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Topological Index in Shadow Graphs

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ABSTRACT: Mathematical modeling of various natural biological activities has gained significant importance in recent times. In the modeling of these activities, the eccentric connectivity index (ECI) is utilized as a distance-based molecular structure descriptor. This index is defined as $\varepsilon^c(G) = \sum_{v \in V(G)} \deg(v)e(v)$, where $\deg(v)$ and $e(v)$ denote the vertex degree and eccentricity of v, respectively. To support its use as a topological structure descriptor, this study calculates the ECI values of shadow graphs of some graphs such as cycle, path, star, complete bipartite and wheel graphs.

Key Words: Graphical indices, chemical graph theory, distance in graph, vertex degree, theoretic methods, and shadow graph.

Contents

1. Introduction

Graph theory has become an important component of mathematics, particularly in natural sciences such as Chemistry and Biology, due to various applications [1,4,9] . Topological indices are numerical parameters that are graph invariants concerning graph isomorphism. Research on topological indices has been intensifying in recent years. A topological index is a numerical quantity in the structural graph of a molecule. Topological indices are numerical indices based on the topology of atoms and their bonds.

In theoretical chemistry, the chemical molecular structure is expressed as a graph: each vertex represents an atom of a molecule, and each corresponding edge between vertices represents the chemical bonds between atoms. This graph obtained from a chemical molecular structure is commonly referred to as a molecular graph [5,9].

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

Researchers in the fields of chemistry and mathematics have introduced several important indices, such as the Zagreb index, PI index, eccentricity index, atom-bond connectivity index, Wiener index, eccentric connectivity index, and more recently, the Sombor index, to predict the properties of drugs, nanomaterials, and other chemical compounds [1,7,8,9,12] .

Recently, research has begun on the eccentric connectivity index, which exhibits higher predictability compared to other topological indices. Structure-property and structure-activity studies related to molecule and drug design have shown that this index has a distinctive feature. This parameter has been successfully applied in the development of numerous mathematical models for the prediction of various biological activities.

All of these studies have motivated us to work on the eccentric connectivity index in this paper. In our study, eccentric connectivity index values have been calculated for specific molecular graphs. The considered molecular graphs include some shadow graphs.

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This paper focuses on simple, finite, and undirected graphs that do not contain loops or multiple edges. Let $G = (V, E)$ represent a graph, where V is the vertex set and E is the edge set. The order of G is determined by $|V(G)| = n$, and the size is defined as $|E(G)| = m$. The neighborhood of a vertex v in $V(G)$ is the set of adjacent vertices, denoted as $N_G(v)$ or simply $N(v)$, and the closed neighborhood of v is given by $N[v] = N(v) \cup \{v\}$. Therefore, $N(v) = \{u \in V(G) \mid uv \in E(G)\}$, and $N(v)$ is referred to as the open neighborhood of v. The degree of a vertex v in V is defined as $\deg(v) = |N(v)|$. A vertex with a degree of zero is considered an isolated vertex or isolate. A vertex with a degree of one is an endvertex or pendant vertex, and its neighbor is referred to as a support vertex. The distance $d(u, v)$ between two vertices u and v in G represents the length of the shortest path connecting them. If u and v are not connected, then $d(u, v) = \infty$, and for $u = v$, $d(u, v) = 0$. The eccentricity $e(v)$of a vertex v in G is defined as the distance from v to the vertex farthest away from v in G. The diameter of G, denoted as $\mathrm{diam}(G)$, is the largest distance between any two vertices in V . Likewise, the radius of G is established as the smallest among the eccentricity values of the vertices in G [2,3,11].

The eccentric connectivity index of a graph G is defined as the sum of the products of the eccentricity and degree of each vertex in G, denoted as $\varepsilon^c(G)$ [6,8,12]. The eccentric connectivity index is defined as:

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

The shadow graph $D(G)$ is formed from a connected graph G by duplicating it into two copies, referred to as G_1 and G_2, and establishing connections between each vertex u in G_1 and the neighbors of the corresponding vertex v in G_2 [4,10].

The paper is organized as follows. In Section 2, we presented some of the studies conducted in the literature on the subject of the eccentric connectivity index. In Section 3, the values of for certain shadow graphs were calculated, and their proofs were provided.

2. Some Related Results

In this section, some of the results from the literature related to the topic of the eccentric connectivity index have been provided. Below are the values previously obtained by Morgan and colleagues in 2011 for the eccentric connectivity index values in some well-known graphs, such as complete, cycle, star, path, and two-partite complete graphs.

