the literature, see for example [2, 4, 7]. Let $u v$ be an edge of $G$. Define $N(u, G)=\left\{x \in V(G) \mid d_{G}(u, x)<d_{G}(u, x)\right\}$. In other words, $N(u, G)$ consists of vertices of $G$ which are closer to $u$ than to $v$. Note that the vertices equidistant to $u$ and $v$ are not included into either $N(u, G)$ or $N(v, G)$. Such vertices exist only if the edge uv belongs to an odd cycle. Hence, in trees, $n_{u}+n_{v}=n$ for all edges of the tree. It is also worth noting that $u \in N(u, G)$ and $v \in N(v, G)$, which implies that $n_{u} \geq 1$ and $n_{v} \geq 1$. The second geometric-arithmetic index $G A_{2}$ is defined in [5] as:

$$
G A_{2}(G)=\sum_{u v \in E(G)} \frac{2 \sqrt{n_{u} n_{v}}}{n_{u}+n_{v}},
$$

where $n_{u}=n_{u}(G)=|N(u, G)|$. See $[1,3,8]$ for more information on this index.
The following statements can be found in [5].
Theorem A. The path $P_{n}$ is the n-vertex tree with maximum second geometric-arithmetic index.

Theorem B. Let $S_{n}$ be a star of order n , then $G A_{2}(G)=\frac{2(n-1) \sqrt{n-1}}{n}$.
In this paper we first present some examples. Then we prove that for any tree $T$ of order $n \geq 2$ with maximum degree $\Delta$,

$$
G A_{2}(T) \leq \frac{2}{n}\left((\Delta-1) \sqrt{n-1}+\sum_{i=1}^{n-\Delta} \sqrt{i(n-i)}\right)
$$

Finally, we prove that for any unicyclic graph $G$ of order $n \geq 3$ with maximum degree $\Delta \geq 3$ and girth $k$, if $k$ is odd, then

$$
\begin{aligned}
G A_{2}(G) & \leq \frac{2}{n}\left((\Delta-2) \sqrt{n-1}+\sum_{i=1}^{n-k-\Delta+2} \sqrt{i(n-i)}\right) \\
& +\frac{2(k-1)}{n-1} \sqrt{\left(\frac{k-1}{2}+\Delta-2\right)\left(n-\frac{k-1}{2}-\Delta+1\right)}+\frac{2}{\Delta+\mathrm{k}-3} \sqrt{\frac{k-1}{2}\left(\frac{k-1}{2}+\Delta-2\right)} \\
& +\frac{2}{n-\Delta+1} \sqrt{\frac{k-1}{2}\left(n-\frac{k-1}{2}-\Delta+1\right)},
\end{aligned}
$$

and if $k$ is even, then

$$
G A_{2}(G) \leq \frac{2}{n}\left((\Delta-2) \sqrt{n-1}+\sum_{i=1}^{n-k-\Delta+2} \sqrt{i(n-i)}+k \sqrt{\left(\frac{k}{2}+\Delta-2\right)\left(n-\frac{k}{2}-\Delta+2\right)}\right)
$$

We also characterize the trees and unicyclic graphs which achieve the upper bounds.

## 2 Examples

Dendrimers are nanostructures that can be precisely designed and manufactured for a wide variety of applications, such as drug delivery, gene delivery and diagnostic tests. In this section we calculate the second geometric-arithmetic index for Dendrimers of types A and B and for Tecto Dendrimers. See Figure 1.


Figure 1: Dendrimers of types A and B and Tecto Dendrimers.
Example 1. In Dendrimers $D[n]$ type $A$, denoted $D[n]_{A}$, there are $4\left(2^{n}-1\right)+1$ vertices and $4\left(2^{n}-1\right)$ edges. Let $e$ be an edge between the $i$ th and the $(i+1)$ th layers. Then

$$
f_{i}(e)=\sqrt{\left(2^{n-i}-1\right)\left(2^{n+2}-2^{n-i}-2\right)} \text { for } \mathrm{i}=1,2, \ldots, \mathrm{n}-1
$$

