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Eccentric and Leap Eccentric Connectivity Indices of Some Mycielski Graphs

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Abstract. In graph theory, topological indices are frequently studied parameters both theoretically and in terms of applications. Two significant indices among these are the eccentric connectivity index and the leap eccentric connectivity index. The eccentric connectivity index value is calculated as the sum of the products of the eccentricity and degree values of the vertices. The leap eccentric connectivity index value is the sum of the products of the eccentricity value of the vertices and their second-degree values. The second-degree value of a vertex is the number of vertices at a distance of two from it. In this study, we examined the Mycielski Graph structure, which structurally resembles the form of chemical molecules. We obtained results for the eccentric and leap eccentric connectivity indices of some special Mycielski Graphs.

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1 Introduction

Graph theory has become a significant component of mathematics, especially with its various applications in natural sciences such as Chemistry

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and Biology. Topological indices are numerical parameters that serve as graph invariants in the context of graph isomorphism. Research on topological indices has intensified recently. A topological index is a numerical quantity associated with the structural graph of a molecule. These indices are numerical values based on the topology of atoms and their bonds. The study of the quantitative structure-activity relationship (QSAR) aims to rapidly and effectively predict the physico-chemical, pharmacological, and toxicological properties of a compound directly from its molecular structure.

Molecules and molecular compounds are typically represented by graphs where the vertices correspond to atom types and the edges represent bonds. In theoretical chemistry, a chemical molecular structure is expressed as a graph: each vertex indicates an atom of a molecule, and each edge between the corresponding vertices signifies the chemical bonds between the atoms. This graph derived from a chemical molecular structure is commonly referred to as a molecular graph [1, 27].

A topological chemical index defined on a molecular graph can be considered a real-valued function $f: G \to R$ that assigns a real number to each molecular structure. Topological indices and graph invariants (such as diameter, radius, etc.) based on the distances between vertices or vertex degrees are widely used to characterize molecular graphs, establish relationships between the structure and properties of molecules, predict the biological activity of chemical compounds, and perform chemical applications.

The parameters derived from this graph-theoretic model of a chemical structure are utilized not only in QSAR studies related to molecular design and pharmaceutical drug design but also in the environmental hazard assessment of chemicals. Over the past several decades, many degree based topological indices have been proposed and extensively studied. Some studies include the so-called degree distance based topological indices refered to reader [2–11, 18, 23, 24, 26, 27, 32, 33]. The focus of this study is on the Eccentric Connectivity Index and the Leap Eccentric Connectivity Index. These indices can aid in measuring chemical, biological, and nano properties commonly used in developing regions. In our study, the values of the eccentric and leap connectivity indices for certain specific molecular graphs have been calculated.

To ensure the readability of the article, some notations and terminology will be provided. We use the books for terminology [12,13]. This notation and these definitions provide a foundational understanding for the subsequent analysis and discussion of graph invariants and topological indices in this study. Let G be a graph with vertex set V(G) and edge set E(G). The degree of a vertex v in G is denoted by deg(v). For two vertices u and v in V(G), d(u, v) denotes the distance between u and v, which is the length of the shortest path connecting them. The eccentricity of a vertex v in V(G), denoted by ec(v), is defined as

$$ec(v) = \max\{d(u, v): \forall u \in V(G), u \neq v\}.$$

The diameter of a graph G is then defined as:

$$diam(G) = \max\{ec(v) : \forall v \in V(G)\}.$$

The eccentric connectivity index, ξ^c , of a graph G is defined as:

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

For a vertex v and a positive integer k, the open k-neighborhood of k in G is represented by $N_k(v)$ and is defined as $N_k(v) = \{u \in V(G) : d_G(u, v) = k\}$. The k-distance degree of a vertex v in G is denoted by $d_k(v)$ and its mean is the cardinality of k-neighbors of the vertex v in G. Simply, it can be symbolized as $d_k(v) = |N_k(v)|$ where $d_1(v) = \deg(v)$ for every $v \in V(G)$. In this paper, we focus on the leap connectivity index introduced by Pawar et al. [25]. Motivated by the eccentric connectivity index, the leap eccentric connectivity index of a graph, denoted by $L\xi^c(G)$, is calculated as the product of the second degree value and the eccentricity value for each vertex. We can mathematically define it as follows:

$$L\xi^{c}(G) = \sum_{v \in V(G)} d_{2}(v)ec(v).$$

These types of topological indices are significant for mathematically modeling various natural activities. For detailed information on the



Figure 1: An illustration of Mycielski graphs $\mu(C_{10})$ (left) and $\mu(P_{10})$ (right)

eccentric connectivity index and the leap eccentric connectivity index, readers are referred to the references [15–17, 19, 25, 28–31, 34–38].