Theorem 2.1 *[7] The eccentric connectivity index values*

a) For the complete graph, K_n, where $n \geq 2$, then $\varepsilon^c(K_n) = n(n-1)$.

b) For the cycle graph C_n

$$\varepsilon^c(C_n) = \begin{cases} n^2 & \text{, if } n \text{ is even} \\ n(n-1) & \text{, if } n \text{ is odd.} \end{cases}$$

c) For the star graph S_n, $\varepsilon^c(S_n) = 3(n-1)$.

d) For the path graph P_n,

$$\varepsilon^c(P_n) = \begin{cases} \frac{1}{2}\left(3n^2 - 6n + 4\right) & \text{, if } n \text{ is even} \\ \frac{3}{2}(n-1)^2 & \text{, if } n \text{ is odd.} \end{cases}$$

e) For the complete bipartite graph, $K_{m,n}$, where $m, n \neq 1$, $\varepsilon^c(K_{m,n}) = 4mn$.

In 2010, Zhou B. and Du Z. established lower and upper bounds for the eccentric connectivity index. These bounds are as follows:

Theorem 2.2 *[12] Let G be a connected graph with m edges. In this case, $2m(rad(G)) \leq \varepsilon^c(G) \leq 2m(diam(G))$. Equality is achieved only when G is a self-centered graph.*

Theorem 2.3 *[12] Let G be a connected graph with $n \geq 4$ vertices, and let $\bar{G}$ be the complement of G, which is also a connected graph. Thus, $\varepsilon^c(G) + \varepsilon^c(\bar{G}) \geq 2n(n-1)$. Equality is achieved only when both G and $\bar{G}$ have a radius of 2 and are self-centered graphs.*

Theorem 2.4 *[12] Let G be a connected graph with $n \geq 4$ vertices. In this case, $\varepsilon^c(G) \geq 3(n-1)$. Equality is achieved only when G is a star graph.*

3. Topological Index Values for Some Shadow Graphs

In this section, we calculate the eccentric connectivity index of shadow graphs for various specific graphs, including cycle graphs, path graphs, star graphs, complete bipartite graphs, and wheel graphs.

Theorem 3.1 *Let $G \cong P_n$ be a path graph with $n \geq 4$. Then, the eccentric connectivity index value of the shadow graph of G is*

$$\varepsilon^c(D(G)) = \begin{cases} 6(n-1)^2 & , \text{if } n \text{ is odd} \\ 3n^2 - 6n + 4 & , \text{if } n \text{ is even} \end{cases}$$

Proof: To prove the theorem, the eccentricity values and degrees of all vertices in the graph should be determined. Let's label the vertices of graph $D(G)$ as

$$\begin{aligned} V(D(G)) &= V(G) \cup V(G') \\ &= \{1, 2, \ldots, n\} \cup \{1', 2', \ldots, n'\}. \end{aligned}$$

Let's first find the degrees of the vertices in the graph.

- For $v \in V(G)$, it can be readily observed that $\deg(1) = \deg(n) = 2$ and for $\forall v \in (V(G) - \{1, n\})$ $\deg(v) = 4$.

- For $v \in V(G')$, it can be readily observed that $\deg(1') = \deg(n') = 2$ and for $\forall v' \in (V(G') - \{1', n'\})$, $\deg(v') = 4$.

Now, let's obtain the eccentricity values of the vertices of the graph. This will be examined in two cases depending on whether n is odd or even.

Case 1. Let n is odd.

In this case, the following equations are derived for the eccentricity values of the vertices in the set $V(G)$.

$$e\left(\frac{n-1}{2}\right) = e\left(\frac{n+1}{2} + 1\right), e\left(\frac{n-3}{2}\right) = e\left(\frac{n+1}{2} + 2\right), \ldots, e(2) = e(n-1), e(1) = e(n).$$

These values are formulated as $e(i) = e(n - (i-1)) = n - i, i \in \left\{1, 2, \ldots, \frac{n-1}{2}\right\}$ and $e\left(\frac{n+1}{2}\right) = n - \frac{n+1}{2}$. The eccentricity values of each vertex in $V(G')$ are the same as the eccentricity values of their corresponding copy vertices in $V(G)$. Thus, these values are

$$e(1') = e(1), e(2') = e(2), \ldots, e(n') = e(n).$$

When we substitute the results we have found into the definition of the eccentric connectivity index, we obtain for $G \cong P_n$ and $n \geq 3$

$$\begin{aligned}
\varepsilon^c(D(G)) &= 2\left[2\left(2(n-1)+\sum_{i=(n+1)/2}^{n-2} 4i\right)+4\left(\frac{n-1}{2}\right)\right] \\
&= 2\left(4(n-1)+8\sum_{i=(n+1)/2}^{n-2} i+2(n-1)\right) = 2\left(6(n-1)+8\sum_{i=(n+1)/2}^{n-2} i\right) \\
&= 12(n-1)+16\left(\frac{(n-2)(n-1)}{2}-\frac{\left(\frac{n+1}{2}-1\right)\left(\frac{n+1}{2}\right)}{2}\right) \\
&= 12(n-1)+8(n-2)(n-1)-2(n-1)(n+1) \\
&= 6(n-1)^2.
\end{aligned}$$

