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Eccentric connectivity index of some central graphs

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Abstract

Graph theory has become an indispensable branch of contemporary mathematics, contributing significantly to both theoretical and applied research., particularly in the realm of natural sciences such as Chemistry and Biology, due to its various applications. Topological indices are numerical parameters associated with graph isomorphism, which have significance in diverse scientific fields. Research on topological indices has been intensifying in recent times. A topological index denotes a numeric value that encapsulates structural information about a molecule's graph representation in the chemical graph theory. These indices are based on the topology and bonds of atoms and serve as numerical descriptors. A wide range of topological indices have been developed to capture and evaluate the physicochemical characteristics of molecular structures. Chemical graph theory models molecules as graphs in which atoms are depicted as vertices and chemical bonds as edges. This study concentrates on a particular topological descriptor known as the eccentric connectivity index (ECI), which combines information about vertex degrees and the shortest path distances between them. Here, we investigate and compute the ECI values for certain central graph structures that exhibit distinctive configurations.

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1. Introduction

Graph theory has emerged as a significant component of mathematics, particularly within the realm of natural sciences such as Chemistry and Biology, due to its diverse range of applications [4-7, 14, 15]. Topological indices are numerical parameters that remain invariant under graph isomorphism and find relevance in graph theory. Research into topological indices has recently witnessed a notable surge in activity.

Chemical graph theory commonly models molecular structures using graphs, where atoms and bonds are abstracted as vertices and edges, respectively. Consequently, many challenges encountered within chemical molecular networks can be resolved using graph theory. Fundamental challenges in the study of chemical molecular graphs include the structural characterization of molecules, establishing quantitative structure–property and structure–activity relationships, and predicting the pharmacological or biological effects of chemical substances [9, 12, 15]. In this context, various topological indices—including the Zagreb, neighbor Zagreb, connectivity, eccentric, Randić, Wiener, and eccentric connectivity indices—have been introduced and widely studied in the framework of graph theory [2, 3, 8, 13, 21, 22]. One such index is *the eccentric connectivity index* (*ECI*).

The ECI, a distance-based topological index along with connectivity, was introduced and employed around the late 1990s. It serves as a parameter with diverse applications in the fields of chemistry and topology. The ECI provides an efficient means to estimate a wide range of chemical, biological, and physicochemical characteristics that can be determined directly based on the molecular configuration of the compound.

In recent times, the ECI has been investigated for its higher predictability compared to other topological indices. It exhibits a distinctive role in analyzing the relationships between molecular structure and both physicochemical properties and biological activities, especially in drug design [3, 6, 13, 14, 15]. This parameter has been successfully employed in developing a wide range mathematical models for predicting different types of biological activities. Despite the various chemical and biological applications, the comprehensive investigation into the mathematical attributes of this index has only begun in recent times.

The eccentric connectivity index (ECI) of a graph G is obtained by summing the products of the eccentricity and degree of each of its vertices, denoted as $\varepsilon^c(G)$, and is defined as $\varepsilon^c(G) = \sum_{v \in V(G)} \deg(v)e(v)$ [10, 22].

We adopt the notation and terminology of graph theory as described in [15]. We examine a graph G, assumed to be simple and connected, with

vertices in $V(G)$ and edges in $E(G)$. The function $d_G(u,v)$ denotes *the shortest path* length between two vertices u and v in G, measured by the smallest number of edges connecting them. *The eccentricity of a vertex* $u \in V(G)$, written as $\mathrm{ec}_G(u)$, is the greatest distance from u to any other vertex in the graph, $\mathrm{ec}_G(u) = \max\{d_G(u,v) \mid v \in V(G)\}$. *The diameter* of a connected graph G is defined as $diam(G) = \max\{\mathrm{ec}_G(u)\}$ and the radius of G is defined as $rad(G) = \min\{\mathrm{ec}_G(u)\}$. A vertex $u \in V(G)$ is called a *central vertex* if its eccentricity is equal to the radius of the graph, i.e., $\mathrm{ec}_G(u) = rad(G)$. *The degree* of a vertex $u \in V(G)$, $\deg_G(u)$, is the number of edges incident to u. A vertex of degree one is called a *pendant vertex*. For a given vertex $v \in V(G)$ in G, its *open neighborhood* is represented by $N_G(v) = \{u \in V(G) : uv \in E(G)\}$, while its *closed neighborhood* is represented by $N_G[v] = N_G(v) \cup \{v\}$ [20].

