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The Eccentric Connectivity Index of Dendrimers

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Abstract

If G is a connected graph with vertex set V, then the eccentric connectivity index of G, $\xi^C(G)$, is defined as $\sum_{v \in V(G)} deg(v)ecc(v)$ where $deg(v)$ is the degree of a vertex v and $ecc(v)$ is its eccentricity. We obtain exact formulas for calculating the eccentric connectivity index of dendrimers.

Mathematics Subject Classification: 05C05, 05C12

Keywords: Eccentricity; Eccentric connectivity index; Dendrimers

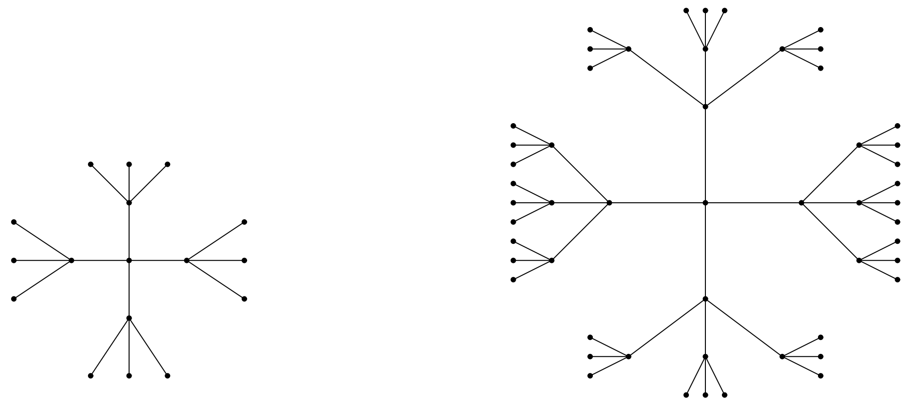
1 Introduction

Let G be a connected graph with the vertex-set $V(G)$ and edge-set $E(G)$, respectively. $|V(G)| = n$, $|E(G)| = m$ are the number of vertices and edges. The degree of a vertex $v \in V(G)$ is the number of vertices joining to v and denoted by $deg(v)$ (or simply as $d_G(v)$, $d(v)$) and $d_G(u, v)$ denote the degree of u and the distance (i.e.,the number of edges on the shortest path) between u and v, respectively.

A critical step in pharmaceutical drug design continues to be the identification and optimization of compounds in a rapid and cost effective way. An important tool in this work is the prediction of physico-chemical, pharmacological and toxicological properties of a compound directly from its molecular structure. This analysis is known as the study of the quantitative structure-activity relationship (QSAR). In chemistry, a molecular graph represents the topology of a molecule, by considering how the atoms are connected. This can be modeled by a graph, where the points represent the atoms, and the edges symbolize the covalent bonds. Relevant properties of these graph models are then studied, giving rise to numerical graph invariants. The parameters derived from this graph-theoretic model of a chemical structure are being used not only in QSAR studies pertaining to molecular design and pharmaceutical drug design, but also in the environmental hazard assessment of chemicals. Many such graph invariant topological indices have been studied. The first, and most well-known parameter, the Wiener index, was introduced in the late 1940s in an attempt to analyze the chemical properties of paraffins (alkanes)(see [1]). This is a distance-based index, whose mathematical properties and chemical applications have been widely researched. Numerous other indices have been defined, and more recently, indices such as the eccentric distance sum, and the adjacency-cum-distance-based eccentric connectivity index have been considered. These topological models have been shown to give a high degree of predictability of pharmaceutical properties, and may provide leads for the development of safe and potent anti-HIV compounds. Refinements of some of these indices have also been considered.

The eccentric connectivity index of the molecular graph G, $\xi^C(G)$, was proposed by Sharma, Goswami and Madan(see [2]). It is defined as $\xi^C(G) = \sum\limits_{v\in V(G)} deg(v)ecc(v)$, where $ecc(v) = \max\{d(x,v)|x \in V(G)\}$, see [3-7] for details. The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G, respectively. Herein, our notation is standard and taken from the standard book of graph theory(see[8]).