Case 2. Let n is even.

In this case, the following equations are derived for the eccentricity values of the vertices in the set $V(G)$.

$$e\left(\frac{n}{2}\right)=e\left(\frac{n}{2}+1\right), .e\left(\frac{n}{2}-1\right)=e\left(\frac{n}{2}+2\right), \ldots ., e(2)=e(n-1), e(1)=e(n)$$

These values are formulated as $e(i)=e(n-(i-1))=n-i, i \in \left\{1,2,\ldots,\frac{n}{2}\right\}$.
The eccentricity values of each vertex in $V(G')$ are the same as the eccentricity values of their corresponding copy vertices in $V(G)$. Thus, these values are

$$e\left(1'\right)=e(1), e\left(2'\right)=e(2), \ldots, e\left(n'\right)=e(n).$$

When we substitute the results we have found into the definition of the eccentric connectivity index, we obtain for $G \cong C_n$ and $n \geq 4$

$$\begin{aligned}
\varepsilon^c(D(G)) &= 2\left(2(n-1)+\sum_{i=n/2}^{n-2} 4i\right) \\
&= 4(n-1)+8\sum_{i=n/2}^{n-2} i = 4(n-1)+8\left(\frac{(n-2)(n-1)}{2}-\frac{\left(\frac{n}{2}-1\right)\left(\frac{n}{2}\right)}{2}\right) \\
&= 4n-4+4\left(n^2-3n+2\right)-n^2+2n = 3n^2-6n+4.
\end{aligned}$$

Thus, the proof of the theorem is completed.

□

Theorem 3.2 *Let $G \cong C_n$ be a cycle graph with $n \geq 4$. Then, the eccentric connectivity index value of the shadow graph of G is $\varepsilon^c(D(G))=8n\left\lfloor\frac{n}{2}\right\rfloor$.*

Proof:

To prove the theorem, the eccentricity values and degrees of all vertices in the graph should be determined. Let's label the vertices of graph $D(G)$ as

$$\begin{aligned}
V(D(G)) &= V(G) \cup V\left(G'\right) \\
&= \{1,2,\ldots,n\} \cup \left\{1',2',\ldots,n'\right\}.
\end{aligned}$$

Let's first find the degrees of the vertices in the graph. For $\forall v \in V(D(G))$, the vertex v has exactly two neighbors in the set $V(G)$. Therefore, according to this definition of the shadow graph, it implies that it should also have two neighbors in the set $V(G')$. Thus, for $\forall v \in V(D(G))$, $\deg(v)=4$ is obtained.

Now, let's find the eccentricity values of the vertices of the graph. There are two cases based on the vertices.

Case 1. Let $\forall u \in V(G) \subset V(D(G))$.

- If $v \in V(G)$, then the shortest distance between vertices u and v is $1 \leq d(u,v) \leq \lfloor \frac{n}{2} \rfloor$.

- If $v = v' \in V(G')$, then the shortest distance between vertices u and v is $1 \leq d(u,v) \leq \lfloor \frac{n}{2} \rfloor$.

Case 2. Let $\forall u \in V(G')$. In this case as well, the obtained shortest distances are the same as in Case 1.

Therefore, from Cases 1 and 2, we find that for all $v \in V(D(G))$, $e(v) = \lfloor \frac{n}{2} \rfloor$. When we substitute the results we have found into the definition of the eccentric connectivity index, we obtain for $G \cong C_n$ and $n \geq 4$

$$\varepsilon^c(D(G)) = \sum \deg(v) \cdot \mathrm{e}(v) \quad = \left(4 \left\lfloor \frac{n}{2} \right\rfloor\right) 2n = 8n \left\lfloor \frac{n}{2} \right\rfloor .$$

Thus, the proof of the theorem is completed.