In addition, there are $2^{i+2}$ edges between the $i$ th and the $(i+1)$ th layers. Therefore, for $n \geq 2$,

$$
\begin{aligned}
G A_{2}\left(D[n]_{A}\right) & =\frac{2}{4\left(2^{n}-1\right)+1}\left(4 \sqrt{\left(2^{n}-1\right)\left(3\left(2^{n}-1\right)+1\right)}+\sum_{i=1}^{n-1} 2^{i+2} f_{i}(e)\right) \\
& =\frac{8}{4\left(2^{n}-1\right)+1}\left(\sqrt{\left(2^{n}-1\right)\left(3\left(2^{n}-1\right)+1\right)}+\sum_{i=1}^{n-1} 2^{i} f_{i}(e)\right) .
\end{aligned}
$$

For examples,

$$
\begin{aligned}
& G A_{2}\left(D[2]_{A}\right)=\frac{8}{13}(\sqrt{30}+2 \sqrt{12})=7.63 \text { and } \\
& G A_{2}\left(D[3]_{A}\right)=\frac{8}{29}(\sqrt{154}+2 \sqrt{78}+4 \sqrt{28})=14.13 .
\end{aligned}
$$

Example 2. In Dendrimers $D[n]$ type $B$, denoted $D[n]_{B}$, there are $3\left(2^{n}-1\right)+1$ vertices and $3\left(2^{n}-1\right)$ edges. Let $e$ be an edge between the $i$ th and the $(i+1)$ th layers. Then

$$
f_{i}(e)=\sqrt{\left(2^{n-i}-1\right)\left(3\left(2^{n}\right)-2^{n-i}-1\right)} \text { for } \mathrm{i}=1,2, \ldots, \mathrm{n}-1
$$

In addition, there are $3\left(2^{i}\right)$ edges between the $i$ th and the $(i+1)$ th layers. Therefore, for $n \geq 2$,

$$
G A_{2}\left(D[n]_{B}\right)=\frac{8}{3\left(2^{n}-1\right)+1}\left(\sqrt{3\left(2^{n}-1\right)\left(2\left(2^{n}-1\right)+1\right)}+\sum_{i=1}^{n-1} 3\left(2^{i}\right) f_{i}(e)\right) .
$$

For example,
$G A_{2}\left(D[2]_{B}\right)=\frac{2}{10}(3 \sqrt{21}+18)=6.35$ and
$G A_{2}\left(D[3]_{B}\right)=\frac{2}{22}(3 \sqrt{105}+6 \sqrt{57}+12 \sqrt{21})=11.91$.
Example 3. In Tecto Dendrimers $D[n]_{T}$, there are $2^{n+2}-2$ vertices and $2^{n+2}-3$ edges. Let $e$ be an edge between the $i$ th and the $(i+1)$ th layers. Then

$$
f_{i}(e)=\sqrt{\left(2^{n-i}-1\right)\left(2^{n+2}-2^{n-i}-1\right)} \text { for } \mathrm{i}=1,2, \ldots, \mathrm{n}-1
$$

In addition, there are $2^{i+2}$ edges between the $i$ th and the $(i+1)$ th layers. Therefore, for $n \geq 2$,

$$
G A_{2}\left(D[n]_{T}\right)=\frac{8}{2^{n+2}-2}\left(4 \sqrt{\left(2^{n}-1\right)\left(3\left(2^{n}\right)-1\right)}+\sum_{i=1}^{n-1} 2^{i+2} f_{i}(e)+2^{n+1}-1\right)
$$

For example,

$$
\begin{aligned}
& G A_{2}\left(D[2]_{T}\right)=\frac{2}{14}(4 \sqrt{33}+8 \sqrt{13}+7)=8.40 \text { and } \\
& G A_{2}\left(D[3]_{T}\right)=\frac{2}{30}(4 \sqrt{161}+8 \sqrt{81}+16 \sqrt{29}+15)=14.93 .
\end{aligned}
$$

## 2 AN UPPER BOUND ON THE SECOND GEOMETRIC-ARITHMETIC OF Trees

In this section we present a sharp upper bound for the second geometric-arithmetic index of trees in terms of their order and maximum degree. We also characterize all trees whose the second geometric-arithmetic index achieves the upper bound. A leaf of a tree $T$ is a vertex of degree 1, a support vertex is a vertex adjacent to a leaf and a strong support vertex is a support vertex adjacent to at least two leaves. An end-support vertex is a support vertex whose all neighbors with exception at most one are leaves. A rooted tree is a tree having a distinguished vertex $v$, called the root. Let $T_{n, \Delta}$ be the set of trees of order $n$ and maximum degree $\Delta$. Let $T$ be a tree of order $n$ and let $f: E(T) \rightarrow \mathrm{Z}^{+}$is a function defined by $f(x y)=$ $\sqrt{n_{x} n_{y}}$. Hence $G A_{2}(T)=\frac{2}{n} \sum_{u v \in E(G)} f(u v)$. We start with an easy but useful observation.