In this study, we calculated the eccentric connectivity and leap eccentric connectivity for the Mycielski structure. The Mycielski graph, an important family of graphs, was defined in the mid-20th century [22]. This family of graphs does not contain any triangle graphs. Let V(G) = $\{v_1, v_2, ..., v_n\}$ be the vertex set of graph G and $V'(G) = \{v'_1, v'_2, ..., v'_n\}$ be the corresponding vertex set where the vertex v'_i is referred to as the duplicate vertex of v_i The Mycielski graph of G is denoted by $\mu(G)$ and its vertex and edge sets are defined as follows:

 $V(\mu(G)) = V(G) \cup V'(G) \cup w$, while vertex w is called the root vertex of $\mu(G).$

and

$$E(\mu(G)) = E(G) \cup \{v_i v'_i : v_i v_i \in E(G)\} \cup \{w v'_i : \forall i \in \{1, ..., n\}\}.$$

Notably, the path and cycle forms of Mycielski structures closely resemble molecular structures in chemistry. Therefore, some topological index values for Mycielski graphs have been found to be significant. Results concerning various topological indices for Mycielski graphs are available in the literature [3–6,14,18,20,23]. The structure of the graph and existing studies have motivated us to conduct this research. Different drawings of the $\mu(C_{10})$ and $\mu(P_{10})$ graphs are provided in Figure 1.

2 The Eccentricity of Some Special Mycielski Graphs

In this section, we calculate the eccentric connectivity index values for the Mycielski graphs of some special graph classes, such as paths, cycles, stars, wheels, and complete graphs.

Theorem 2.1. Let G be a path graph with n vertices, P_n provided that $n \geq 8$. Then, the eccentric connectivity of Mycielski path graph is

$$\xi^{c}(\mu(G)) = 27n - 22.$$

Proof. In order to prove the theorem, the eccentricity and degree of all vertices of P_n should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{v_1, ..., v_n\} \cup \{v'_1, ..., v'_n\} \cup \{w\}$. According to the form of the graph, $\deg(v_1) = \deg(v_n) = 2$ provided that v_1 and v_n are pendant vertices of P_n , and for the corresponding duplicate vertices of v_1 and v_n , deg (v'_1) = deg (v'_n) = 2, and for the remaining vertices of P_n and their copies, $\deg(v_j) = 4$, $\deg(v'_j) = 3$, 1 < j < n, and $\deg(w) = n$. In addition, the eccentricity values of all vertices of the graph can be calculated in three cases:

Case 1: First, let us consider the vertices v_i of $V(P_n)$. Consider the distance of each vertices on P_n to all other vertices on P_n except itself on Mycielski structure. For each vertex to have a distance of at least 4 to at least one vertex on P_n , provided that $n \ge 8$. In this case, in the Mycielski construction, we have $1 \leq d(v_i, v_j) \leq 4$, for $i \neq j$.

Now let us examine the relationship between each vertex v_i and copy vertices. Given the Mycielski form, for each $i, j \in \{1, 2, ..., n\}$, we have $1 \le d(v_i, v'_i) \le 3.$

Next, if we examine the relationship between each vertex v_i and the root vertex w, it is obtained that $d(v_i, w) = 2$ for each $i \in \{1, 2, ..., n\}$.

Therefore, for each vertex v_i , we conclude that $ec(v_i) = 4$.

Case 2: Similarly, when considering the duplicate vertices v'_i , the distance between one duplicate vertex and another duplicate vertex, when considered through the shortest path obtained using the vertex w, is given by $1 \leq d(v'_i, v'_i) \leq 3$, for $i \neq j$. As examined in Case 1, the distances between the vertices v_i and the copy vertices range between 1

and 3. Also, the distance of any vertex v'_i to the vertex w is always 1. Thus, $ec(v'_i) = 3$ for all $i \in \{1, 2, ..., n\}$.

