College of Natural and Computational Sciences

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ON THE GENERAL ECCENTRIC CONNECTIVITY COINDEX OF GRAPHS

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Certificate

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As a member of the Board of Examiners of the MSc Thesis-Open Defense Examination, this is to certify that the MSc Graduate thesis prepared by Helen Tizazu, entitled: **ON General Eccentric Connectivity Coindex of a Trees** and submitted in fulfillment of the requirements for the Degree of Master of Science in Mathematics (Combinatory).

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Declaration

I hereby declare and affirm that this thesis is my own work and has not been previously submitted to another university or for another qualification review or completion of any postgraduate degree.

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Helen Tizazu

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Abstract

In this thesis, we introduce the general eccentric connectivity coindex, $ECCI_a$ of connected graphs. For a connected graph G order n, we define the general eccentric connectivity coindex as

$$ECCI_a(G) = \sum_{v \in V(G)} ecc_G^a[n-1-d_G(v)]$$

for $a \in \mathbb{R}$, where $E(G)$ is the edge set of graph G , $d_G(v)$ is the degree of vertex v and $V(G)$ is the vertex set of graph G.

We study, the general eccentric connectivity coindex of tree graphs of a given graph parameters. We determine trees with the maximum and minimum general eccentric connectivity coindex among all trees of a given graph parameters for $a > 1$.

Chapter 1

Introduction and Preliminaries

This chapter presents a mathematical model known as topological indices and defines the standard terminology from graph theory that will be utilized throughout the thesis. Next, we give an explanation of the reason behind our work and some important background results. When necessary, terms that are not specified in this chapter will be clarified in later chapters.

1.1 Basic Graph Theory Terminology and properties

This section presents a few definitions and graph properties. [3] [11] [31] [5] [35] [37] [7]

Definition of Graph A graph G is a pair (V,E), in which E is a set of 2-element subsets of V, and V is a set (which is generally always finite). Vertices in V and edges in E are the respective elements of each element. We designate V as the vertex set and E as the edge set of G. It is common practice to shorten the edge $\{x,y\}$ to just xy for ease. But keep in mind that $xy \in E$ and $yx \in E$ have the same identical meanings. Two different vertices from V are x and y. Graph G's order and size are commonly referred to as the cardinalities of $V(G)$ and $E(G)$, respectively. In actuality, $|G|$ is frequently used to indicate $|V(G)|$ and $||G||$ to indicate $|E(G)|$. A graph G is formally a pair of disjoint sets (V,E) that are ordered, with $E \subseteq V \times V$.
Finite graph A graph is finite if its vertex and edge sets are finite sets. Otherwise, it is called an infinite graph. Most commonly in graph theory, it is implied that the graphs discussed are finite. If the graphs are infinite, that is usually specifically stated.
Simple graph A graph with no loops or multiple edges is called a simple graph.

Throughout the thesis, the letter G denotes a graph and we look at a simple and finite graph.

In order for two graphs to be the same, they must have the same set of vertices and the same set of edges. This is rather limiting, and typically the only thing we want to know is if they are basically the same, meaning that they are just different labels for the same basic structure. A formal definition of this idea is given below.

Isomorphic graphs If G and H are two graphs then an isomorphism between G and H is a bijection $\phi : V(G) \to V(H)$ such that for any $v, w \in V(G)$ the number of edges between v and w in G is the same as the number of edges between ϕ in G, and ϕ in H. If such a bijection exists we say that G and H are isomorphic and write $G \cong H$.

By proving the necessary isomorphism and then confirming that the incidence relation is preserved, we can prove that the two graphs are isomorphic with ease. In fact, all we actually need is the capacity to calculate the number of edges between any two vertices in both graphs, as well as a bijection between the edges of G and H. Given that those counts coincide between the relevant pairs in the vertex set of H and the pairs of vertices in the vertex set of G, we know an isomorphism exists. It can be more difficult to demonstrate that two graphs are not isomorphic. When two graphs differ on some function or statement that is preserved by isomorphism, we can demonstrate that they are not isomorphic in many situations by demonstrating that they do not share an isomorphism invariant. One straightforward illustration of this would be vertex size: we are limited to creating bijections between sets that have an equal amount of components. In the same way, edge size is an invariant of isomorphism.

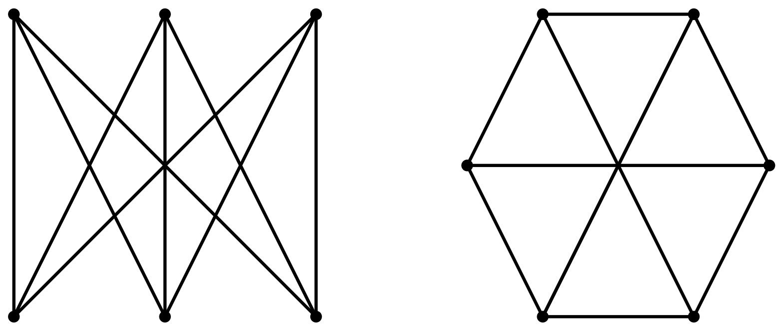

Figure 1.1: Isomoprphic graphs

FIGURE 1.1 Example of an isomorphic graphs.

In graph theory, and especially in this thesis, there are a few exceptional graphs that come a lot. Some are the following.

Complete graph A complete graph is a graph in which each pair of vertices is joined by an edge. A complete graph contains all possible edges, and denoted by K_n where n is the order of G.

Neighborhood of a vertex Each edge in $E(G)$ connects two vertices from $V(G)$, called the ends or endpoints of this edge. For an edge e with endpoints u and v , we say that u and v are adjacent to each other and that u and v are incident to e. The set of all vertices adjacent to a specific vertex v is called the (open) neighborhood of v and is denoted by $N_G(v)$ (or just $N(v)$ for short). The set $N[v] = N(v) \cup v$ that also includes v itself is called the closed neighborhood.

Degree of a vertex The number of edges that a vertex v is incident to in G is called the degree of v, denoted by $deg_G(v)$ or simply $deg(v)$. Note that $deg(v) = |N(v)|$. A vertex of degree 0 is isolated. The number $\delta(G) := min\{deg(v)|v \in V(G)\}$ is the minimum degree of G, the number $\Delta(G) := max\{deg(v)|v \in V(G)\}$ its maximum degree. If all vertices of G have the same degree k, then G is k-regular or simply regular.

A vertex of degree 1 is called a pendant vertex or a leaf, a vertex of degree at least 2 is called an internal vertex, and a vertex of degree at least 3 is called a branching vertex. See Figure 1.2 for an example of these definitions.

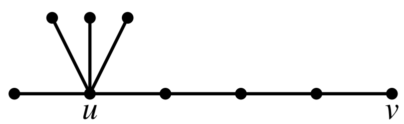

Figure 1.2: Leaf

FIGURE 1.2 An example where v is a leaf, u is a branching vertex of degree 5.

