International Journal of Physics and Mathematical Sciences ISSN: 2277-2111 (Online)
An Open Access, Online International Journal Available at http://www.cibtech.org/jpms.htm
2014 Vol. 4 (3) July- September, pp. 1-4/Jayenthi and Therese

Research Article

ON ECCENTRIC CONNECTIVITY INDEXES OF SOME SPECIAL GRAPHS

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ABSTRACT

The eccentric connectivity index ξ^c is a novel distance based molecular structure descriptor that was recently used for mathematical modeling of biological activities of diverse nature. If *G* is a connected graph, then the eccentric connectivity index of *G* is defined as $\xi^c(G) = \sum_{v \in V(G)} \deg(v).\varepsilon(v)$, where $\deg(v)$ and $\varepsilon(v)$ denotes the vertex degree and eccentricity of *v* respectively. We present the explicit formulae for the values of eccentric connectivity index for some special graphs.

Keywords: *Barbell Graph, Corona Graph, Double-Wheel Graph, Eccentric Connectivity Index and Gear Graph*

INTRODUCTION

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 physic-chemical, pharmacological and toxicological properties of a compound directly using its molecular structure. This analysis is known as the study of the *Quantitative Structure Activity Relationship* (*QSAR*) (Diudea, 2000). Topological descriptors are derived from hydrogen-suppressed molecular graphs, in which the atoms are represented by vertices and the bonds by edges. The connections between the atoms can be described by various types of topological matrices, which can be mathematically manipulated so as to derive a single number, usually known as graph invariants, graph-theoretical index or topological index.

The first and most well-known parameter, the *Wiener index* (Wiener, 1947) was introduced in an attempt to analyze the chemical properties of *paraffin* (alkenes). This is a distance based index, whose mathematical properties and chemical applications have been widely explored. 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.

A *graph* $G = (V,E)$ is a finite nonempty set of objects called vertices together with a set of unordered pairs of distinct vertices of *G* called edges. The vertex set of *G* is denoted by $V(G)$, while the edge set is denoted by $E(G)$. The *degree of a* vertex *v* in a graph *G* is the number of edges of *G* incident with *v*, which is denoted by $\deg_G v$ or simply by $\deg v$. The *distance* $d_G(u,v)$ from a vertex *u* to a vertex *v* in a connected graph *G*, or simply $d(u, v)$ if the graph *G* is clear, is the minimum of the lengths of the $u - v$ paths in *G*. The *eccentricity*, $\varepsilon(v)$ of a vertex $v \in V(G)$ is the maximum distance between *u* and any other vertex in *G*.

The eccentric connectivity index (Sharma *et al.*, 1997) is an adjacency-cum-distance base topological index. The eccentric connectivity index of a graph G is defined as

$$\xi^c(G) = \sum_{v \in V(G)} \deg(v).\varepsilon(v)$$

The barbell graph B_n is defined as the simple graph obtained by connecting two copies of a complete graph K_n by a bridge. The Gear graph G_n is also known as bipartite wheel graph. It is a wheel graph with a graph vertex added between each pair of adjacent graph vertices of the outer cycle. The Double-Wheel graph DW_{2n+1} is defined as the graph $2C_n + K_1$, where K_1 is the singleton graph and C_n is the cycle graph. The corona graph operation (Frucht, 1970) $G_1 * G_2$ of two graphs G_1 and G_2 is a new graph obtained by taking n_1 copies of the graph G_2 and then joining i^{th} vertex of G_1 to every vertex in the i^{th} copy of G_2 respectively.

Preliminaries

For a connected graph *G*, the radius $r(G)$ and diameter $D(G)$ are the minimum and maximum eccentricity among all vertices of *G*. A connected graph is called self- centred graph if all its vertices have the same eccentricity. First we give two useful estimations of the eccentric connectivity index and in the following we present explicit formulae for eccentric connectivity index of various families of graphs.

For every vertex $v \in V(G)$, there holds $r(G) \le \varepsilon(v) \le D(G)$. Using the known result $\sum_{v \in V(G)} \deg(v) = 2m$, it follows that $2m.r(G) \le \xi^c(G) \le 2m.D(G)$.Then, a graph G is said to be self-centred if and only if $r(G) = D(G)$. Let k be the number of vertices of degree $n - 1$ in the graph $G \ne K_n$, with $r(G) = 1$.

For $1 \le k \le n - 1$, we have $\xi^c(G) = \sum_{v \in V(G)} \deg(v).\varepsilon(v) \ge (n-1)k + 2(2m - (n-1)k) = 4m - k(n-1)$

with equality hold if and only if all $n - k$ vertices of degree lass than $n - 1$ have eccentricity two.

Let P_n and S_n be respectively the path and the star with n vertices. Let K_n be the complete graph with n vertices. Let C_n be the cycle with $n \ge 3$ vertices. Let $K_{n,m}$ be the complete bipartite graph with n vertices in one vertex-class and m vertices in the other vertex-class.