Dendrimers[10-14] are a new class of polymeric materials. They are highly branched, mono-disperse macromolecules. The structure of these materials has a great impact on their physical and chemical properties. As a result of their unique behavior dendrimers are suitable for a wide range of biomedical and industrial applications[9]. Consider the molecular graph regular dendrimer $T_{k,d}$ is a central tree with center v_0 and having every non-pendent vertex is of degree d, and the distance from v_0 to each pendent vertex is k. $T_{2,4}$ and $T_{3,4}$ are depicted in Figure 1.



$T_{2,4}$ $T_{3,4}$

Figure 1. Dendrimers $T_{k,d}$ for $k = 2, d = 4$ and $k = 3, d = 4$

2 Main Results

These are the main results of the paper.

For special classes of graphs we have the following useful results.

Lemma 2.1 *For the complete graph K_n and bipartite graph $K_{a,b}$, we have*

$$\xi^C(K_n) = n(n-1) \quad (\text{for } n \geq 2) \tag{1}$$

$$\xi^C(K_{a,b}) = n(n-1) \quad (\text{for } a, b \neq 1) \tag{2}$$

and the index reaches its maximum for $K_{a,b}$ when $a = b = \frac{n}{2}$.

For the star, cycle and path of order n,

Lemma 2.2 *For the star S_n, cycle C_n and path P_n, we have*

$$\xi^C(S_n) = 3(n-1) \tag{3}$$

$$\xi^C(C_n) = \begin{cases} n^2, & \text{for } n \text{ even;} \\ n(n-1), & \text{for } n \text{ odd.} \end{cases} \tag{4}$$

$$\xi^C(P_n) = \begin{cases} \frac{1}{2}(3n^2 - 6n + 4), & \text{for } n \text{ even;} \\ \frac{3}{2}(n-1)^2, & \text{for } n \text{ odd.} \end{cases} \tag{5}$$

Note that the order of $T_{k,d}$ is $n(T_{k,d}) = 1 + \frac{d}{d-2}[(d-1)^k - 1]$.

Theorem 2.3 *For any pair of integers (k,d), where $d \geq 3$.*

$$\xi^C(T_{k,d}) = \begin{cases} dk + \frac{d^2k[1-(d-1)^{k-1}]}{2-d} + 2dk(d-1)^{k-1} + d^2[\frac{1-(d-1)^{k-1}}{(2-d)^2} \\ +\frac{k-1}{d-2}(d-1)^{k-1}], \quad when\ d \geq 3; \\ 6k^2, \quad when\ d = 2. \end{cases} \tag{6}$$

Proof. For the convenience of the computation, we classified the vertices of $T_{k,d}$ into k classes.

(i) For the vertices v_0, the vertex for the contribution to the eccentric connectivity index is $\xi_1^C = dk$;

(ii)For the vertices x with $d(v_0,x) = i, i = 1,2,\cdots,k-1$: their contribution to eccentric connectivity index are $d^2(d-1)^{i-1}(k+i)$, respectively, summing up, we have

$$\begin{aligned} &\xi_2^C \\ = \ & d^2 \times \sum_{i=1}^{k-1}(d-1)^{i-1}(k+i) \\ = \ & d^2 \times \{\tfrac{k}{2-d}[1-(d-1)^{k-1}] + \tfrac{1-(d-1)^{k-1}}{(2-d)^2} + \tfrac{k-1}{d-2}(d-1)^{k-1}\} \end{aligned}$$

(iii) For the vertices x with $d(v_0,x) = k$: their total contribution to eccentric connectivity index is $\xi_3^C = 2dk(d-1)^{k-1}$.

Summing up, we arrive at the desired result.

The chemically most interesting cases of equation (1) correspond to $d = 3,4$:

Theorem 2.4 *For the fixed k, we have*

$$\xi^C(T_{k,3}) = 3(4k-3)\cdot 2^k - 3(2k-3) \tag{7}$$

$$\xi^C(T_{k,4}) = 4(2k-1)\cdot 3^k - 4(k-1) \tag{8}$$

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