Lemma 1.1. *(Handshaking Lemma). The sum of the degrees of a graph's vertices equals twice the number of edges. That is* $\sum_i deg(v_i) = 2|E|$.

Regular graph A regular graph is a graph in which each vertex has the same number of neighbors, i.e., every vertex has the same degree. A regular graph with vertices of degree k is called a k-regular graph or regular graph of degree k.

Walk, trial, path A walk of graph G is an alternating sequence of vertices and edges beginning and ending with vertices, in which each line is incident with two vertices immediately proceeding and following it. This walk joins v_0 and v_n. It is sometimes called $v_0 - v_n$ walk. It is a closed walk if $v_0 = v_n$ and is open otherwise. A walk is called a trial if all the edges in the walk are distinct and a path if all the vertices are distinct.

1.1.1 Cycle graph

A simple graph with n vertices $(n \geq 3)$ and m edges is called a cycle graph that consists of a single cycle. The cycle graph with n vertices is called C_n. The number of vertices in C_n equals the number of edges, and every vertex has degree 2; that is, every vertex has exactly two edges incident with it.

Bipartite graph A bipartite graph is a simple graph in which the vertex set can be partitioned into two non-empty and disjoint sets, W and X, so that no two vertices in W share a common edge and no two vertices in X share a common edge.

Complete bipartite graph A complete bipartite graph is a bipartite graph the vertex set is the union of two disjoint sets, W and X, so that every vertex in W is adjacent to every vertex in X but there are no edges within W or X. The complete bipartite graph with $n = |W|$ and $m = |X|$ vertices is denoted by $K_{n,m}$.

Star graph The star graph S_n of order n, sometimes simply known as an n-star is a tree on n vertices with one vertex having vertex degree $n-1$ and the other $n-1$ having vertex degree 1. The star graph S_n is therefore isomorphic to the complete bipartite graph $K_{(1,n-1)}$.

Complement graph The complement of a graph G denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are adjacent, i.e., connected by an edge uv, if and only if they are not adjacent in G.

Connected graph A graph G is connected if each pair of vertices in G belongs to a path, otherwise, G is disconnected. The maximal connected subgraphs are called components.

Corollary 1.1. *Any simple graph with n vertices and more than $\frac{(n-1)(n-2)}{2}$ edges is connected.*

Acyclic graph An acyclic graph is a graph having no graph cycles. Acyclic graphs are bipartite.

Trees A tree is a connected acyclic graph. A graph that is only acyclic, but not necessarily connected, is also called a forest (it can be seen as a union of trees).

The well-known fact that the number of edges in a tree T is the number of edges is one less than the number of vertices. $|E(T)| = |V(T)| - 1$. This may be easily shown using induction. It will often be important that every tree with at least two vertices has at least two leaves. It is also worth mentioning that all trees are bipartite.

Two trees of order n will occur particularly frequently: the path P_n is the only tree with only two leaves, and the star S_n is the only tree with $n-1$ leaves (Figure 1.3). Intuitively, the path is the most "stretched out" among all trees of the same order, and the star is the most "compact" among all trees of the same order. In fact, the path and the star turn out to be the extremal structures in the studies of many topics in chemical graph theory.

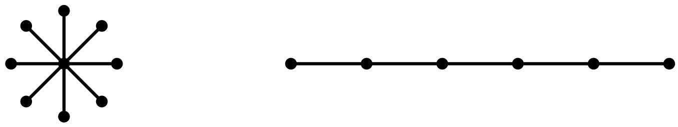

Figure 1.3: Star and path graph

FIGURE 1.3 A path (on the right) and a star (on the left).

Theorem 1.1. *The following assertions are equivalent to a tree:*

1. *Any two vertices of T are linked by a unique path in T;*
2. *T is minimally connected, i.e.T is connected but $T-e$ is disconnected for every edge of $e \in T$;*
3. *T is maximally acyclic, i.e. T contains no cycles but $T+xy$ does, for any two non-adjacent vertices $x, y \in T$*

Corollary 1.2. *The vertices of a tree can always be enumerated, say as $v_1, \dots, v_n$, so that every v_i with $i \geq 2$ has a unique neighbor in $\{v_1, \dots, v_{i-1}\}$.*

Corollary 1.3. *A connected graph with n vertices is a tree if and only if it has $n-1$ edges.*

Unicyclic graph A unicyclic graph is a connected graph containing exactly one cycle. The number of edges and vertices of a unicyclic graph are equal.

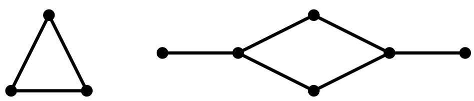

Figure 1.4: Unicyclic graph

FIGURE 1.4 An example of a unicyclic graph.

Distance in graph The distance $d_G(u,v)$ between two vertices $u, v \in V(G)$ is the minimum number of edges on a path in G between u and v. If u and v are in different components of G, then $d_G(u,v) = \infty$.

Eccentricity of a vertex The eccentricity of a vertex v in a graph G is the maximum distance from v to any vertex in G.

If u is a vertex such that $d_G(u,v) = ecc_G(v)$, then u is called an eccentric vertex of v in G. If there is only one such vertex u, then u is called the unique eccentric point v.

Lemma 1.2. *Let T be a tree with at least three vertices.*

1. *If v is a leaf of T and w is its neighbor, then $ecc(w) = ecc(v) - 1$*

2. *If u is a central vertex of T, then $deg(u) \geq 2$.*

Lemma 1.3. *Let v and w be two vertices in a tree T such that w is of maximum distance from v (i.e., $ecc(v) = d(v,w)$). Then w is a leaf.*

Lemma 1.4. *Let T be a tree with at least three vertices, and let T^* be the subtree of T obtained by deleting from T all its leaves. If v is a vertex of T^*, then*

$$ecc_T(v) = ecc_{T^*}(v) + 1.$$

Diameter of a graph The diameter of G is the maximum distance between any two vertices in G. Defined as $d(G) = max_{\{u,v\} \subseteq V(G)} d_G(u,v)$.

Diameteral Path A diametral path of a graph is the shortest path whose length is equal to the diameter of the graph.

Center of a Graph The center of a graph is the set of all vertices of minimum eccentricity, that is, the set of all vertices u where the greatest distance $d(u,v)$ to other vertices v is minimal. Equivalently, it is the set of vertices with eccentricity equal to the graph's radius. Thus vertices in the center (central points) minimize the maximal distance from other points in the graph.

Graph operation A graph operations are those that takes initial graphs and create new ones from them. They consist of binary (two inputs) as well as unary (one input) operations. Binary operation includes sum, disjunction, symmetric difference, corona product and etc.

