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Eccentricity based Geometrical-Arithmetic Indices of Dendrimers

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Abstract: ***Eccentricity of a node is the longest path connecting this node to any other node in the network. The eccentricity-based Geometrical-arithmetic index is defined as $GA_4(G) = \sum_{uv \in E(G)} 2\frac{\sqrt{\epsilon(u)\epsilon(v)}}{\epsilon(u)+\epsilon(v)}$, Where $\epsilon(u)$ is eccentricity of vertex u. In this paper Geometrical-arithmetic index $GA_4(G)$ and multiplicative $GA_4(G)$ are investigated for the dendrimers $T_{k,d}$ where k = 2,d = 4 and k = 3,d = 4 .***

Keywords: Distance, eccentricity, topological indices, geometric-arithmetic index, dendrimers

1. Introduction

Let G = (V, E) be a molecular graph. The set of vertex and edge are denoted by V =V(G) and E = E(G) respectively. The distance between any two vertices u and v of a graph is the length of shortest path connecting u and v is denoted by d (u,v). The eccentricity of a vertex is the farthest distance from it to any other vertex [1].For a disconnected network; all nodes are defined to have infinite eccentricity. In other words eccentricity is ecc(v) = $\mathrm{Max}\{d(u,v) \mid \forall u \in V(G)\}$. The diameter of G is the maximum eccentricity among the vertices of graph. The maximum eccentricity over all vertices of G is called the diameter of G and is denoted by D(G).The eccentricity-based topological indices are widely studied in the literature [2-13].Our notations are standard and mainly taken from standard books of graph theory [14-17]. Distance is important concept in graph theory in general and distance-based topological indices in particular [18]. A class of highly branched molecules, called dendrimers is known to be suitable for a number of biomedical applications [9]. A regular dendrimer $T_{k,d}$ is a tree with a unique central vertex v_o. Every non-pendent vertex of $T_{k,d}$ is of degree $d \geq 2$ and the radius k, the distance from v_o to each pendent vertex [19]. A network with eccentricity of each node indicated is shown in figure 1.

A topological index for molecular graph is a numerical quantity which is invariant under automophisms of the graph. There are several topological indices defined and studied which are degree-based and distance-based. These topological indices found many applications in modeling chemical, pharmaceutical and other properties of molecules.

2. Materials and Methods

A molecular graph is constructed by representing nodes and edges. The eccentricity of a node is the longest path connecting this node to any other node in the molecular graph.

The first geometric-arithmetic index is degree-based topological index and is defined as [20],

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

Where uv denotes the edge of the graph G connecting the vertices u and v and d_u denotes the degree of the vertex u. The different forms of Geometric-arithmetic indices are widely studied. The eccentricity version geometric-arithmetic index called the fourth GA index. Ghorbani et al. introduced $GA_4(G)$ index based on eccentricity of vertices [21-22], it is defined as

$$GA_4 = \sum_{uv \in E(G)} 2\frac{\sqrt{\epsilon(u)\epsilon(v)}}{\epsilon(u)+\epsilon(v)}$$

Where $\epsilon(u)$eccentricity of vertex u.The network with eccentricity indicated is shown in figure (1).The multiplicative geometric-arithmetic eccentricity version of $GA_4(G)$ is defined as,

$$\text{Multiplicative } GA_4(G) = \prod_{uv \in E(G)} 2\frac{\sqrt{\epsilon(u)\epsilon(v)}}{\epsilon(u)+\epsilon(v)}$$

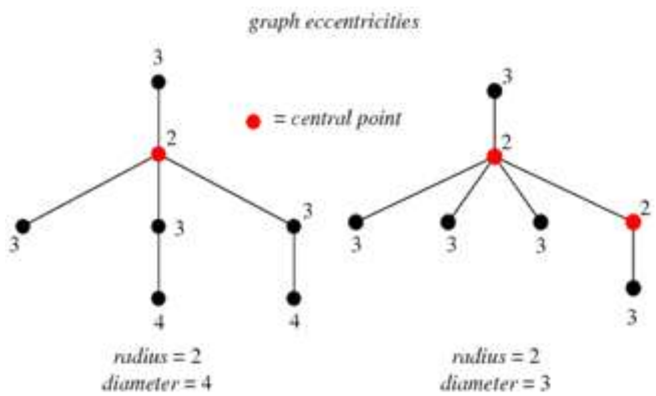

Figure 1: A network with the eccentricity of each node

The maximum entry for a given row/column of the distance matrix of an undirected (strongly connected directed) graph is known as the eccentricity of the node. The maximum distance from any vertex to other vertex is counted for dendrimers $T_{k,d}$ with k= 2, d= 4 and k= 3, d= 4 figure (2).