Observation 4. Let $x \geq y \geq 1$ and $n \geq x+y+2$ be positive integers. Then for every $1 \leq k \leq y,(x+k)(n-x-k)>(y-k+1)(n-y+k-1)$.

Proof. First note that $(x+k)(n-x-k)-(y-k+1)(n-y+k-1)=n(2 k+x)-$ $(x+k)^{2}$. Since $n \geq x+y+2$, it follows that $n(2 k+x)-(x+k)^{2}>0$. So the result follows.

Lemma 5. Let $T$ be a tree of order $n$ with maximum degree $\Delta$ and $v$ be a vertex of maximum degree. If $T$ has a vertex of degree at least three different from $v$, then there is a tree $T^{\prime} \in T_{n, \Delta}$ such that $G A_{2}(T)<G A_{2}\left(T^{\prime}\right)$.

Proof. Let $T$ be the rooted tree at $v$. Let $u \neq v$ be a vertex of degree $\operatorname{deg}(u)=k \geq 3$ such that $d(u, v)$ is as large as possible and let $N(u)=\left\{u_{1}, u_{2}, \ldots, u_{k-2}, u_{k-1}, u_{k}\right\}$. Now we distinguish three cases.

Case 1. $u$ is an end-support vertex.
We may assume that $u_{k}$ is the parent of $u$. Let $S=\left\{u u_{1}, u u_{2}, \ldots, u u_{k-2}, u u_{k-1}\right\}$ and let $T^{\prime}$ be the tree obtained by attaching the path $u u_{1} u_{2} \ldots u_{k-2} u_{k-1}$ to $T-\left\{u_{1}, u_{2}, \ldots, u_{k-1}\right\}$. Suppose that $S^{\prime}=\left\{u u_{1}, u_{1} u_{2}, \ldots, u_{k-2} u_{k-1}\right\}$. Clearly, $T^{\prime} \in T_{n, \Delta}$ and

$$
\sum_{u v \in E(T)-s} f(u v)=\sum_{u v \in E\left(T^{\prime}\right)-s^{\prime}} f(u v) .
$$

By definition

$$
\begin{align*}
& \quad \frac{n}{2} G A_{2}(T)=\sum_{u v \notin S} f(u v)+\sum_{u v \in S} f(u v)=\sum_{u v \in E(T)-S} f(u v)+(k-1) \sqrt{n-1},  \tag{1}\\
& \text { and } \\
& \frac{n}{2} G A_{2}\left(T^{\prime}\right)=\sum_{u v \notin S^{\prime}} f(u v)+\sum_{u v \in S^{\prime}} f(u v)=\sum_{u v \in E\left(T^{\prime}\right)-S^{\prime}} f(u v)+\sum_{i=1}^{k-1} \sqrt{i(n-i)} . \tag{2}
\end{align*}
$$

Combining (1), (2) and the fact that $k \geq 3$, we obtain $G A_{2}(T)<G A_{2}\left(T^{\prime}\right)$, as desired.
Case 2. $u$ is a support vertex.
By Case 1 , we may assume that $u$ is not an end-support vertex and $\operatorname{deg}\left(u_{1}\right)=1$. Suppose $\operatorname{deg}\left(u_{2}\right)=2$ and $T_{u_{2}}$ is the component of $T-u u_{2}$ containing $u_{2}$. Since, by the choice of vertex $u$, $d(u, v)$ is as large as possible, we may assume that $T_{u_{2}}$ is the path $u_{2} x_{1} x_{2} \ldots x_{t}, t \geq 1$. Let $T^{\prime}$ be the tree obtained from $T-u u_{1}$ by adding the pendant edge $x_{t} u_{1}$ to this graph. Let $S=\left\{u u_{1}, u u_{2}, u_{2} x_{1}, x_{1} x_{2}, \ldots, x_{t-1} x_{t}\right\} \quad$ and $S^{\prime}=\left\{u u_{2}, u_{2} x_{1}, x_{1} x_{2}, \ldots, x_{t-1} x_{t}, u_{1} x_{t}\right\}$. Clearly, $T^{\prime} \in T_{n, \Delta}$ and

$$
\sum_{u v \in E(T)-S} f(u v)=\sum_{u v \in E\left(T^{\prime}\right)-S^{\prime}} f(u v) .
$$