By direct calculation, the following formula holds

$\xi^c(K_n) = n(n-1)$, $\xi^c(K_{n,m}) = 4mn$, for n, $m \ge 2$, $\xi^c(S_n) = 3(n-1)$, $\xi^c(C_n) = 2n\left[\frac{n}{2}\right]$,

$\xi^c(P_n) = \left[\frac{3(n-1)^2 + 1}{2}\right]$. For P_n we have two classes based on the parity of n. If $n \ge 2$ is even, then

$$\xi^c(P_n) = 2\left(n - 2 + \sum_{i=n/2}^{n-2} 2i\right) = 4\sum_{i=n/2}^{n-1} i - 2(n-1)$$
$$= n\left(\frac{n}{2} + n - 1\right) - 2(n-1) = \frac{3(n-1)^2 + 1}{2}$$

and if $n \ge 3$ is odd, then

$$\xi^c(P_n) = 2\left(n - 1 + \sum_{i=(n+1)/2}^{n-2} 2i\right) + 2.\frac{n-1}{2} = 4\sum_{i=(n+1)/2}^{n-1} i - (n-1)$$
$$= (n-1)\left(\frac{n+1}{2} + n - 1\right) - (n-1) = \frac{3(n-1)^2}{2}$$

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It is sometimes interesting to consider the sum of eccentricities of all vertices of a given graph *G*. We call this quantity, the total eccentricity of a graph *G* and denote it by $\varsigma(G)$. For a *k*-regular graph G, we have $\xi^{c}(G) = k\,.\,\varsigma(G)$.

RESULTS AND DISCUSSION

Results

In this section, we derived an expression for the eccentric connectivity index of the Barbell graphs, Gear graphs, Double Wheel graphs and Corona graphs.

Theorem 1: The eccentric connectivity index of the Barbell graph B_n is

$$\xi^{(c)}(B_n) = 6n^2 - 8n + 6, \quad for\ n \geq 3.$$

Proof:

The cardinality of the vertex set of the graph B_n is 2*n*, among which 2(*n* -1) vertices are of degree (*n* -1), and the remaining vertices are the vertices of an edge (bridge) connecting two copies of K_n of degree *n*.

The vertices of degree (*n* -1) are of eccentricity 3 and the vertices of degree *n* are of eccentricity 2.

Hence, $\xi^{(c)}(B_n) = 2(n-1).(n-1).3 + 2.n.2 = 6n^2 - 8n + 6, \quad for\ the\ case\ n \geq 3.$

Theorem 2: The eccentric connectivity index of Double Wheel graph DW_{2n+1}

$$\xi^{(c)}(DW_{2n+1}) = 14n, \quad for\ n \geq 3.$$

Proof:

The Double-Wheel graph DW_{2n+1} contains the subgraphs *inner cycle* (C_n), the *outer cycle* (C_n) and the *hub* of the wheel. The *n* vertices in the outer cycle and *n* vertices in the inner cycle are of degree 3 and eccentricity 2 respectively.

The *hub* of the wheel is of degree 2n and the eccentricity is 1.

Hence, for all $n \geq 3$, $\xi^{(c)}(DW_{2n+1}) = n.3.2 + n.3.2 + 1.2n.1 = 14n.$

Theorem 3: The eccentric connectivity index of Gear graph G_n is

$$\xi^{(c)}(G_n) = \begin{cases} 51, & for\ n = 3, \\ 19n, & for\ n \geq 4. \end{cases}$$

Proof:

The Gear graph G_n is a wheel graph with a graph vertex added between each pair of adjacent graph vertices of the outer cycle.

The graph G_n contains 2*n* vertices in the *cycle* and a single vertex in the *hub* respectively.

For all *n*, $n \geq 3$, the hub of the graph is of degree *n* and is of eccentricity 2.

Among 2*n* vertices, the *n* vertices are of degree 3 and the remaining *n* vertices are of degree 2.

For the case, *n* = 3, the 2*n* vertices are of eccentricity 3.For the case, *n* ≥ 4,the *n* vertices are of eccentricity 3 and remaining *n* vertices are of eccentricity 4.

Hence,

$$\xi^{(c)}(G_n) = 2.n + 3.3.n + 2.3.n = 17n = 51, \ for\ the\ case\ n = 3.$$

$\xi^{(c)}(G_n) = 2.n + 3.3.n + 2.4.n = 19n$, *for the case* $n \geq 4$.

Theorem 4.1: Let C_n and K_1 be two graphs, then the eccentric connectivity index of corona graph $C_n * K_1$ is

$$\xi^{(c)}(C_n * K_1) = \begin{cases} 2n^2 + 3n, & \text{when } n \geq 3 \text{ and } n \text{ is odd}, \\ 2n^2 + 5n, & \text{when } n > 3 \text{ and } n \text{ is even}. \end{cases}$$

Proof:

C_n and K_1 are two graphs with *n* vertices and single vertex respectively. The corona graph $C_n * K_1$ is the graph obtained by taking *n* copies of K_1 and then joining i^{th} vertex of C_n to every vertex in the i^{th} copy of K_1 .

In general, for all $n \geq 3$, the *n* vertices of C_n are of degree 3 and the vertices of *n* copies of K_1 are of degree 1.

For all values of $n \geq 3$ and *n* is odd, the *n* vertices of C_n are of eccentricity $\frac{n+1}{2}$ and the vertices of *n* copies of K_1 are of eccentricity $\left(\frac{n+3}{2}\right)$.

For all values of $n > 3$ and *n* is even, the *n* vertices of C_n are of eccentricity $\frac{n}{2}+1$ and the vertices of *n* copies of K_1 are of eccentricity $\left(\frac{n}{2}+2\right)$.

Hence,

$\xi^{(c)}(C_n * K_1) = 2n^2 + 3n,$ *for the case* $n \geq 3$ *and* n *is odd*.

$\xi^{(c)}(C_n * K_1) = 2n^2 + 5n,$ *for the case* $n > 3$ *and* n *is even.*

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