Corollary 1.4. *Let T be an n-vertex tree. Then the center $Z(G)$ is either a single vertex or a single edge.*

Connectivity of a graph The connectivity number $\kappa(G)$ is defined as the minimum number of vertices whose removal from G results in a disconnected graph or in the trivial graph (a single vertex). A graph G is said to be $\kappa-$connected if $\kappa(G) \geq \kappa$. The connectivity number $\lambda(G)$ is defined as the minimum number of edges whose removal from G results in a disconnected graph or in the trivial graph (a single vertex). A graph G is said to be k-edge-connected if $\lambda(G) \geq k$.

Matching in a graph A matching in a simple graph G is a set of edges without common vertices. A maximum matching is a matching that contains the largest possible number of edges. The matching number of G, denoted by $\beta(G)$, is the size of a maximum matching of G.

Independent set An independent set in a simple graph G is a subset of $V(G)$ in which no two vertices are adjacent to each other. The independence number of G, usually denoted by $\alpha(G)$, is the size of a maximum independent set of G.

Theorem 1.2. *A set $S \subseteq V$ is an independent set of G if and only if V is a covering of G.*

This paper considers only finite, simple, connected graphs. Let G be a connected graph with the edge set $E(G)$ and vertex set $V(G)$, respectively. The numbers of vertices and edges are $|V(G)| = n, |E(G)| = m$. The complement of a graph G is denoted by $\overline{G}$. The number of vertices joining v is the degree of a vertex $v \in V(G)$. It is represented by $deg(v)$, also known as $d_G(v)$ and $d_G(u,v)$ denote the distance (i.e., the number of edges on the shortest path) The distance between v and any vertex in G that is furthest from v is the eccentricity of v, $ecc(v)$. $ecc_G = maxd_G(u,v)$. The diameter (radius, resp.) of G is the maximum (lowest, resp.) eccentricity over all vertices of G.

1.2 Topological Indices

Topological indices which are invariant to structure are numerical characteristics of a molecular graph that describe the bonding topology of a molecule. The primary goal of topological index research is to determine, by theoretical means how to extract and translate the information contained in a molecular structure into one or more numbers known as topological indices, which is then utilized to quantify the relationships between molecular structures and other experimental properties, biological activities and other properties. Quantitative structure-activity relationships (QSARs), in which a wide range of molecular properties, from physicochemical and thermodynamic properties to chemical activity and biological activity, are correlated with their chemical structure are developed using topological indices. Properties from physicochemical and thermodynamic properties to chemical activity and biological activity are correlated with their chemical structure and are developed using topological indices.

The study of topological indices started in 1947 when Harold Wiener [36] introduced the Wiener index to establish the relationships between the physical-chemistry properties of alkenes and the structures of their molecular graphs.

The Wiener index's definition in terms of the distances between vertices of a graph was first defined as

$$W(G) = \sum_{u,v \in V(G)} d_G(u,v).$$

There were also many distance-based topological indexes: The hyper-Wiener index, as a generalization of the Wiener index, is traditionally denoted by $WW(G)$. The hyper-Wiener index of acyclic graphs was introduced by Milan Randi ´c [28] in 1993 and extended to all connected graphs by Klein et al[8] . The hyper-Wiener index of a connected graph G is defined as

$$WW = \frac{1}{2} \sum_{u,v \in V(G)} (d(u,v) + d^2(u,v)).$$

For the purpose of characterizing molecular graphs, Plavši ´c et al.[6] and Ivanciuc et al.[19] in 1993 introduced the Harary index of a molecular graph G, indicated by $H(G)$, in this Journal. The Harary index is defined as follows:

$$H = H(G) = \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)}.$$

The graph invariants that are now known as Zagreb indices were historically the first degree-based structural descriptors [13]. In the present day, M_1 is referred to as the "first Zagreb index" and M_2 as the "second Zagreb index". The term "Zagreb group index" was soon shortened to "Zagreb index". The first and second Zagreb indices are defined as:

$$M_1(G) = \sum_{v \in V(G)} d_G^2(v) = \sum_{uv \in E(G)} [d_G(u) + d_G(u)], \qquad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

The other degree-based topological index is: The Randić index was invented in 1975 by Milan Randić [28]. His index was defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg(u)deg(v)}}.$$

With summation going over all pairs of adjacent vertices of the molecular graph G. Randić called it the "branching index," but it was shortly renamed to the "connectivity index". The popularity of the Randić index led to several modifications and generalizations, including the sum-connectivity index and the universal sum-connectivity index. The harmonic index $H(G)$ is also another variant of the Randić index, which is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{deg(u)+deg(v)}.$$

The distance and adjacency topological descriptor known as the eccentric connectivity index was first introduced by Sharma, Goswami, and Madan [2] in 1997. The eccentric connectivity index is defined as

$$\xi(G) = \sum_{u \in V(G)} d(u)\varepsilon(u)$$

The eccentric connectivity index is a graph invariant with a great deal of potential in structure-activity (property) interactions. It can be used to predict biological and physical properties. It has been applied to the development of several mathematical models for predicting biological processes with different characteristics. The mathematical properties of this index have been discussed by several authors.

The total eccentricity of graph G, denoted by $\xi(G)$, is defined as the sum of eccentricities of all vertices of graph G [29], i.e.,

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

Since then numerous studies have been conducted on the mathematical characteristics of eccentricity-based topological indices. Hua and Miao [17] consider the total eccentricity sum of all non-adjacent vertex pairs, they call this new eccentricity-based graph invariant the eccentric connectivity coindex defined as

$$ECCI(G) = \sum_{uv \notin E(G)} (ecc_G(u) + ecc_G(v))$$

They studied the extremal problems of *ECCI* for connected graphs of a given order, connected graphs of given order and size, and the trees, unicyclic graphs, bipartite-containing cycles, and triangle-free graphs of a given order, respectively additionally, they established various lower bound for *ECCI* in terms of several other graph parameters.

1.3 Literature Review

A topological graph index, also called a molecular descriptor, is a mathematical formula that can be applied to any graph that models some molecular structure. From this index, it is possible to analyze mathematical values and further investigate some physicochemical properties of a molecule. Therefore, it is an efficient method for avoiding expensive and time-consuming laboratory experiments. Topological indices of molecular graphs are one of the oldest and most widely used descriptors for quantitative structure activity relationship (QSAR) and quantitativity structure property relationship (QSPR) studies. Before many years the first topological index called the Wiener index was introduced in 1947 by chemist Harold Wiener [36] as the sum of the distance between all vertices of a graph G. Many topological indices were introduced by many mathematicians and they were classified based on degree (Randic index, first and second Zagreb index, Harmonic index, etc), eccentricity (eccentric connectivity index, total eccentricity index, etc), distance (Wiener index, hyper-Wiener index, Harary index, etc) and others.