In this research, we direct our attention to the evaluation of the ECI value within central graphs. The notion of central graphs was introduced by Viven et al. in their works [19]. A central graph, denoted as $C(G)$, is derived from graph G by subdividing each edge exactly once, thereby establishing adjacency between all initially non-adjacent vertices of G. Throughout this paper, we use n and m to represent the cardinalities of the vertex set and the edge set of the graph G, respectively (denoted by $|V(G)| = n$ and $|E(G)| = m$). Consequently, within a central graph, there exist n vertices, each with a degree of $n-1$, as well as m vertices with a degree of 2. Thus, the total edge number in $C(G)$ amounts to $\binom{n}{2} + m$. Furthermore, it is important to note that a central graph is connected at all times and devoid of any 3-cycles. From a structural point of view, central graphs can be regarded as a specific type of split graphs, where the vertices are divided into two distinct subsets: one forming a clique and the other forming an independent set. [1, 11, 16-19]. The core focus of our investigation centers on elucidating the properties and characteristics of central graphs. Thus, we study about ECI of some central graphs.

Theorem 1.1 [10]

- *Complete graph,* K_n *where* $n \geq 2$. *Then,* $\varepsilon^c(K_n) = n(n-1)$.
- *Cycle graph,* C_n. *Then,* $\varepsilon^c(C_n) = \begin{cases} n^2, & n \text{ even} \\ n(n-1), & n \text{ odd} \end{cases}$.

- Star graph, S_n. Then, $\varepsilon^c(S_n) = 3(n-1)$.
- Path graph, P_n. Then, $\varepsilon^c(P_n) = \begin{cases} \frac{1}{2}(3n^2 - 6n + 4), & n \text{ even} \\ \frac{3}{2}(n-1)^2, & n \text{ odd} \end{cases}$.
- Comlete bipartite graph, $K_{m,n}$ where $m, n \neq 1$. Then, $\varepsilon^c(K_{m,n}) = 4mn$.

Theorem 1.3: [22] *Let G be connected graph with* $|E(G)| = m$ *edges. It yields*

$$2m(\text{rad}(G)) \leq \varepsilon^c(G) \leq 2m(\text{diam}(G)).$$

2. On the ECI values corresponding to some special graphs

In this section, the ECI of the central graphs of some graphs were calculated. To make the proofs of the theorems more understandable, the labeling given below is used. The vertex set of the graph $C(G)$ is divided into two parts as $V(C(G)) = V_1 \cup V_2$ in Theorems 2.1, 2.2 and 2.3. Here, label the sets as $V_1 = V(G) = \{1, 2, \ldots, n\}$ and $V_2 = \{n+1, n+2, \ldots, |E(G)|\}$. V_2 is the set of vertices of the subdivision added to the graph G. However, in Theorems 2.4 and 2.5, the set V_1 is considered as $V_1 = V(G) = \{1, 2, \ldots, n-1\} \cup \{c\}$, where c is central vertex.

Theorem 2.1: *Let G be isomorphic to the cycle graph,* C_n, *including n vertices and its corresponding central cycle graph is denoted by* $C(G)$. *Then, the ECI of* $C(G)$ *is* $\varepsilon^c(C(G)) = 2n^2 + 4n$.

Proof: To compute the ECI of the graph $C(G)$, it is essential to determine both the degree and the eccentricity of each vertex. Initially, the vertex degrees are computed.

- Every vertex belonging to the set V_1 is connected to exactly two vertices in V_2. Additionally, according to the definition of a central graph, each vertex must be adjacent to $n-3$ vertices in $C(G)$ that are not neighbors in G. Therefore, for $\forall v \in V_1$, we have $\deg(v) = n-1$.
- The vertices in V_2 are obtained by subdividing each edge exactly once. Thus, for $\forall v \in V_2$, we have $\deg(v) = 2$.

Now, we need to determine the eccentricities of the vertices in $C(G)$. There are two cases according to the vertices.

Case 1: For every vertex $v \in V_1$, the shortest geodesic lengths connecting v to every other vertex u in $C(G)$, excluding v itself, is $d(v,u) \leq 2$. Therefore, for every $v \in V_1$, the vertex eccentricity is $ec(v) = 2$.