By definition

$$
\begin{equation*}
\frac{n}{2} G A_{2}(T)=\sum_{u v \in E(T)-s} f(u v)+\sum_{i=1}^{t+1} \sqrt{i(n-i)}+\sqrt{n-1} \tag{3}
\end{equation*}
$$

and

$$
\begin{equation*}
\frac{n}{2} G A_{2}\left(T^{\prime}\right)=\sum_{u v \in E\left(T^{\prime}\right)-s^{\prime}} f(u v)+\sum_{i=1}^{t+2} \sqrt{i(n-i)} . \tag{4}
\end{equation*}
$$

By (3), (4) and the fact that $n \geq t+4$, we obtain $G A_{2}(T)<G A_{2}\left(T^{\prime}\right)$.

Case 3. $u$ is not a support vertex.

Suppose $T_{u_{1}}$ and $T_{u_{2}}$ are the components of $T-\left\{u u_{1}, u u_{2}\right\}$ containing $u_{1}$ and $u_{2}$, respectively. By the choice of vertex $u$, we may assume that $T_{u_{1}}=u_{1} x_{1} x_{2} \ldots x_{s}, s \geq 1$ and $T_{u_{2}}=u_{2} y_{1} y_{2} \ldots y_{t}, t \geq 1$. Then $\operatorname{deg}\left(x_{i}\right)=\operatorname{deg}\left(y_{j}\right)=2,1 \leq i \leq s-1,1 \leq$ $j \leq t-1$, and $\operatorname{deg}\left(x_{s}\right)=\operatorname{deg}\left(y_{t}\right)=1$. Let $T^{\prime}$ be the tree obtained from $T-T_{u_{2}}$ by adding the path $x_{s} y_{t} y_{t-1} \ldots y_{1} u_{2}$ to this graph. Let

$$
S=\left\{u u_{1}, u_{1} x_{1}, x_{1} x_{2}, \ldots, x_{s-1} x_{s}\right\} \cup\left\{u u_{2}, u_{2} y_{1}, y_{1} y_{2}, \ldots, y_{t-1} y_{t}\right\}
$$

and

$$
S^{\prime}=\left\{u u_{1}, u_{1} x_{1}, x_{1} x_{2}, \ldots, x_{s-1} x_{s}\right\} \cup\left\{x_{s} y_{t}, u_{2} y_{1}, y_{1} y_{2}, \ldots, y_{t-1} y_{t}\right\}
$$

Clearly, $T^{\prime} \in T_{n, \Delta}$ and

$$
\sum_{u v \in E(T)-S} f(u v)=\sum_{u v \in E\left(T^{\prime}\right)-S^{\prime}} f(u v) .
$$

By definition we have

$$
\begin{equation*}
\frac{n}{2} G A_{2}(T)=\sum_{u v \in E(T)-S} f(u v)+\sum_{i=1}^{s+1} \sqrt{i(n-i)}+\sum_{i=1}^{t+1} \sqrt{i(n-i)} \tag{5}
\end{equation*}
$$

and

$$
\begin{equation*}
\frac{n}{2} G A_{2}\left(T^{\prime}\right)=\sum_{u v \in E\left(T^{\prime}\right)-s^{\prime}} f(u v)+\sum_{i=1}^{s+t+2} \sqrt{i(n-i)} . \tag{6}
\end{equation*}
$$

Applying Observation 4 and inequalities (5) and (6), we conclude that $G A_{2}(T)<G A_{2}\left(T^{\prime}\right)$. This complete the proof.

A spider is a tree with at most one vertex of degree more than 2 , called the center of the spider (if no vertex is of degree more than two, then any vertex can be the center). A leg of a spider is a path from the center to a vertex of degree 1 . Thus, a star with $k$ edges is a spider of $k$ legs, each of length 1 , and a path is a spider of 1 or 2 legs.