Case 3: Considering Case 1 and Case 2, where the distance of the vertex w to the vertices v_i and v'_i , $\forall i \in \{1, 2, ...n\}$ is examined, it is clear that ec(w) = 2. Thus, the total eccentric connectivity value is obtained as follows:

$$\begin{split} \xi^c(\mu(G)) &= \sum_{v \in V(\mu(G))} \deg(v) ec(v) \\ &= 2.2.4 + (n-2).4.4 + 2.2.3 + (n-2).3.3 + 2.n \\ &= 27n - 22. \end{split}$$

Remark 2.2. The result concerning the Mycielski C_n graph, which we will present in detail below, has previously been mentioned in Theorem 3.6 of [29]. However, a detailed proof is not provided in that work. Due to the lack of a rigorous demonstration, we found it necessary to re-examine and rigorously establish this result. The proof presented in our study fills the gaps in the previous work and provides a clearer theoretical foundation for the result.

Theorem 2.3. Let G be a cycle graph with n vertices, C_n provided that $n \ge 8$. Then, the eccentric connectivity of Mycielski cycle graph is

$$\xi^c(\mu(G)) = 27n.$$

Proof. In order o prove the theorem, the eccentricity and degree of all vertices of C_n should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{v_1, ..., v_n\} \cup \{v'_1, ..., v'_n\} \cup \{w\}$. According to the form of the graph, $\deg(v_i) = 4$ and for the corresponding duplicate vertices of v_i , $\deg(v'_i) = 3$ where $i \in \{1, ..., n\}$, and $\deg(w) = n$. In addition, the eccentricity values of all vertices of the graph can be calculated in three cases:

Case 1: First, let us consider the vertices v_i of $V(C_n)$. Consider the distance of each vertices on C_n to all other vertices on C_n except itself on Mycielski structure. As considered in Theorem 2.1, for each vertex to have a distance of at least 4 to at least one vertex on C_n ,

provided that $n \geq 8$. In this case, in the Mycielski construction, we have $1 \leq d(v_i, v_j) \leq 4$, for $i \neq j$.

Now let us examine the relationship between each vertex v_i and copy vertices v'_j . Given the Mycielski form, for each $i, j \in \{1, 2, ..., n\}$, we have $1 \leq d(v_i, v'_j) \leq 3$.

Next, if we examine the relationship between each vertex v_i and the root vertex w, it is obtained that $d(v_i, w) = 2$ for each $i \in \{1, 2, ..., n\}$.

Therefore, for each vertex v_i , we conclude that $ec(v_i) = 4$.

Case 2: Similarly, when considering the duplicate vertices v'_i , the distance between one duplicate vertex and another duplicate vertex, when considered through the shortest path obtained using the vertex w, is given by $1 \leq d(v'_i, v'_j) \leq 3$, for $i \neq j$. As examined in Case 1, the distances between the vertices v_i and the copy vertices range between 1 and 3. Also, the distance of any vertex v'_i to the vertex w is always 1. Thus, $ec(v'_i) = 3$ for all $i \in \{1, 2, ..., n\}$.

Case 3: Considering Case 1 and Case 2, where the distance of the vertex w to the vertices v_i and v'_i , $\forall i \in \{1, 2, ..., n\}$ is examined, it is clear that ec(w) = 2. Thus, the total eccentric connectivity value is obtained as follows:

$$\begin{aligned} \xi^{c}(\mu(G)) &= \sum_{v \in V(\mu(G))} \deg(v) ec(v) \\ &= n.4.4 + n.3.3 + 2.n \\ &= 27n. \end{aligned}$$

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Theorem 2.4. Let G be a star graph with n vertices, $S_{1,n-1}$ provided that $n \ge 3$. Then, the eccentric connectivity of Mycielski star graph is

$$\xi^{c}(\mu(G)) = 16n - 12$$

Proof. In order 0 prove this, the eccentricity and degree of all vertices of $S_{1,n-1}$ should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{c, v_1, ..., v_{(n-1)}\} \cup \{c', v'_1, ..., v'_{(n-1)}\} \cup \{w\}$. According to the form of the graph, deg(c) = 2n - 2, deg $(v_i) = \text{deg}(v'_i) = 2, \forall i \in \{1, ..., (n-1)\}$ and deg(w) = n. Also, the eccentricity of all vertices of the graph is 2.