□

Theorem 3.3 *Let $G \cong S_{1,n-1}$ be a star graph with $n \geq 3$. Then, the eccentric connectivity index value of the shadow graph of G is $\varepsilon^c(D(G)) = 16(n-1)$.*

Proof:

To prove the theorem, the eccentricity values and degrees of all vertices in the graph should be determined. Let's label the vertices of graph $D(G)$ as

$$\begin{aligned} V(D(G)) &= V(G) \cup V(G') \\ &= \{c, 1, 2, \ldots, n\} \cup \{c', 1', 2', \ldots, n'\}. \end{aligned}$$

Let's first find the degrees of the vertices in the graph. The center vertex c is is adjacent to $n-1$ vertices except itself in the set $V(G)$, and also to all $n-1$ vertices except the copy vertex c' in cluster in the set $V(G')$. Similarly, the same applies to the vertex c'. Hence, we obtain $\deg(c) = \deg(c') = 2(n-1)$. It can be easily observed that the neighbors of the vertex $\forall v \in (V(D(G)) - \{c, c'\})$ are $N_{D(G)}(v) = \{c, c'\}$. From this, for $\forall v \in (V(D(G)) - \{c, c'\})$, we have $\deg(v) = 2$.

Now, let's find the eccentricity values of the vertices of the graph. There are two cases based on the vertices.

Case 1. Let $\forall u \in V(G)$.

- If v is the center vertex c, then we obtain $d(v,i) = 1, \quad i \in \{1, \ldots, n-1, 1', \ldots, (n-1)'\}$, and $d(v, c') = 2$.

- If $v = i, \quad i \in \{1, 2, \ldots, n-1\}$, then we have $d(v,c) = d(v,c') = 1$, and for $u \neq v$, $d(v,u) = 2$, $u \in \{1, 2, \ldots, n-1, 1', \ldots, (n-1)'\}$.

Case 2. Let $\forall u \in V(G')$. In this case as well, the obtained shortest distances are the same as in Case 1.

Therefore, from Cases 1 and 2, we find that for all $v \in V(D(G))$, $e(v) = 2$. When we substitute the results we have found into the definition of the eccentric connectivity index, we obtain for $G \cong S_{1,n-1}$ and $n \geq 3$

$$\begin{aligned} \varepsilon^c(D(G)) &= \sum \deg(v) e(v) \\ &= (2n-1) \cdot 2 \cdot 2 + 2 \cdot 2 \cdot (2n-2) = 16(n-1). \end{aligned}$$

Thus, the proof of the theorem is completed.

□

Theorem 3.4 *Let $G \cong W_{1,n-1}$ be a wheel graph with $n \geq 3$. Then, the eccentric connectivity index value of the shadow graph of G is $\varepsilon^c(D(G)) = 32(n-1)$.*

Proof:

To prove the theorem, the eccentricity values and degrees of all vertices in the graph should be determined. Let's label the vertices of graph $D(G)$ as

$$\begin{aligned} V(D(G)) &= V(G) \cup V(G') \\ &= \{c, 1, 2, \ldots, n\} \cup \{c', 1', 2', \ldots, n'\}. \end{aligned}$$

Let's first find the degrees of the vertices in the graph. The center vertex c is is adjacent to $n-1$ vertices except itself in the set $V(G)$, and also to all $n-1$ vertices except the copy vertex c' in cluster in the set $V(G')$. Similarly, the same applies to the vertex c'. Hence, we obtain $\deg(c) = \deg(c') = 2(n-1)$. For $\forall v \in (V(D(G)) - \{c, c'\})$, the vertex v has exactly three neighbors in the set $V(G)$, one of which is the center vertex c. Therefore, according to the definition of the shadow graph, it implies that it should also have three neighbors in the set $V(G')$. Thus, for $\forall v \in (V(D(G)) - \{c, c'\})$, we obtain $\deg(v) = 6$.

Now, let's find the eccentricity values of the vertices of the graph. There are two cases based on the vertices.

- Let $v = c, c'$. If $v = c$, then the shortest distance between $v = c$ and $\forall u \in V(D(G) - \{c'\})$ is $d(v, u) = 1$, while the shortest distance between $v = c$ and its copy vertex c' is $d(v, c') = 2$. Similarly, the same values are obtained when the vertex $v = c'$.

- If $v \in (V(D(G)) - \{c, c'\})$, then the shortest distance between the vertex v and the vertex $\forall u \in \left(V(D(G)) - N_{D(G)}(v)\right)$ is $d(v, u) = 2$.

  Therefore, for $\forall v \in V(D(G))$, we have $e(v) = 2$.