Degree-based topological indices have been widely explored due to their simplicity and effectiveness in capturing molecular structure information, with the first and second Zagreb indices being one of the pioneering indices in this field. Gutman [12] established the first and second Zagreb indices about thirty years ago. Gutman [14] introduced the Gutman index, which is also referred to as the Schultz index of the second kind. The Randić index, known for its effectiveness in structure-property and structure-activity relationship studies, has been significant attention as a molecular descriptor. Its mathematical properties have been extensively explored in graph theory, to explore more see [28]. Then, Ashrafi [1] looked at the total contribution of every pair of a non-adjacent vertex in a graph and came up with two new indices of the Zagreb type: the first and second Zagreb coindices. Li [21] presented the idea of the first general Zagreb index of G. After more than 40 years, Furtula [9] restarted and established a few of its fundamental characteristics known as the F-index or forgotten topological index, it is represented by the symbol $F(G)$. Melaku.B.B [22] proposed a more generalized coindex known as the first general Zagreb coindex, which was inspired by the first Zagreb coindex and the F-coindex.

In 1997, Sharma [33] presented the eccentric-connectivity index, an important eccentricity-based topological index. A graph invariant with a significant deal of potential in structure activity (property) interactions is the eccentric connectivity index. Predicting biological and physical attributes is possible with it. Morgan discovered an exact lower limit, an asymptotically sharp upper bound, and a sharp lower bound for graphs of prescribed order and diameter for the eccentric connectivity index on [23][27]. Among the connected graphs with a given number of vertices and edges, the graphs with the highest eccentric connectivity index were determined by Zhang [42]. The least eccentric connectivity index, for all connected graphs with a specific order and a given order with a pendant vertex were described in detail by Devillez [10]. The minimum degree and order of a connected graph determine the sharp lower bound of the eccentric connectivity index established by Wu and Chen [41]. Lower bounds on vertex connected bipartite graphs with a given diameter in terms of the number of edges were obtained by Zhang.[25]. Zhang developed a sharp upper bound on the eccentric connectivity index of graphs of diameter 2 with a specified minimum degree and a sharp lower bound on the eccentric connectivity index of cacti with a given radius. [24]. The eccentric connectivity index of generalizations of thorn graphs was computed by Balachandran, Venkatakrishnan, and Kannan [38]. the topological indices of the three fence graphs the ladder, circular ladder, and Möbius ladders as well as the corresponding line graphs were given by Farooq and Malik [26]. Bounds, either upper or lower, on the connective eccentricity index in terms of some graph invariants and the maximal connective eccentricity index of the cactus on n-vertices with k cycles were studied by Yu [39]. Wang [34] demonstrated a lower bound for graphs of given order and clique number. For any tree with a given order and matching number, some lower and upper boundaries on the connective eccentricity index were given by Xu [20]. The eccentricity connective index for each path-thorn graph family was given in [18]. The greatest eccentric distance sum of the extremal trees and graphs and explicit formulae for the values of eccentric distance sum for the Cartesian product characterized by Ili´c [40]. The sharp upper bound on the eccentric connectivity index of graphs with matching numbers that belong to the class of provided vertex connected bipartite graphs determined by Li. Javaid [16].

Motivated by Ashrafi et.al's [1] definition for Zagreb coindices, Hua and Miao [17] consider the total eccentricity sum of all non-adjacent vertex pairs, similar to Ashrafi [1] definition for Zagreb coindices, they call this new eccentricity based graph invariant the eccentric connectivity coindex defined as

$$ECCI(G) = \sum_{uv \notin E(G)} (ecc_G(u) + ecc_G(v))$$

They studied the extremal problems of ECCI for connected graphs of given order. Additionally, they explored ECCI in trees, unicyclic graphs, bipartite graphs with cycles, and triangle-free graphs of a given order. Moreover, they established various lower bounds for ECCI in terms of several other graph parameters. The eccentric connectivity coindex under graph operations was presented by Mahedieh [4], for the eccentric connectivity coindex of a number of graph operations, including sum, disjunction, symmetric difference, lexicographic product, generalized hierachial product, cartesion product, rooted product, corona product, and strong product, he provided precise formulae or sharp lower bounds. Again the eccentric connectivity coindex in graph presented by Hogzhuan Wang,Xianhao Shi and Ber-Linyu [15] they presented the sharp lower bound on ECCI for general connected graph and they identified the cacti with the smallest eccentric connectivity coindex for a given order and several cycles. They also aimed to characterize the graph with the minimum and maximum eccentric connectivity coindex among all trees with a specified order and diameter. Additionally, they determined the smallest eccentric connectivity coindex for unicyclic graphs with a given order and diameter, and described the corresponding extremal graph. Bipartite graphs' eccentric connectivity coindex was presented by Tomáš Vetríc, Mesfin Masre, and Selvaraj Balachandran [30]. They introduced extremal graphs and provided lower bounds on the eccentric connectivity and connectivity coindex for bipartite graphs of given order and vertex connectivity, order matching number, and odd diameter.

The structure of this thesis is as follows. In Chapter 2, we collect relevant results concerning graph theoretical terms and eccentric-based topological indices. In Chapter 3, we explore the eccentric connectivity coindex of graphs in terms of different parameters. In Chapter 4, we explore the general eccentric connectivity coindex of trees of a given graph parameters. In Chapter 5, we give conclusions and future works.

Chapter 2

Eccentric Connectivity Coindex of Trees and Unicyclic Graph

In this chapter, we will discuss the extremal value of the eccentric connectivity coindex of a tree and unicyclic graph by using different graph parameters and different operations and visualize the extremal graphs.

2.1 Trees of a given order

Corollary 2.1. *[17] Let T be a tree of order n. Then*

$$ECCI(T) \geq 2n^2 - 6n + 4$$

with equality if and only if $T \cong S_n$.

Theorem 2.1. *[15] Let T be a tree on n vertices. Then*

$$2n^2 - 6n + 4 \leq ECCI(T) \leq f_2(n, n-1)$$

For $d = n-1$, where

$$f_2(n,d) = \begin{cases} \sum_{i=1}^{\frac{d}{2}-1}(d-i)(2n-6) + \frac{6d^2-3nd+2n^2d-2nd^2+2n-2-7d}{2} & \text{if } n \text{ is even}, \\ \sum_{i=1}^{\frac{d-1}{2}}(d-i)(2n-6) + 3d^2 - 2nd + n^2d - nd^2 + n - 1 - 2d & \text{if } n \text{ is odd}, \end{cases}$$

The left equality holds if and only if $T \cong S_n$ and the right equality holds if and only if $T \cong P_n$.

2.2 Trees of given order and diameter

In this section, we shall determine the tree of diameter d with the minimum and maximum *ECCI* respectively.