Lemma 6. Let $T$ be a spider of order $n$ with $k \geq 3$ legs. If $T$ has two legs of length at least 2 , then there is a spider $T^{\prime}$ of order $n$ with $k$ legs such that $G A_{2}(T)<G A_{2}\left(T^{\prime}\right)$.

Proof. Let $v$ be the center of $T$ and $N(v)=\left\{v_{1}, v_{2}, \ldots, v_{k}\right\}$. Root $T$ at $v$. Assume, without loss of generality, that $\operatorname{deg}\left(v_{1}\right)=\operatorname{deg}\left(v_{2}\right)=2$ and let $v_{1} x_{1} x_{2} \ldots x_{s}$ and $v_{2} y_{1} y_{2} \ldots y_{t}$ be two legs of $T$. Let $T^{\prime}$ be the tree obtained from $T$ be deleting the edges $x_{1} x_{2}, \ldots, x_{s-1} x_{s}$ and adding the edges $x_{1} y_{t}, x_{1} x_{2}, \ldots, x_{s-1} x_{s}$. Suppose

$$
S=\left\{v v_{1}, v_{1} x_{1}, x_{1} x_{2}, \ldots, x_{s-1} x_{s}\right\} \cup\left\{v v_{2}, v_{2} y_{1}, y_{1} y_{2}, \ldots, y_{t-1} y_{t}\right\},
$$

and

$$
S^{\prime}=\left\{v v_{1}, y_{t} x_{1}, x_{1} x_{2}, \ldots, x_{s-1} x_{s}\right\} \cup\left\{v v_{2}, v_{2} y_{1}, y_{1} y_{2}, \ldots, y_{t-1} y_{t}\right\}
$$

Clearly

$$
\sum_{u v \in E(T)-s} f(u v)=\sum_{u v \in E\left(T^{\prime}\right)-s^{\prime}} f(u v) .
$$

By definition we have

$$
\begin{equation*}
\frac{n}{2} G A_{2}(T)=\sum_{u v \in E(T)-s} f(u v)+\sum_{i=1}^{s+1} \sqrt{i(n-i)}+\sum_{i=1}^{t+1} \sqrt{i(n-i)} \tag{7}
\end{equation*}
$$

and

$$
\begin{equation*}
\frac{n}{2} G A_{2}\left(T^{\prime}\right)=\sum_{u v \in E\left(T^{\prime}\right)-s^{\prime}} f(u v)+\sum_{i=1}^{s+t+1} \sqrt{i(n-i)}+\sqrt{n-1} . \tag{8}
\end{equation*}
$$

By Observation 4, equalities (7) and (8) and the fact that $n \geq s+t+4$ we obtain $G A_{2}(T)<G A_{2}\left(T^{\prime}\right)$.

We are now ready to prove the main theorem of this section.
Theorem 7. For any tree $T \in T_{n, \Delta}$ of order $n \geq 2$,

$$
G A_{2}(T) \leq \frac{2}{n}\left((\Delta-1) \sqrt{n-1}+\sum_{i=1}^{n-\Delta} \sqrt{i(n-i)}\right)
$$

The equality holds if and only if $T$ is a spider with at most one leg of length at least two.
Proof. Let $T_{1}$ be a tree of order $n \geq 2$ with maximum degree $\Delta$ such that
$G A_{2}\left(T_{1}\right)=\max \left\{G A_{2}(T) \mid T\right.$ is a tree of order $n$ with maximum degree $\left.\Delta\right\}$.
Let $v$ be a vertex with maximum degree $\Delta$. Root $T_{1}$ at $v$. If $\Delta=2$, then $T_{1}$ is a path of order $n$ and the result follows by Theorem A. Let $\Delta \geq 3$. By the choice of $T_{1}$, we deduce from Lemma 5 that $T_{1}$ is a spider with center $v$. It follows from Lemma 6 and the choice of $T_{1}$ that $T_{1}$ has at most one leg of length at least two. First let all legs of $T_{1}$ have length one. Then $T_{1}$ is a star of order $n$ and the result follows by Theorem B. Now let $T_{1}$ have only one leg of length at least two. Then

$$
G A_{2}(T)=\frac{2}{n}\left((\Delta-1) \sqrt{n-1}+\sum_{i=1}^{n-\Delta} \sqrt{i(n-i)}\right)
$$

This completes the proof.

