The First Geometric–Arithmetic Index of Some Nanostar Dendrimers

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Abstract. Dendrimers are highly branched organic macromolecules with successive layers or generations of branch units surrounding a central core [1, 4]. These are key molecules in nanotechnology and can be put to good use. In this article, we compute the first geometric-arithmetic index of two infinite classes of dendrimers.

Keywords: nanostar dendrimer, the first geometric-arithmetic index.

1. Introduction

Investigations of topological indices based on end–vertex degrees of edges have been conducted over 35 years. One of them is the first geometric–arithmetic index \((GA_1)\). The \((GA_1)\) index defined as:

\[
GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{2(d_u + d_v)}
\]

has been introduced less than a year ago [2, 3, 5]. Here \(d_u\) denotes degree of vertex \(u\) and so on.

Dendrimer is a synthetic 3-dimentional macromolecule that is prepared in a step-wise fashion from simple branched monomer units. The nanostar dendrimer is a part of a new group of macromolecules that appear to photon funnels just like artificial antennas. In this article many attempt have been made to compute the first geometric-arithmetic index for two types of nanostar dendrimers.

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2. RESULTS AND DISCUSSION

Lemma 1. Consider the complete graph $K_n$ of order $n$. The first geometric-arithmetic index of this graph is computed as follow:

$$GA_1(K_n) = \frac{1}{2} n(n-1).$$

Proof. The degree of all the vertices of a complete graph of order $n$ is $n-1$ and the number of edges for $K_n$ is equal $\frac{1}{2} n(n-1)$, thus

$$GA_1(K_n) = \sum_{uv \in E(K_n)} \frac{\sqrt{d_u d_v}}{2(d_u + d_v)} = \frac{1}{2} n(n-1) \frac{\sqrt{(n-1)^2}}{\frac{1}{2} 2(n-1)} = \frac{1}{2} n(n-1).$$

Lemma 2. If $G$ is a regular graph of degree $r>0$, then

$$GA_1(G) = \frac{nr}{2}.$$

Proof. A regular graph $G$ on $n$ vertices, having degree $r$, possesses $\frac{nr}{2}$ edges, thus

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{2(d_u + d_v)} = \frac{nr}{2} \frac{\sqrt{r^2}}{\frac{1}{2} 2(r + r)} = \frac{nr}{2}.$$

Lemma 3. Let $S_n$ be a star on $n+1$ vertices (Figure 1), then

$$GA_1(S_n) = \frac{2n\sqrt{n}}{n+1}.$$

Proof. It is easily seen that there are $n$ vertices of degree 1 and a vertex of degree $n$. Therefore,

$$GA_1(S_n) = \sum_{uv \in E(K_n)} \frac{\sqrt{d_u d_v}}{2(d_u + d_v)} = \frac{2n\sqrt{n}}{n+1}.$$

Figure 1. Star graph with $n+1$ vertices.
2.1 The First Geometric-arithmetic Index of the First Class of Nanostar Dendrimers

Consider a graph $G$ on $n$ vertices, where $n \geq 2$. The maximum possible vertex degree in such a graph is $n-1$. Suppose $d_{ij}$ denote the number of edges of $G$ connecting vertices of degrees $i$ and $j$. Clearly, $d_{ij} = d_{ji}$. We now consider two infinite classes $NS_1[n]$ and $NS_2[n]$ of nanostar dendrimers, Figures 2 and 3. The aim is to compute the first geometric-arithmetic index for two of these nanostar dendrimers.

We consider the molecular graph of $K(n) = NS_1[n]$ with four similar branches and three extra edges, where $n$ is steps of growth in this type of dendrimer nanostars (Figure 2). Define $d_{23}$ to be the number of edges connecting a vertex of degree 2 with a vertex of degree 3, $d_{13}$ to be the number of edges connecting a vertex of degree 1 with a vertex of degree 3, $d_{22}$ to be the number of edges connecting two vertices of degree 2 and $d_{12}$ to be the number of edges connecting a vertex of degree 1 with a vertex of degree 2. Also $d'_{ij}$ denote the number of edges connecting vertices of degrees $i$ and $j$ in each branch ($i, j \leq 4$).