Case 2: For every vertex $v \in V_2$, the shortest geodesic lengths connecting v to every other vertex u in $C(G)$, excluding v itself, is $d(v,u) \leq 3$. Therefore, for every $v \in V_2$, the vertex eccentricity is $ec(v) = 3$.

When substituting the obtained values into the definition of the ECI, we get $\varepsilon^c(C(G)) = n.(n-1).2 + n.2.3 = 2n^2 + 4n$.

Theorem 2.2: *Let be G be isomorphic to the path graph, P_n, including n vertices and its corresponding central path graph is denoted by $C(G)$. Then, the ECI of $C(G)$ is $\varepsilon^c(C(G)) = 2n^2 + 4n - 6$.*

Proof: To compute the ECI of the graph $C(G)$, it is essential to determine both the degree and the eccentricity of each vertex. Initially, the vertex degrees are computed.

- Each vertex in the set V_1 is adjacent to exactly two vertices in the set V_2. Thus, for all $v \in V_1$, $\deg(v) = n - 2 + 1 = n - 1$ is obtained.
- The vertices in the set V_2 are new vertices added to each edge of the graph *G*. The vertices in the set V_2 are obtained by performing the subdivision process once for each edge. Thus, for all $v \in V_2$, $\deg(v) = 2$ is obtained.

Now we need to find the eccentricity of the vertices in the graph $C(G)$. There are two cases for vertices.

Case 1: For all $v \in V_1$, the shortest geodesic lengths connecting v to every other vertex u vertices in $C(G)$ except itself is at most 2. Thus, the vertex eccentricity for all $v \in V_1$ is $ec(v) = 2$.

Case 2: For all $v \in V_2$, the shortest geodesic lengths connecting v to every other vertex u vertices in $C(G)$ except itself is at most 1. Thus, the vertex eccentricity for all $v \in V_2$ is $ec(v) = 1$.

When the obtained values are substituted into the definition of the ECI, we get

$$\varepsilon^c(C(G)) = n \cdot (n-1) \cdot 2 + (n-1) \cdot 2 \cdot 1 = 2n^2 - 2n + 2n - 2 = 2n^2 + 4n - 6.$$

Theorem 2.3: *Let G be isomorphic to the complete graph, K_n, including n vertices and its corresponding central complete graph is denoted by $C(G)$ Then, the ECI of $C(G)$ is $\varepsilon^c(C(G)) = 7n^2 - 7n$.*

Proof: To compute the ECI of the graph $C(G)$, it is required to determine both the degree and the eccentricity of each vertex. Initially, the vertex degrees are computed.

- Each vertex in set V_1 is adjacent to $n-1$ vertices in set V_2. Thus, for all $v \in V_1$, we have $\deg(v) = n-1$.
- The vertices in set V_2 are the subdivision vertices added to every edge of graph G. Since G is a complete graph, the graph contains exactly $|E(K_n)| = \frac{n(n-1)}{2}$ edges and thus, the number of newly added subdivision vertices to each edge is $|V_2| = \frac{n(n-1)}{2}$. Each of these subdivision vertices is added exactly once for each edge through subdivision process. Therefore, for all $v \in V_2$, $\deg(v) = 2$.

Now, we need to determine the vertex eccentricity values in graph $C(G)$. There are two cases based on vertices:

Case 1: For all $v \in V_1$, the shortest geodesic lengths connecting v to every other vertex u in $C(G)$ excluding itself is $d(v,u) \le 3$. Thus, for all $v \in V_1$, the vertex eccentricity v is $ec(v) = 3$.

Case 2: For all $v \in V_2$, the shortest geodesic lengths connecting v to every other vertex u in $C(G)$ excluding itself is $d(v,u) \le 4$. Thus, for all $v \in V_2$, the vertex eccentricity v is $ec(v) = 4$.

Substituting the obtained values into the definition of the ECI, we get

$$\varepsilon^c(C(G)) = n \cdot (n-1) \cdot 3 + \frac{n(n-1)}{2} \cdot 2 \cdot 4 = 7n^2 - 7n.$$

Theorem 2.4: *Let G be isomorphic to the star graph, $S_{1,n-1}$, including n vertices and its corresponding central star graph is denoted by $C(G)$. Then, the ECI of $C(G)$ is $\varepsilon^c(C(G)) = 2n^2 - 4n$.*

Proof: To compute the ECI of the graph $C(G)$, it is required to determine both the degree and the eccentricity of each vertex. Initially, the vertex degrees are computed.