When we substitute the results we have found into the definition of the eccentric connectivity index, we obtain for $G \cong W_{1,n-1}$ and $n \geq 3$

$$\begin{aligned} \varepsilon^c(D(G)) &= \sum \deg(v) e(v) \\ &= 2.(2n-2) \cdot 2 + (2n-2) \cdot 6 \cdot 2 = 32(n-1). \end{aligned}$$

Thus, the proof of the theorem is completed.

□

Theorem 3.5 *Let $G \cong K_n$ be a complete graph with $n \geq 3$. Then, the eccentric connectivity index value of the shadow graph of G is $\varepsilon^c(D(G)) = 8n(n-1)$.*

Proof:

To prove the theorem, the eccentricity values and degrees of all vertices in the graph should be determined. Let's label the vertices of graph $D(G)$ as

$$\begin{aligned} V(D(G)) &= V(G) \cup V(G') \\ &= \{1, 2, \ldots, n\} \cup \{1', 2', \ldots, n'\}. \end{aligned}$$

Let's first find the degrees of the vertices in the graph. The graph $D(G)$ contains two graphs $G \cong K_n$. According to the definition of $D(G)$, the vertex $\forall v \in V(D(G))$ is adjacent to all vertices except its copy vertex v'. Thus, the degree of the vertex $\forall v \in V(D(G))$ is $\deg(v) = 2n - 2$.

Also, since $N_{D(G)}(v) = V(D(G)) - \{v'\}$, the shortest distances between any vertex $\forall v \in V(D(G))$ and all other vertices in the graph $D(G)$ are as follows:

- If $u \in N_{D(G)}(v)$, then the shortest distance between u and v is $d(u, v) = 1$.
- If $u \notin N_{D(G)}(v)$, then the shortest distance between u and v is $d(u, v) = 2$.

Therefore, for $\forall v \in V(D(G))$, we have $e(v) = 2$.

When we substitute the results we have found into the definition of the eccentric connectivity index, we obtain for $G \cong K_n$ and $n \geq 3$

$$\begin{aligned}\varepsilon^c(D(G)) &= \sum \deg(v)e(v) \\ &= 2n.(2n-2) \cdot 2 \cdot 2 = 8n(n-1).\end{aligned}$$

Thus, the proof of the theorem is completed. □

Theorem 3.6 *Let $G \cong K_{m,n}$ be a complete bipartite graph with $m \leq n$. Then, the eccentric connectivity index value of the shadow graph of G is $\varepsilon^c(D(G)) = 16mn$.*

Proof:
To prove the theorem, the eccentricity values and degrees of all vertices in the graph should be determined. Let's label the vertices of graph $D(G)$ as

$$\begin{aligned}&V(D(G)) = V_1 \cup V_2 \cup V_3 \cup V_4, \text{ where} \\ &V_1 = \{1, 2, \ldots, m\} \\ &V_2 = \{m+1, m+2, \ldots, m+n\} \\ &V_3 = \{1', 2', \ldots, m'\} \\ &V_4 = \{(m+1)', (m+2)', \ldots, (m+n)'\}\,.\end{aligned}$$

In the graph $D(G)$, the copies of vertices in set V_1 correspond to vertices in set V_3, while the copies of vertices in set V_2 correspond to vertices in set V_4.

Let's first find the degrees of the vertices in the graph.

- For $\forall v \in V_1$ or $\forall v \in V_3$, we have $N_{D(G)}(v) = V_2 \cup V_4$, which implies $\deg(v) = |V_2| + |V_4| = n + n = 2n$.
- For $\forall v \in V_2$ or $\forall v \in V_4$, we have $N_{D(G)}(v) = V_3 \cup V_1$, which implies $\deg(v) = |V_3| + |V_1| = m + m = 2m$.

Now, let's find the eccentricity values of the vertices in the graph. Let v be any vertex in a set $V_i, \quad i \in \{1, 2, 3, 4\}$, of the graph.

- If $u \notin N_{D(G)}(v)$, then the shortest distance between vertices v and u is $d(v,u) = 2$.

- If $u \in N_{D(G)}(v)$, then the shortest distance between vertices v and u is $d(v,u) = 1$.

Therefore, for $\forall v \in V(D(G))$, we have $e(v) = 2$.

When we substitute the results we have found into the definition of the eccentric connectivity index, we obtain for $G \cong K_{m,n}$

$$\begin{aligned}\varepsilon^c(D(G)) &= \sum \deg(v)e(v)\\ &= 2m \cdot 2n \cdot 2 + 2n.2m \cdot 2 = 16mn.\end{aligned}$$

Thus, the proof of the theorem is completed.

□

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