It is obvious that $d_{12} = 4d'_{22} + 1$, $d_{22} = 4d'_{22} + 1$, $d_{13} = 4$, $d'_{13}$ and $d_{23} = 4d'_{23} + 2$. On the other hand a simple calculation shows that $d_{12}' = 2^{n-1}$. Therefore, $d_{12}' = 4d'_{12} = 2^n$. Using a similar argument, one can see that $d_{22}' = 3(n-1)$ then $d_{22}' = 12.2^n - 11$, $d_{13}' = 2^n - 1$ then $d_{13}' = 4d'_{13} = 4.2^n - 4$ and finally $d_{23}' = 3(2^n - 1) + (2^{n-1} - 1)$ then $d_{23}' = 4d'_{23} + 2 = 14.2^n - 14$.

**Theorem 4.** The first geometric-arithmetic index of $K(n) = NS_1[n]$ is

$$G_{A_1}(K(n)) = \left(\frac{4\sqrt{3}}{3} + 12 + 2\sqrt{3} + \frac{28\sqrt{6}}{5}\right)2^n - (11 + 2\sqrt{3} + \frac{28\sqrt{6}}{5}).$$

**Proof.** We have $G_{A_1}(K(n)) = \sum_{uv \in E(K(n))} \frac{d_u d_v}{2(d_u + d_v)}$. Then

$$G_{A_1}(K(n)) = \left(\frac{2\sqrt{2}}{3} + (12.2^n - 11) + (4.2^n - 4)\frac{\sqrt{3}}{2} + (14.2^n - 4)\frac{2\sqrt{6}}{5}\right)2^n$$

$$= G_{A_1}(K(n)) = \left(\frac{4\sqrt{3}}{3} + 12 + 2\sqrt{3} + \frac{28\sqrt{6}}{5}\right)2^n - (11 + 2\sqrt{3} + \frac{28\sqrt{6}}{5}).$$

2.2 The First Geometric-arithmetic Index of the Second Class of Nanostar Dendrimers

We consider the second class $H(n) = NS_2[n]$, where $n$ is steps of growth. Since the molecular graph of $H$ has four similar branches and five extra edges (Figure 3), $d_{12} = 4d'_{12}$,
\[ d_{22} = 4d'_{22} + 3 \quad \text{and} \quad d_{23} = 4d'_{23} + 2. \] By a routine calculation we have \( d'_{12} = 2^{n-1} \), \( d'_{22} = 2(2^n - 1) \) and \( d'_{23} = 3.2^{n-1} - 2 \). One can prove that \( d_{12} = 2^{n+1} \), \( d_{22} + 8.2^n - 5 \) and \( d_{23} = 6.2^n - 6 \).

**Figure 2.** \( NS_1[1] \) and \( NS_1[n] \) PAMAM Dendrimer.

**Theorem 5.** The first geometric-arithmetic index of \( H(n) = NS_2[n] \) is computed as follows:

\[
GA_1(H(n)) = \left( \frac{4\sqrt{2}}{3} + 8 + \frac{12\sqrt{6}}{5} \right)2^n - (5 + \frac{12\sqrt{6}}{5})
\]

**Proof.** By definition, we have:

\[
GA_1(H(n)) = \sum_{uv \in E(H(n))} \frac{\sqrt{d_ud_v}}{\frac{1}{2}(d_u + d_v)}
\]

\[
= 2^{n+1} \frac{2\sqrt{2}}{3} + (8.2^n - 5) + (6.2^n - 6) \frac{2\sqrt{6}}{5}
\]

\[
= \left( \frac{4\sqrt{2}}{3} + 8 + \frac{12\sqrt{6}}{5} \right)2^n - (5 + \frac{12\sqrt{6}}{5}).
\]
Figure 3. $\text{NS}_2[1]$ and $\text{NS}_2[n]$ Polypropylenimin octaamin Dendrimer.

In Table 1, this topological index are calculated for two classes of dendrimers.


Table 1. GA$_1$ Index for some Dendrimer Graphs.

<table>
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<tr>
<th>n</th>
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REFERENCES