- Each vertex in the set V_1 forms a complete graph structure in $C(G)$. The number of vertices in the set V_1 is $|V_1| = n-1$. Therefore, $C(G)$

contains the subgraph K_{n-1}. Thus, for all $v \in V_1$, $\deg(v) = n-1$ is obtained.

- The vertices in the set V_2 are new vertices added to each edge of the graph *G*. The vertices in the set V_2 are obtained by performing the subdivision process once for each edge. Thus, for all $v \in V_2$, $\deg(v) = 2$ is obtained.
- In the graph, the central vertex *c* is incident to exactly $n-1$ edges. So, deg(*c*)= $n-1$.

Now we need to find the vertex eccentricity values in the graph $C(G)$. Due to the structure of the graph $C(G)$, it is easily observed that for all $v \in V(C(G))$, the vertex eccentricity is $e_c(v) = 2$.

When the obtained values are substituted into the definition of the ECI, we have

$$\varepsilon^c(C(G)) = (n-1)\cdot(n-1)\cdot 2 + (2n-2)\cdot 2\cdot 2 + 1\cdot(n-1)\cdot 2 = 2n^2 + 2n - 4.$$

Theorem 2.5: *Let G be isomorphic to the wheel graph, $W_{1,n-1}$ including n vertices and its corresponding central wheel graph is denoted by $C(G)$. Then, the ECI of $C(G)$ is $\varepsilon^c(C(G)) = 3n^2 + 9n - 12$.*

Proof: To compute the ECI of the graph $C(G)$, it is essential to determine both the degree and the eccentricity of each vertex. Initially, the vertex degrees are computed.

- The vertices in the set V_1 form a complete graph structure in $C(G)$. The number of vertices in the set V_1 is $|V_1| = n-1$. Therefore, $C(G)$ contains the subgraph K_{n-1}. Thus, for all $v \in V_1$, $\deg(v) = n-1$ is obtained.
- The vertices in the set V_2 are new vertices added to each edge of the graph *G*. The vertices in the set V_2 are obtained by performing the subdivision process once for each edge. Thus, for all $v \in V_2$, $\deg(v) = 2$ is obtained.
- The central vertex *c* of the graph *G* has $n-1$ degree.

Now we need to find the vertex eccentricity values in the graph $C(G)$. There are three cases for vertices.

Case 1: For all $v \in V_1$,

- The shortest geodesic lengths connecting v to every other vertex u in $C(G)$ except itself in the set V_1 is at most 2; for all $v \in V_1$, $(v \neq u) \Rightarrow d(v,u) \leq 2$ is obtained.
- The shortest geodesic lengths connecting v to every other vertex u in the set V_2 is at most 3; for all $v \in V_2 \Rightarrow d(v,u) \leq 3$ is obtained.
- The shortest geodesic lengths connecting v to the central vertex c is at most 2; for $v = c \Rightarrow d(v,u) \leq 2$ is obtained.

Thus, the vertex eccentricity value for all $v \in V_1$ is $ec(v) = 3$.

Case 2: For all $v \in V_2$,

- The shortest geodesic lengths connecting v to every other vertex u in $C(G)$ except itself in the set V_2 is at most 3; for all $v \in V_2$, $(v \neq u) \Rightarrow d(v,u) \leq 3$ is obtained.
- The shortest geodesic lengths connecting v to every other vertex u in the set V_1 is at most 3; for all $v \in V_1 \Rightarrow d(v,u) \leq 3$ is obtained.
- The shortest geodesic lengths connecting v to the central vertex c is at most 3; for $v = c \Rightarrow d(v,u) \leq 3$ is obtained.

Thus, the vertex eccentricity value for all $v \in V_2$ is $ec(v) = 3$.

Case 3: Let $v = c$ be the central vertex. Due to Case 1 and Case 2, it is observed that the eccentricity of the central vertex $v = c$ is $ec(v = c) = 3$.