Therefore, the eccentric connectivity value of the $S_{1,n-1}$ is:

$$\xi^{c}(\mu(G)) = \sum_{v \in V(\mu(G))} \deg(v) ec(v) = 16n - 12.$$

Theorem 2.5. Let G be a complete graph with n vertices, K_n provided that $n \ge 2$. Then, the eccentric connectivity of Mycielski complete graph is

$$\xi^{c}(\mu(G)) = 6n^{2} - 2n$$

Proof. In order o prove the theorem, the eccentricity and degree of all vertices of K_n should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{v_1, ..., v_n\} \cup \{v'_1, ..., v'_n\} \cup \{w\}$. According to the form of the graph, $\deg(v_i) = 2n - 2$, $\deg(v'_i) = \deg(w) = n$, $\forall i \in \{1, ..., n\}$. In addition, the eccentricity values of all vertices of the graph is 2. Thus, the eccentric connectivity value of the K_n is:

$$\xi^{c}(\mu(G)) = \sum_{v \in V(\mu(G))} \deg(v) ec(v) = 6n^{2} - 2n.$$

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Theorem 2.6. Let G be a wheel graph with n vertices, $W_{1,n-1}$ provided that $n \ge 4$. Then, the eccentric connectivity of Mycielski wheel graph is

$$\xi^c(\mu(G)) = 28n - 24$$

Proof. In order 0 prove this, the eccentricity and degree of all vertices of $W_{1,n-1}$ should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{c, v_1, ...\}$

 $(v_{(n-1)}) \cup \{c', v'_1, ..., v'_{(n-1)}\} \cup \{w\}$. According to the form of the graph, $\deg(c) = 2n - 2, \ \deg(v_i) = 6, \ \deg(v'_i) = 4, \forall i \in \{1, ..., (n-1)\}$ and $\deg(w) = n$. In addition, the eccentricity values of all vertices of the graph is 2. Thus, the eccentric connectivity value of the $W_{1,n-1}$ is:

$$\xi^{c}(\mu(G)) = \sum_{v \in V(\mu(G))} \deg(v) ec(v) = 28n - 24.$$

3 The Leap Eccentricity of Some Special Mycielski Graphs

In this section, we calculate the leap eccentric connectivity index values for the Mycielski graphs of some special graph classes, such as paths, cycles, stars, wheels, and complete graphs.

Theorem 3.1. Let G be a star graph with n vertices, $S_{1,n-1}$ provided that $n \geq 3$. Then, the leap eccentric connectivity of Mycielski star graph is

$$L\xi^{c}(\mu(G)) = 4(n+1) + 16(n-1)^{2}.$$

Proof. In order o prove this, the eccentricity and the second distance degree of all vertices of $S_{1,n-1}$ should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{c, v_1, ..., v_{(n-1)}\} \cup \{c', v'_1, ..., v'_{(n-1)}\} \cup \{w\}$. As calculated in the proof of Theorem 2.4, the eccentricity of all vertices of the graph is 2. In addition, according to the form of the graph, the second disance degrees of each vertices are $d_2(c) = 2$, $d_2(v_i) = d_2(v'_i) = 2n - 2$ where $1 \le i \le n - 1$, $d_2(c') = n$ and $d_2(w) = n$. Therefore,

$$L\xi^{c}(\mu(G)) = \sum_{v \in V(\mu(G))} d_{2}(v)ec(v)$$

= 2.2 + 2.2.(2n - 2)(n - 1) + 2n + 2n
= 4(n + 1) + 16(n - 1)^{2}.

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Theorem 3.2. Let G be a wheel graph with n vertices, $W_{1,n-1}$ provided that $n \ge 4$. Then, the leap eccentric connectivity of Mycielski wheel graph is

$$L\xi^{c}(\mu(G)) = 8(n^{2} - 3n + 3).$$

Proof. In order 0 prove this, the eccentricity and second distance degree of all vertices of $W_{1,n-1}$ should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{c, v_1, ..., v_{(n-1)}\} \cup \{c', v'_1, ..., v'_{(n-1)}\} \cup \{w\}$. As calculated in the proof of Theorem 2.6, the eccentricity of all vertices of the graph is 2. In addition, according to the form of the graph, the second distance degrees of each vertices are $d_2(c) = 2$, $d_2(v_i) = 2(n-3)$ and $d_2(v'_i) =$