The graph generated by joining a vertex in S to the central vertex of P_{d+1}, given a path P_{d+1} and a set S of $n-d-1$ vertices, is called the volcano graph $V_{n,d}$. It follows that P_{d+1} has a single center if d is even (see Figure 2.1). P_{d+1} has two central vertices if d is odd (see Figure 2.2). [15]

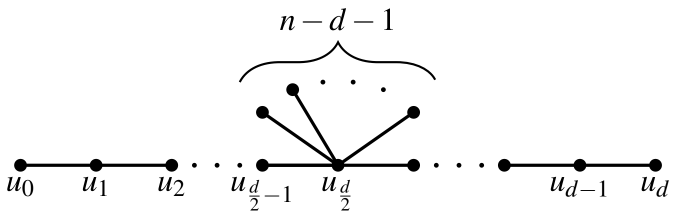

Figure 2.1: $V_{n,d}$

d is even

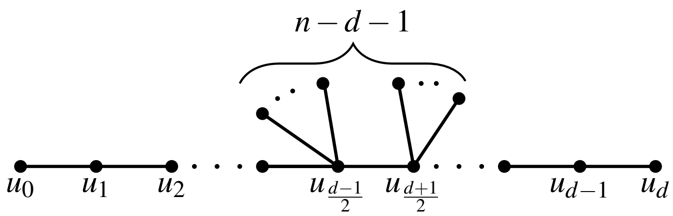

Figure 2.2: $V_{n,d}$

d is odd

Let

$$f_1(n,d) = \begin{cases} \sum_{i=1}^{\frac{d}{2}-1}(d-i)(2n-6) + \frac{n^2d-nd^2-nd+2n^2-6n-4d+3d^2+4}{2} & \text{if } n \text{ is even,} \\ \sum_{i=1}^{\frac{d-1}{2}-1}(d-i)(2n-6) + \frac{n^2d-nd^2+3nd-8n+3d^2-4d+1}{2} & \text{if } n \text{ is odd,} \end{cases}$$

Theorem 2.2. *[15] Let T be a tree on $n \geq 5$ vertices with diameter $d \geq 2$.Then*

$$ECCI(T) \geq f_1(n,d)$$

The equality holds if and only if $T \cong V_{n,d}$.

By attaching the two star centers, $K_{1,p}$ and $K_{1,q}$, to the ends of path P_{d-2}, where $p+q=n-d-1$, we can obtain a double star-like tree, which we indicate by $H(p,n,q)$. The broom graph $B_{n,d}$ is made up of a path P_{d-1} and $n-d$ pendent vertices that are all adjacent to the same pendent vertex of P_{d-1}. It is clear that $B_{n,d}=H(0,n,n-d-1)$; for further information, see Figures 2.3 and 2.4. According to [15]

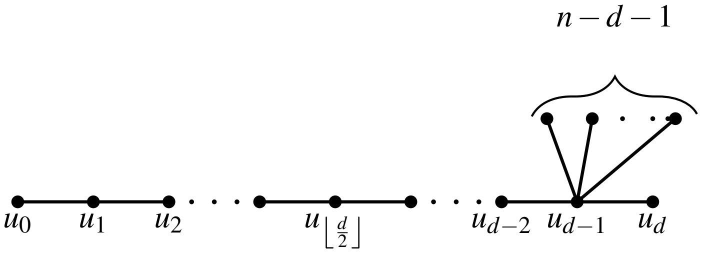

Figure 2.3: $B_{n,d}$

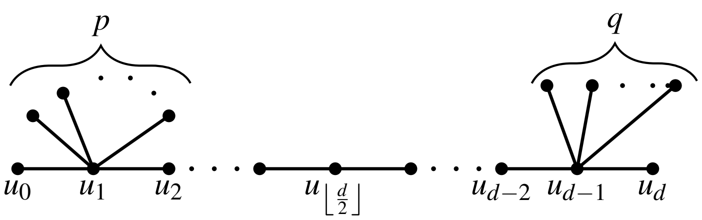

Figure 2.4: $H(p,n,q)$

For any tree $T \in H(p,n,q)$, we have $ECCI(T)=ECCI(B_{n,d})=f_2(n,d)$. Let

$$f_2(n,d)=\begin{cases} \sum_{i=1}^{\frac{d}{2}-1}(d-i)(2n-6)+\frac{6d^2-3nd+2n^2d-2nd^2+2n-2-7d}{2} & \text{if n is even,} \\ \sum_{i=1}^{\frac{d-1}{2}}(d-i)(2n-6)+3d^2-2nd+n^2d-nd^2+n-1-2d & \text{if n is odd,} \end{cases}$$

Theorem 2.3. *[15] If T is a tree of order n and diameter d,then*

$$ECCI(T) \le f_2(n,d)$$

The equality holds if and only if $T \cong H(p,n,q)$.

2.3 Unicyclic graph of a given order and diameter

In this section, we consider the minimum *ECCI* of unicyclic graphs with given diameter. The unicyclic graph with order n and diameter d is denoted by G_n^d. In order to create $V_{n,d}^1$ for an even d, we first need to construct the graph $P_{d+1} = u_0u_1...u_d$. This graph is then constructed by connecting $n-d-1$ pendant edges to $u_{\frac{d}{2}}$ and adding an edge between $u_{\frac{d}{2}+1}$ and one of the pendant vertices attached to $u_{\frac{d}{2}}$. The graph $V_{n,d}^2$ is formed from $P_{d+1} = u_0u_1 \ldots u_d$ by attaching $n-d-1$ pendant edges to $u_{\frac{d}{2}}$ and adding an edge between two of the pendant vertices connected to $u_{\frac{d}{2}}$ (see Figure).

Consider $V_{n,d}^3$ as the unicyclic graphs for odd d, characterized by s and t pendant vertices (where $s+t = n-d-2$) adjacent to $u_{\frac{d-1}{2}}$ and $u_{\frac{d+1}{2}}$ on the diametral path, respectively. Similarly, let $V_{n,d}^4$ denote the unicyclic graphs with p and q pendant vertices (where $p+q = n-d-3$) attached to $u_{\frac{d-1}{2}}$ and $u_{\frac{d+1}{2}}$ on the diametral path, respectively (see Figure).

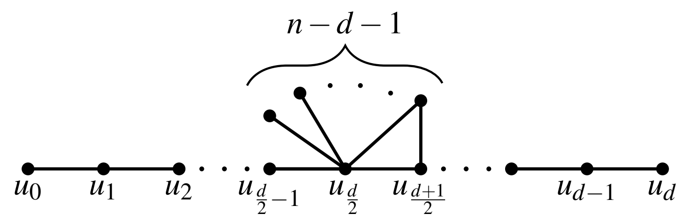

Figure 2.5: $V_{n,d}^1$ (when d is even)

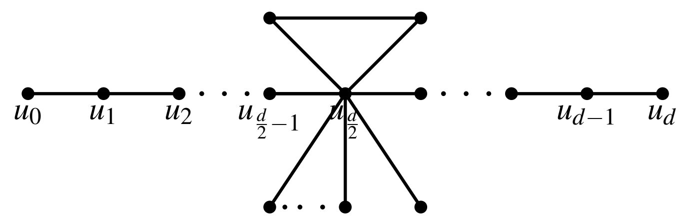

Figure 2.6: $V_{n,d}^2$ (when d is even)