3. Results and discussion

Eccentricity of a node is the longest path connecting this node to any other node in the molecular graph .The graph eccentricities; radius and diameter for graph are given in figure (1).

$GA_4(G)$ based on eccentricity of vertices [21-22], defined as

$$GA_4(G) = \sum_{uv \in E(G)} 2\frac{\sqrt{\in(u)\in(v)}}{\in(u)+\in(v)}.$$

The dendrimers $T_{2,4}$ and $T_{3,4}$ are shown in figure (2). The eccentricities for each vertex in dendrimer $T_{2,4}$ are 2,3 and 4. The pendent vertex of a molecular graph has degree 1. There are 12 pendent vertices and having the maximum distance from any node of the molecular graph as 4.The middle vertex has maximum distance as 2.The eccentricities for all vertices are counted on $T_{2,4}$ (Table 1).The dendrimer $T_{3,4}$ has vertices 51 and edges 50.The eccentricity of each node from molecular graph fig.2 used in computing fourth geometric-arithmetic index and multiplicative fourth geometric-arithmetic index. The distance based and eccentricity based indices may be used to derive quantitative structure property or activity relationships (QSPR/QSAR) [23].

Table 1: Edges of the type uv ∈ E (G) and eccentricity for dendrimers$T_{2,4}$ and $T_{3,4}$.

Dendrimer	Edges of the type uv ∈ E(G) with eccentricity	frequency
$T_{2,4}$	(4,3)	12
	(3,2)	4
$T_{3,4}$	(6,5)	36
	(4,5)	12
	(4,3)	4

The method to compute eccentricity based topological indices is as given below. The eccentricity based geometric -arithmetic index,

$$GA_4(G) = \sum_{uv \in E(G)} 2\frac{\sqrt{\in(u)\in(v)}}{\in(u)+\in(v)}$$

$$= 12 * 2\frac{\sqrt{4*3}}{4+3} + 4 * 2\frac{\sqrt{3*2}}{3+2}$$

$$= 15.7961.$$

The multiplicative version of geometric-arithmetic for dendrimer $T_{2,4}$ (Table 1) is computed as,

$$\text{Multiplicative } GA_4(G) = \prod_{uv \in E(G)} 2\frac{\sqrt{\in(u)\in(v)}}{\in(u)+\in(v)}$$

$$12 * 2\frac{\sqrt{4*3}}{4+3} * 4 * 2\frac{\sqrt{3*2}}{3+2}$$

$= 46.5477$.

The values of $GA_4(G)$ and Multiplicative $GA_4(G)$ are given in table (2).

Table 2: The values of $GA_4(G)$ and multiplicative $GA_4(G)$ of Dendrimers $T_{2,4}$ and $T_{3,4}$.

Dendrimer	Geometric-arithmetic eccentricity index $GA_4(G)$	Multiplicative version of geometric-arithmetic eccentricity index $GA_4(G)$
$T_{2,4}$	15.7961	46.5477
$T_{3,4}$	51.7357	1692.56

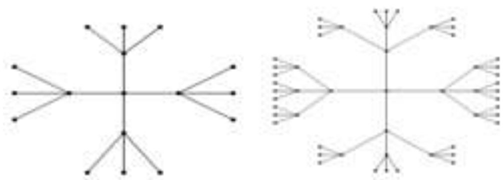

Figure 2: Dendrimers $T_{k,d}$ for k= 2, d= 4 and k= 3, d= 4.

4. Conclusion

Distance is important concept in molecular graph theory for studying eccentricity-based topological indices. The eccentricity is the maximum distance of each node from any other node. Dendrimers has many biomedical applications. In this paper we have computed eccentricity–based $GA_4(G)$ topological index and Multiplicative version of $GA_4(G)$ for dendrimers $T_{2,4}$ and $T_{3,4}$. Multiplicative eccentricity based geometric-arithmetic version has greater value than $GA_4(G)$.

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