## 3 UNICYCLIC GRAPHS

A connected graph with precisely one cycle is called a unicyclic graph. Let the set $\varphi_{n, \Delta, k}$ consist of all unicycle graphs of order $n$, maximum degree $\Delta \geq 3$ and grith $k$, where $3 \leq k \leq n$. Note that if $G$ is a cycle of order $n$, then $G A_{2}(G)=n$. Let $G \in \varphi_{n, \Delta, k}$. In this section we assume that the $k$-cycle of $G$ is $C_{k}=\left(w_{1}, w_{2}, \ldots, w_{k}\right)$. In addition for a vertex $u \in V\left(C_{k}\right)$ we let $T_{u}$ be the connected component of $G \backslash E\left(C_{k}\right)$ containing $u$. Note that $T_{u}$ is a tree and we assume $u$ is the root of this tree. Without loss of generality, we also assume one of the vertices of $T_{w_{1}}$, say $v$, is of degree $\Delta$.

Lemma 8. Let $G \in \varphi_{n, \Delta, k}$ and $v$ be a vertex of maximum degree $\Delta$. Let $C$ be the only cycle of $G, u \in V(C)$ and $u \neq v$. If $T_{u}$ is a spider with at least two legs, then there is a graph $G^{\prime} \in \varphi_{n, \Delta, k}$ such that $G A_{2}(G)<G A_{2}\left(G^{\prime}\right)$.

Proof. Assume $T_{u}$ has $\ell$ legs with lengths $t_{1}, t_{2}, \ldots, t_{\ell}$ and $\sum_{i=1}^{\ell} t_{i}=s$. Let the graph $G^{\prime}$ be obtained from $G \backslash E\left(T_{u}\right)$ by attaching a path $P_{s}$ to vertex $u$. Obviously, $G^{\prime} \in \varphi_{n, \Delta, k}$. A simple calculation shows that

$$
G A_{2}\left(G^{\prime}\right)-G A_{2}(G)=\frac{2}{n}\left[\sum_{i=1}^{s} \sqrt{i(n-i)}-\sum_{j=1}^{\ell} \sum_{i=1}^{t_{j}} \sqrt{i(n-i)}\right]
$$

Apply Observation 4 to obtain $G A_{2}\left(G^{\prime}\right)-G A_{2}(G)>0$.

Lemma 9. Let $G \in \varphi_{n, \Delta, k}$ and $\operatorname{deg}(u) \geq 3$, where $u \in T_{w_{i}}, u \neq w_{i}$, for some $2 \leq i \leq k$. Then there is a graph $G^{\prime} \in \varphi_{n, \Delta, k}$ such that $G A_{2}(G)<G A_{2}\left(G^{\prime}\right)$.

Proof. Without loss of generality, we may assume $u$ has the largest distance from $w_{i}$ among all the vertices of $T_{w_{i}}$ whose degree is at least 3 . This implies that $T_{u}$ is a spider with at least two legs. Let $G^{\prime}$ be the graph obtained from $G$ by replacing $T_{u}$ with a path with the same order as $T_{u}$. A calculation similar to that presented in Lemma 8 shows that $G A_{2}\left(G^{\prime}\right)-$ $G A_{2}(G)>0$.

Lemma 10. Let $G \in \varphi_{n, \Delta, k}$ and $T_{w_{i}}$ and $T_{w_{j}}$ be paths of length at least 1 for some $2 \leq$ $i, j \leq k, i \neq j$. Then there is a graph $G^{\prime} \in \varphi_{n, \Delta, k}$ such that $G A_{2}(G)<G A_{2}\left(G^{\prime}\right)$.

Proof. Let $\ell_{1}$ and $\ell_{2}$ be the length of the paths $T_{w_{i}}$ and $T_{w_{j}}$, respectively. Let $G^{\prime}$ be the graph obtained from $G$ by removing $T_{w_{i}}$ and $T_{w_{j}}$ and attaching a path of length $\ell_{1}+\ell_{2}$ to the vertex $u$. Then as before one can see that $G A_{2}(G)<G A_{2}\left(G^{\prime}\right)$.