By direct calculation, for even d,

$$ECCI(V_{n,d}^1) = ECCI(V_{n,d}^2) = \sum_{i=1}^{\frac{d}{2}-1} (d-i)(2n-6) + 2d(n-2) + \frac{d(d-2)}{2} + \frac{(d+2)((n-2)(n-d)-n)}{2}$$

For odd d , any $G \in V_{n,d}^3$ we have,

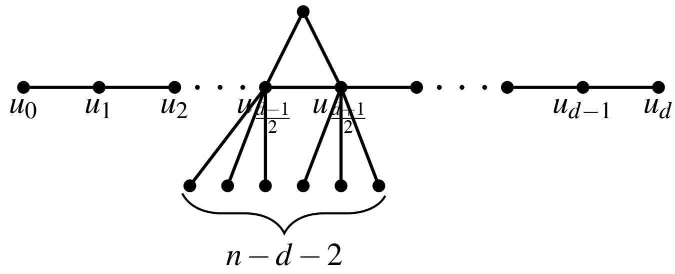

Figure 2.7: $V^3_{n,d}$ (when d is odd)

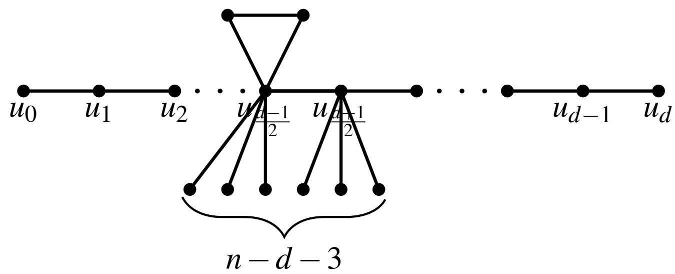

Figure 2.8: $V^4_{n,d}$ (when d is odd)

$$ECCI(G) = \sum_{i=1}^{\frac{d-1}{2}-1} (d-i)(2n-6) + 2d(n-2) + \frac{(d+1)(2n+d-9)}{2} + \frac{(n-2)(d+3)(n-d-2)}{2}.$$

If $G_1 \in V^3_{n,d}$ and $G_2 \in V^4_{n,d}$. By direct calculation, $ECCI(G_1) < ECCI(G_2)$. Let

$$f_3(n,d) = \begin{cases} \sum_{i=1}^{\frac{d}{2}-1} (d-i)(2n-6) + \frac{3d^2-6d+n^2d-nd^2+2n^2-6n-nd}{2} & \text{if n is even,} \\ \sum_{i=1}^{\frac{d-1}{2}-1} (d-i)(2n-6) + \frac{3d^2-nd-6d-10n+n^2d-nd^2+3n^2+3}{2} & \text{if } n \text{ is odd,} \end{cases}$$

Theorem 2.4. *[15] Let G be a unicyclic graph on $n \geq 7$ vertices with diameter $d \geq 2$. Then*

$$ECCI(G) \geq f_3(n,d)$$

The equality holds if and only if $G \cong V^1_{n,d}$ or $G \cong V^2_{n,d}$ for even d and $G \cong V^3_{n,d}$ for odd.

Corollary 2.2. *[17] Let G be a unicyclic graph of order n. Then,*

$$ECCI(G) \geq 2n^2 - 6n$$

with equality if and only if $G \cong S^3_n$, where S^3_n is the graph obtained by introducing an edge *between two pendent vertices of the star S_n.*

Chapter 3

Eccentric Connectivity Coindex of General Graphs

In this chapter, we characterize extremal graphs among all connected graphs with the maximum and minimum eccentric connectivity coindex of general graphs of a given graph parameters.

3.1 Connected Graphs with Given Parameters

In [17], the authors identified the extremal graphs having the maximum and minimum eccentric connectivity coindex among all connected graphs of order n.

Theorem 3.1. *[17] Among all connected graphs of order n, the graphs with the minimum and maximum ECCI are K_n and P_n, respectively.*

Theorem 3.2. *[17] Let G be a connected graph of order n, size m and diameter d. Then*

$$ECCI(G) \geq 2n(n-1) - 4m$$

with equality if and only if $d \leq 2$.

Corollary 3.1. *[17] Let G be a cycle-containing bipartite graph of order n. Then,*

$$ECCI(G) \geq \begin{cases} n^2 - 2n + 1 & \text{if } n \text{ is odd,} \\ n^2 - 2n & \text{if } n \text{ is even.} \end{cases}$$

Each of above equalities holds if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

Theorem 3.3. *[17] Let G be a connected graph of order n with p pendent vertices. Then,*

$$ECCI(G) \geq 4np - 6p - 2p^2$$

with equality if and only if $G \cong K_n^p$

Theorem 3.4. *[17] Let G be a connected graph of order n with independence number* α*. Then,*

$$ECCI(G) \leq 2\alpha^2 - 2\alpha$$

with equality if and only if $G \cong \alpha K_1 \vee K_{n-\alpha}$

Lemma 3.1. *[17] Suppose that G is a graph of order n with matching number* β*. Then,*

$$n - 2\beta = max\{o(G-S) - |s| :\subseteq V(G)\},$$

where $o(G)$ *denotes the number of odd components in G.*

Theorem 3.5. *[17] Let G be a connected graph of order n with matching number* $\beta \leq 1$*.*

1. *If* $\beta = \lceil \frac{n}{2} \rceil$*, then*

$$ECCI(G) \geq 0$$

   with equality if and only if $G \cong K_n$.

2. *If* $1 \leq \beta < \lceil \frac{n}{2} \rceil$ *, then*

$$ECCI(G) \geq 2n^2 - 4n\beta + 2\beta^2 - 2n + 2\beta$$

with equality if and only if $G \cong K_\beta \vee (n-\beta)K_1$

Theorem 3.6. *[15] Let* $G(\neq K_n)$ *be a connected graph of order n with minimum degree* γ*. Then*

$$ECCI(G) \geq 4(n-1-\gamma)$$

with equality if and only if $G \cong K_n^\gamma(\gamma < n-1)$*. Where* K_n^γ *is a connected graph of order n obtained by joining a vertex to the* γ *vertices in* K_{n-1}*.*

Theorem 3.7. *[30] Let G be any connected bipartite graph with n vertices and matching number q, where* $2 \leq q \leq \lceil \frac{n}{2} \rceil$*. Then*

$$ECCI(G) \geq 2[q(q-1)+(n-q)(n-q-1)]$$

with equality if only if G is $K_{q,n-q}$

3.2 Eccentric connectivity coindex under graph operations

In this section, we will examine the behavior of the eccentric connectivity coindex across various graph operations [4].

The complement of G, denoted by $\overline{G}$. For two graphs, G_1 and G_2, the numbers n_i and m_i represent the vertices and edges of G_i, respectively, and $\overline{m_i}$ denotes the number of edges in $\overline{G_i}$, where $i = 1,2$. $\tau(G)$ represents the overall eccentricity of G, which is the sum of the eccentricities of all of its vertices.