2(n-2) where $1 \le i \le n-1$, $d_2(c') = n$ and $d_2(w) = 2(n-2)$. Therefore, the leap eccentric connectivity value is

$$\begin{split} L\xi^c(\mu(G)) &= \sum_{v \in V(\mu(G))} d_2(v) ec(v) \\ &= 2.[2+2(n-3)(n-1)+n+n+2(n-2)(n-1)] \\ &= 8(n^2-3n+3). \end{split}$$

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Theorem 3.3. Let G be a complete graph with n vertices, K_n provided that $n \ge 2$. Then, the leap eccentric connectivity of Mycielski complete graph is

$$L\xi^c(\mu(G)) = 2n(n+3).$$

Proof. In order o prove the theorem, the eccentricity and second distance degree of all vertices of K_n should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{v_1, ..., v_n\} \cup \{v'_1, ..., v'_n\} \cup \{w\}$. As calculated in the proof of Theorem 2.5, the eccentricity of all vertices of the graph is 2. According to the form of the graph, the second disance degrees of each vertices are $d_2(v_i) = 2$, $d_2(v'_i) = n$, for all $i \in \{1, ..., n\}$, and $d_2(w) = n$. Therefore, the leap eccentric connectivity value is

$$L\xi^{c}(\mu(G)) = \sum_{v \in V(\mu(G))} d_{2}(v)ec(v)$$

= 2.[n.2 + n.n + 1.n]
= 2n(n + 3).

Theorem 3.4. Let G be a path graph with n vertices, P_n provided that $n \ge 8$. Then, the leap eccentric connectivity of Mycielski path graph is

$$L\xi^{c}(\mu(G)) = 3n^{2} + 32n - 32.$$

Proof. In order to prove the theorem, the eccentricity and second distance degree of all vertices of P_n should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{v_1, ..., v_n\} \cup \{v'_1, ..., v'_n\} \cup \{w\}$. As calculated

in the proof of Theorem 2.1, the eccentricity value varies according to vertices. According to the form of the graph, the second disance degrees of each vertices are $d_2(v_1) = d_2(v_2) = d_2(v_{n-1}) = d_2(v_n) = 4$, $d_2(v_j) = 6$ where $3 \leq j \leq n-2$, $d_2(v'_1) = d_2(v'_2) = d_2(v'_{n-1}) = d_2(v'_n) = n+1$, $d_2(v_j) = n+2$ where $3 \leq j \leq n-2$, and $d_2(w) = n$. Therefore, the total values of second distance degrees are $\sum_{i=1}^n d_2(v_i) = 6n-8$, and $\sum_{i=1}^n d_2(v'_i) = n^2 + 2n - 4$. Thus, the leap eccentric connectivity value can be calculated using eccentricity value of P_n from the proof of Theorem 2.1:

$$L\xi^{c}(\mu(G)) = \sum_{v \in V(\mu(G))} d_{2}(v)ec(v)$$

= $4 \cdot \sum_{i=1}^{n} d_{2}(v_{i}) + 3 \cdot \sum_{i=1}^{n} d_{2}(v'_{i}) + 2d_{2}(w)$
= $3n^{2} + 32n - 32.$

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Theorem 3.5. Let G be a path graph with n vertices, C_n provided that $n \ge 8$. Then, the leap eccentric connectivity of Mycielski path graph is

$$L\xi^{c}(\mu(G)) = 3n^{2} + 32n.$$

Proof. In order to prove the theorem, the eccentricity and second distance degree of all vertices of C_n should be calculated. Let vertex set of the graph be $V(\mu(G)) = \{v_1, ..., v_n\} \cup \{v'_1, ..., v'_n\} \cup \{w\}$. As calculated in the proof of Theorem 2.3, the eccentricity value varies according to vertices. According to the form of the graph, the second disance degrees of each vertices are $d_2(v_i) = 6$, $d_2(v'_i) = n + 2$, and $d_2(w) = n$. Therefore, the total values of second distance degrees are $\sum_{i=1}^n d_2(v_i) = 6n$, and $\sum_{i=1}^n d_2(v'_i) = n(n+2)$. Thus, the leap eccentric connectivity value can be calculated using eccentricity value of C_n from the proof of Theorem 2.3:

$$L\xi^{c}(\mu(G)) = \sum_{v \in V(\mu(G))} d_{2}(v)ec(v)$$

= $4 \cdot \sum_{i=1}^{n} d_{2}(v_{i}) + 3 \cdot \sum_{i=1}^{n} d_{2}(v'_{i}) + 2d_{2}(w)$
= $3n^{2} + 32n$.

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