Lemma 11. Let $G \in \varphi_{n, \Delta, k}$ and assume the vertices of the cycle $C_{k}$ are all of degree two except $w_{1}$ and $w_{i}, i \neq 1$. If the distance of $w_{i}$ from $w_{1}$ is not $\lceil(k-1) / 2\rceil$, then there is a graph $G^{\prime} \in \varphi_{n, \Delta, k}$ such that $G A_{2}(G)<G A_{2}\left(G^{\prime}\right)$.

Proof. Let $G^{\prime}$ be the graph obtained from $G$ by removing $T_{w_{i}}$ and attaching it to vertex $w_{j}$, where $j=\lceil(k-1) / 2\rceil$. Then one can see that $G A_{2}(G)<G A_{2}\left(G^{\prime}\right)$.

Now we consider the graph $G \in \varphi_{n, \Delta, k}$ with $\operatorname{deg}\left(w_{i}\right)=2$ for all $2 \leq i \leq k, i \neq$ $\lceil(k-1) / 2\rceil$ and $\operatorname{deg}\left(w_{j}\right) \geq 2$, where $j=\lceil(k-1) / 2\rceil$. By Lemma 9, in order to maximize $G A_{2}(G), T_{v}$ must be a spider and $\operatorname{deg}_{G}\left(w_{1}\right)=3$ if $w_{1} \neq v$.

Lemma 12. Let $G \in \varphi_{n, \Delta, k}$ and $w_{1} \neq v$. Then there is a graph $G^{\prime} \in \varphi_{n, \Delta, k}$ such that $G A_{2}(G)<G A_{2}\left(G^{\prime}\right)$.

Proof. Let $G^{\prime}$ be the graph obtained from $G \backslash T_{w_{1}}$ by attaching a path of order $\left|V\left(T_{w_{1}}\right)\right|-\Delta+2$ to the end vertex of the path $T_{w_{j}}$ which is different from $w_{j}, j=$ $\lceil(k-1) / 2\rceil$ and adding $\Delta-2$ pendant edges at vertex $w_{1}$. Obviously, $G^{\prime} \in \varphi_{n, \Delta, k}$ and it is straightforward to verify that $G A_{2}(G)<G A_{2}\left(G^{\prime}\right)$.

By Lammas 8-12 we obtain the following result.

Corollary 13. Let $H \in \varphi_{n, \Delta, k}$ be the graph which consists of a cycle $C_{k}=\left(w_{1}, w_{2}, \ldots, w_{k}\right)$ with $\Delta-2$ pendant edges at vertex $w_{1}$ and a path of order $n-k-\Delta+2$ at vertex $w_{j}$, where $j=\lceil(k-1) / 2\rceil$. Then for every $G \in \varphi_{n, \Delta, k}, G A_{2}(G) \leq G A_{2}(H)$.

We are now ready to state the main theorem of this section.
Theorem 14. For any unicycle graph $G$ of order $n$, girth $k$ and maximum degree $\Delta \geq 3$, if $k$ is odd, then

$$
\begin{aligned}
G A_{2}(G) & \leq \frac{2}{n}\left((\Delta-2) \sqrt{n-1}+\sum_{i=1}^{n-k-\Delta+2} \sqrt{i(n-i)}\right) \\
& +\frac{2(k-1)}{n-1} \sqrt{\left(\frac{k-1}{2}+\Delta-2\right)\left(n-\frac{k-1}{2}-\Delta+1\right)}+\frac{2}{\Delta+\mathrm{k}-3} \sqrt{\frac{k-1}{2}\left(\frac{k-1}{2}+\Delta-2\right)} \\
& +\frac{2}{n-\Delta+1} \sqrt{\frac{k-1}{2}\left(n-\frac{k-1}{2}-\Delta+1\right)},
\end{aligned}
$$

and if $k$ is even, then

$$
G A_{2}(G) \leq \frac{2}{n}\left((\Delta-2) \sqrt{n-1}+\sum_{i=1}^{n-k-\Delta+2} \sqrt{i(n-i)}+k \sqrt{\left(\frac{k}{2}+\Delta-2\right)\left(n-\frac{k}{2}-\Delta+2\right)}\right)
$$

The equality holds if and only if $G$ is the graph $H$ given in Corollary 13 .

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