Theorem 3.8. *(Sum) The eccentric connectivity coindex of* $G_1 + G_2$ *is given by*

$$ECCI(G_1+G_2) = 4(\overline{m_1}+\overline{m_2}).$$

Theorem 3.9. *(Disjunction) The eccentric connectivity coindex of* $G_1 \vee G_2$ *is given by*

$$ECCI(G_1 \vee G_2) = 4(n_1\overline{m_2}+n_2\overline{m_1}+2\overline{m_1}\,\overline{m_2}).$$

Theorem 3.10. *(Symmetric difference) The eccentric connectivity coindex of* $G_1 \oplus G_2$ *is* *given by*

$$ECCI(G_1 \oplus G_2) = 4(n_1\overline{m_2} + n_2\overline{m_1} + 2\overline{m_1}\overline{m_2} + 2m_1m_2).$$

Theorem 3.11. *(Lexicographic product) The eccentric connectivity coindex of $G_1[G_2]$ is given by*

$$ECCI(G_1[G_2]) = n_2 EccI(G_1) + 2\overline{m_2}(n_{n_1-1}(G_1) + \tau(G_1)).$$

Corollary 3.2. *(Cartesian product) The eccentric connectivity coindex of $G_1 \Box G_2$ is given by*

$$ECCI(G_1 \Box G_2) = n_2 ECCI(G_1) + n_1 ECCI(G_2) + 2(n_1\tbinom{n_2}{2} - m_2)\tau(G_1) + 2(n_2\tbinom{n_1}{2} - m_1)\tau(G_2).$$

Corollary 3.3. *(Rooted product) Let G_2 be a nontrivial rooted graph and let w denote its root vertex. The eccentric connectivity coindex of $G_1\{G_2\}$ is given by*

$$\begin{aligned} ECCI(G_1\{G_2\}) &= ECCI(G_1) + [(n_2-1)(n_1n_2+n_1-1) - 2m_2]\tau(G_1) + 2n_2\tbinom{n_1}{2}D_{G_2}(w) \\ &+ 2ecc_{G_2}(w)[n_2^2\tbinom{n_1}{2} + n_1\overline{m_2} - m_1] + n_1 ECCI(w). \end{aligned}$$

Corollary 3.4. *(Corona product) The eccentric connectivity coindex of $G_1 \circ G_2$ is given by*

$$ECCI(G_1 \circ G_2) = ECCI(G_1) + (n_1n_2^2 + 2n_1n_2 - 3n_2 - 2m_2)\tau(G_1) + 2[(n_2+1)(2n_2+1)\tbinom{n_1}{2} + 2n_1\overline{m_2} - m_1].$$

Chapter 4

General Eccentric Connectivity Coindex of Trees

In this chapter, we study the main results of this thesis. We define the general eccentric connectivity coindex of a connected graph G as

$$ECCI(G)_a = \sum_{v \in V(G)} ecc_G^a [|V(G)| - 1 - d_G(v)]$$

for $a \in \mathbb{R}$, where $E(G)$ is the edge set of graph G, $d_G(v)$ is the degree of vertex v and $V(G)$ is the vertex set of graph G.

We study, the general eccentric connectivity coindex of tree graphs of a given graph parameters. We determine trees with the maximum and minimum general eccentric connectivity coindex among all trees with given parameters.

4.1 Trees of a given order

This section determines the tree graph of order n with the minimum general ECCI among all trees of n order, given $a > 1$.

The following Lemma is applied in the proofs of our main results.

Lemma 4.1. *[32] Let* $1 \leq x < y$ *and* $c > 0$. *For* $a > 1$ *or* $a < 0$, *we have*

$$(x+c)^a - x^a < (y+c)^a - y^a.$$

If $0 < a < 1$, *then*

$$(x+c)^a - x^a > (y+c)^a - y^a.$$

Theorem 4.1. *Let T be a tree of order n. Then for $a > 1$*

$$ECCI_a(S_n) \leq ECCI_a(T)$$

the equality holds if and only if T is S_n

Proof. Let T' be a tree with the smallest $ECCI_a$ among trees with n vertices. We prove that T' is star (S_n). On the contrary, suppose that T' is not a star. Let $u_0u_1 \dots u_d$ be diametral path in T'. Clearly $d \geq 3$. Let $d_{T'}(u_1) = p$ and $d_{T'}(u_{d-1}) = q$. It is possible to assume that $p \leq q$ without loss of generality. Let us assume that $E(T'') = \{u_0u_{d-1}\} \cup E(T') \setminus \{u_0u_1\}$ and that $V(T'') = V(T')$. Then $d_{T''}(u_1) = p-1$, $d_{T''}(u_{d-1}) = q+1$, $ecc_{T'}(u_1) = d-1$, $ecc_{T''}(u_1) = d-1$, $ecc_{T'}(u_{d-1}) = d-1$, $d-2 \leq ecc_{T''}(u_{d-1}) \leq d-1$, $ecc_{T'}(u_0) = d$, $ecc_{T''}(u_0) = ecc_{T''}(u_{d-1}) + 1 \geq d-1$, $d_{T'}(u_0) = 1 = d_{T''}(u_0)$. For all $y \in V(T') \backslash \{u_1, u_{d-1}\}$, $d_{T'}(y) = d_{T''}(y)$ and $ecc_{T'}(y) \geq ecc_{T''}(y)$. Thus

$$\begin{aligned}
ECCI_a(T') - ECCI_a(T'') &\geq ecc^a_{T'}(u_1)(n-1-d_{T'}(u_1)) - ecc^a_{T''}(u_1)(n-1-d_{T''}(u_1)) \\
&+ ecc^a_{T'}(u_{d-1})(n-1-d_{T'}(u_{d-1})) - ecc^a_{T''}(u_{d-1})(n-1-d_{T''}(u_{d-1})) \\
&\geq (d-1)^a(n-1-p) - (d-1)^a(n-p) + (d-1)^a(n-1-q) - (d-1)^a(n-q-2) \\
&+ d^a(n-1-1) - (d-1)^a(n-1-1) \\
&\geq (d-1)^a[n-1-p-n+p+n-1-q-n+q+2-n+2] + d^a(n-2) \\
&\geq (d-1)^a(2-n) + d^a(n-2) \\
&\geq (n-2)[d^a - (d-1)^a] \\
&> 0.
\end{aligned}$$

So $ECCI_a(T') > ECCI_a(T'')$, which is a contradiction. Therefore, S_n is the tree with the smallest $ECCI_a$. □

4.2 Trees of given order and diameter

This section presents bounds on the general eccentric connectivity coindex for trees with n vertices and diameter d.

Let $\mathbb{T}_{n,d}$ be set of trees of order n and diameter d obtaining from the path $v_0v_1v_2\dots v_d$ by attaching all the other $n-d-1$ vertices at v_1 or v_{d-1}. We can easily show that all the trees in $T_{n,d}$ have the same general eccentric connectivity coindex. Let $B_{n,d}$ be a tree in $\mathbb{T}_{n,d}$.