When the obtained values are substituted into the definition of the ECI, we get

$$\varepsilon^c(C(G)) = (n-1)\cdot(n-1)\cdot 3 + (2n-2)\cdot 2\cdot 3 + 1\cdot(n-1)\cdot 3 = 3n^2 + 9n - 12.$$

Theorem 2.6: *Let G be isomorphic to the complete bipartite graph, $K_{m,n}$, including m+n vertices and its corresponding central complete bipartite graph is denoted by $C(G)$. Then, the ECI of $C(G)$ is $\varepsilon^c(C(G)) = 2m^2 + 2n^2 + 10nm - 2m - 2n$.*

Proof: The vertex set of graph $C(G)$ is split into three components as $V(C(G)) = V_1 \cup V_2 \cup V_3$, where $V_1 = \{1, 2, \ldots, m\}$, $V_2 = \{n+1, n+2, \ldots, n+m\}$ and $V_3 = \{n+m+1, n+m+2, \ldots, nm\}$. $V_1 \cup V_2 = V(G)$ and V_3 is the subdivision vertices set added to the graph G. To compute the ECI of the graph $C(G)$, it is required to determine both the degree and the eccentricity of each vertex. Initially, the vertex degrees are computed.

- Each vertex in the V_1 set is adjacent to all vertices except itself in the v_2 set. Thus, for all $v \in V_1$, $\deg(v) = n + m - 1$ is obtained.
- Each vertex in the V_2 set is adjacent to all vertices except itself in the v_1 set. Thus, for all $v \in V_2$, $\deg(v) = m + n - 1$ is obtained.

Therefore, for all $v \in (V_1 \cup V_2 = V(G))$, $\deg(v) = n + m - 1$ is obtained.

- The vertices in the V_3 set are new vertices added to each edge of the G graph. Since the number of edges in a two-component complete graph with m and n vertices is $m \cdot n$, the number of new vertices added to each edge is $m \cdot n$. These vertices are obtained by performing the subdivision process exactly once for each edge. Thus, for all $v \in V_3$, $\deg(v) = 2$ is obtained.

Now we need to find the vertex eccentricity values in the $C(G)$ graph. There are three cases for vertices.

Case 1: For all $v \in V_1$,

- The shortest geodesic lengths connecting v to u in $C(G)$ except itself in the set V_1 is 1; for all $v \in V_1, (v \neq u) \Rightarrow d(v,u) = 1$ is obtained.
- The shortest geodesic lengths connecting v to u in V_2 is 1; for all $v \in V_2 \Rightarrow d(v,u) = 2$ is obtained.
- The shortest geodesic lengths connecting v to u in V_3 is 1; for all $v \in V_3 \Rightarrow d(v,u) \leq 2$ is obtained.

Thus, the vertex eccentricity for all $v \in V_1$ is $ec(v) = 2$.

Case 2: For all $v \in V_2$,

- The shortest geodesic lengths connecting v to u in $C(G)$ except itself in V_2 is 1; for all $v \in V_2, (v \neq u) \Rightarrow d(v,u) = 1$ is obtained.
- The shortest geodesic lengths connecting v to u in V_1 is 1; for all $v \in V_1 \Rightarrow d(v,u) = 2$ is obtained.
- The shortest geodesic lengths connecting v to u in V_3 is 1; for all $v \in V_3 \Rightarrow d(v,u) \leq 2$ is obtained.

Thus, the vertex eccentricity for all $v \in V_2$ is $ec(v) = 2$.

Case 3: For all $v \in V_3$,

- The shortest geodesic lengths connecting v to u in $C(G)$ except itself in the set V_3 is 1; for all $v \in V_3, (v \neq u) \Rightarrow d(v,u) \leq 3$ is obtained.
- The shortest geodesic lengths connecting v to u in V_1 is 1; for all $v \in V_1 \Rightarrow d(v,u) \leq 2$ is obtained.
- The shortest geodesic lengths connecting v to u in V_2 is 1; for all $v \in V_2 \Rightarrow d(v,u) \leq 2$ is obtained.

Thus, the vertex eccentricity for all $v \in V_3$ is $ec(v) = 3$.

When the obtained values are substituted into the definition of the ECI, we have $\varepsilon^c(C(G)) = m \cdot (n+m-1) \cdot 2 + n \cdot (m+n-1) \cdot 2 + (n \cdot m) \cdot 2 \cdot 3 = 2m^2 + 2n^2 + 10nm - 2m - 2n$.

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