ON ECCENTRIC CONNECTIVITY INDEXES OF SOME SPECIAL GRAPHS

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ABSTRACT

The eccentric connectivity index $\xi^c$ 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 $\xi^c (G) = \sum_{v \in V(G)} \deg(v) \cdot \varepsilon(v)$, 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 physico-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 based topological index. The eccentric connectivity index of a graph $G$ is defined as

$$\xi^c (G) = \sum_{v \in V(G)} \deg(v) \cdot \varepsilon(v)$$
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) \( G_1 \ast G_2 \) of two graphs \( G_1 \) and \( G_2 \) is a new graph obtained by taking \( n_i \) 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 if and only 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 \( r(G) \leq e(v) \leq D(G) \). Using the known result \( \sum_{v \in V(G)} \deg(v) = 2m \), it follows that \( 2m \cdot r(G) \leq \xi^c(G) \leq 2m \cdot D(G) \). 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 \( G \neq K_n \), with \( r(G) = 1 \).

For \( 1 \leq k \leq n - 1 \), we have \( \xi^c(G) = \sum_{v \in V(G)} \deg(v) \cdot e(v) \geq (n - 1)k + 2(2m - (n - 1)k) = 4m - k(n - 1) \)

with equality hold if and only if all \( n - k \) vertices of degree less 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 \( n \geq 3 \) 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

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

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

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

and if \( n \geq 3 \) is odd, then

\[
\xi^c(P_n) = 2\left(n - 1 + \sum_{i=(n+1)/2}^{n-2} 2i\right) + 2 \cdot \frac{n-1}{2} = 4 \sum_{i=(n+1)/2}^{n-1} i - (n - 1) = (n - 1)\left(\frac{n+1}{2} + n - 1\right) - (n - 1) = \frac{3(n - 1)^2}{2}
\]
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 \( \xi(G) \). For a \( k \)-regular graph \( G \), we have \( \xi^c(G) = k \cdot \xi(G) \).

**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

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

**Proof:**

The cardinality of the vertex set of the graph \( B_n \) is \( 2n \), 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, \( \xi^c(B_n) = 2(n-1).(n-1).3 + 2n.2 = 6n^2 - 8n + 6 \), for the case \( n \geq 3 \).

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

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

**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

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

**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 \( 2n \) 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 \( 2n \) vertices, the \( n \) vertices are of degree 3 and the remaining \( n \) vertices are of degree 2. For the case, \( n = 3 \), the \( 2n \) vertices are of eccentricity 3. For the case, \( n \geq 4 \), the \( n \) vertices are of eccentricity 3 and remaining \( n \) vertices are of eccentricity 4. Hence,

\[
\xi^c(G_n) = 2n + 3.3n + 2.3n = 17n = 51, \quad \text{for the case } n = 3.
\]
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\[ \xi^{(c)}(G_n) = 2n + 3.3n + 2.4n = 19n \], 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 \( C_n \ast K_1 \) is

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

**Proof:**

\( C_n \) and \( K_1 \) are two graphs with \( n \) vertices and single vertex respectively. The corona graph \( C_n \ast K_1 \) 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 \( \frac{n+3}{2} \).

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 \( \frac{n}{2} + 2 \).

Hence,

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

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

**REFERENCES**