Theorem 4.2. *Let T be a tree of order $n\geq 5$ with diameter d. Then for $a>1$, we have*

$$ECCI_a(T)\leq ECCI_a(B_{n,d}),$$

the equality holds if and only if T is in $\mathbb{T}_{n,d}$.

Proof. Let T be a tree with the largest $ECCI_a$ among trees with a given order and diameter we want to show that T is $B_{n,d}$. Let $P=u_0u_1\dots u_d$ be a diametral path in T. Assume T is not the graph $B_{n,d}$, then there exists a pendant vertex v of T, $v\neq u_0,u_d$ in which the vertex u, where $u\neq u_{d-1}$ and $u\neq u_1$, is adjacent to v. Let $v_1,v_2,\dots,v_k$ represent the set of pendant vertices adjacent to u, where $v_i\neq u_0,u_d$ for $i=1,2,\dots,k$.

Suppose $T'=T-\{uv_1,uv_2,\dots,uv_k\}+\{u_{d-1}v_1,u_{d-1}v_2,\dots,u_{d-1}v_k\}$. Clearly, T and T' have an equal number of vertices and the same diameter.

Let $d_T(u_{d-1})=r\geq 2$. Then $d_{T'}(u_{d-1})=r+k$ and $d_{T'}(x)=d_T(x)$, for all $x\in V(T)\setminus\{u,u_{d-1}\}$. We have $ecc_{T'}(v_i)>ecc_T(v_i)$, $ecc_{T'}(u)=ecc_T(u)<ecc_{T'}(u_{d-1})=ecc_T(u_{d-1})$. Let us consider two cases.

Case 1: u lies on the path P. In this case, $d_T(u)=k+2\geq 3$ and $d_{T'}(u)=2$. Thus

$$\begin{aligned}
ECCI_a(T')-ECCI_a(T) &= \sum_{i=1}^{k} ecc^a_{T'}(v_i)(n-1-d_{T'}(v_i))-\sum_{i=1}^{k} ecc^a_T(v_i)(n-1-d_T(v_i))\\
&+ecc^a_{T'}(u)(n-1-d_{T'}(u))-ecc^a_T(u)(n-1-d_T(u))\\
&+ecc^a_{T'}(u_{d-1})(n-1-d_{T'}(u_{d-1})-ecc^a_T(u_{d-1})(n-1-d_{u_{d-1}})\\
&=k(n-2)[ecc^a_{T'}(v_i)-ecc^a_T(v_i)]+ecc^a_T(u)(n-3)-ecc^a_T(u)(n-k-3)\\
&+ecc^a_{T'}(u_{d-1})(n-1-r-k)-ecc^a_{T'}(u_{d-1})(n-1-r)\\
&=k(n-2)[ecc^a_{T'}(v_i)-ecc^a_T(v_i)]+ecc^a_T(u)[n-3-n+k+3]\\
&+ecc^a_{T'}(u_{d-1})[n-1-r-k-n+1+r]\\
&\geq k(n-2)[ecc^a_{T'}(v_i)-ecc^a_T(v_i)]-k[ecc^a_{T'}(u_{d-1})-ecc^a_T(u)]\\
&=k(n-2)[(1+ecc_{T'}(u_{d-1}))^a-(1+ecc_T(u))^a]-k[ecc^a_{T'}(u_{d-1})-ecc^a_T(u)]\\
&>k[(1+ecc_{T'}(u_{d-1}))^a-(1+ecc_T(u))^a]-k[ecc^a_{T'}(u_{d-1})-ecc^a_T(u)]\\
&=k[(1+ecc_{T'}(u_{d-1}))^a-ecc^a_{T'}(u_{d-1})+ecc^a_T(u)-(1+ecc_T(u))^a]\\
&>0,
\end{aligned}$$

by Lemma 4.1. We have $ECCI_a(T') > ECCI_a(T)$, which is a contradiction.

Case 2: u is not on the path P. In this case $d_T(u) = k+1$ and $d_{T'}(u) = 1$. Thus

$$
\begin{aligned}
ECCI_a(T') - ECCI_a(T) &= \sum_{i=1}^{k} ecc^a_{T'}(v_i)(n-1-d_{T'}(v_i)) - \sum_{i=1}^{k} ecc^a_{T}(v_i)(n-1-d_{T}(v_i)) \\
&+ ecc^a_{T'}(u)(n-1-d_{T'}(u)) - ecc^a_{T}(u)(n-1-d_{T}(u)) \\
&+ ecc^a_{T'}(u_{d-1})(n-1-d_{T'}(u_{d-1}) - ecc^a_{T}(u_{d-1})(n-1-d_{u_{d-1}}) \\
&= k(n-2)[ecc^a_{T'}(v_i) - ecc^a_{T}(v_i)] + ecc^a_{T'}(u)(n-2) - ecc^a_{T}(u)(n-k-2) \\
&+ ecc^a_{T'}(u_{d-1})(n-1-r-k) - ecc^a_{T'}(u_{d-1})(n-1-r) \\
&\geq k(n-2)[ecc^a_{T'}(v_i) - ecc^a_{T}(v_i)] + ecc^a_{T'}(u)[n-2-n+k+2] \\
&+ ecc^a_{T'}(u_{d-1})[n-1-r-k-n+1+r] \\
&= k(n-2)[ecc^a_{T'}(v_i) - ecc^a_{T}(v_i)] + k[ecc^a_{T'}(u) - ecc^a_{T'}(u_{d-1}] \\
&> k[(1+ecc_{T'}(u_{d-1}))^a - (1+ecc_T(u))^a] + k[ecc^a_{T'}(u) - ecc^a_{T'}(u_{d-1})] \\
&= k[(1+ecc_{T'}(u_{d-1}))^a - ecc^a_{T'}(u_{d-1}) + ecc^a_{T}(u) - (1+ecc_T(u))^a] \\
&> 0,
\end{aligned}
$$

by Lemma 4.1. We have $ECCI_a(T') > ECCI_a(T)$, which is also a contradiction. Thus the extremal tree is in $\mathbb{T}_{n,d}$. $\square$

Let $\mathbb{L}_{n,d}$ be set of trees of order n and diameter d obtaining from the path $v_0v_1v_2\ldots v_d$ by attaching all the other $n-d-1$ vertices at $v_{\lfloor \frac{d}{2} \rfloor}$ or $v_{\lceil \frac{d}{2} \rceil}$. Let $V_{n,d}$ be a tree in $\mathbb{L}_{n,d}$. We can easily show that all the trees in $\mathbb{L}_{n,d}$ have the same general eccentric connectivity coindex. If d is even, then $V_{n,d}$ is the only tree in $\mathbb{L}_{n,d}$.

Theorem 4.3. *Let T be any tree of order n and diameter d, for $3 \leq d \leq n-2$. Then for $a > 1$, we have*

$$ECCI_a(T) \geq ECCI_a(V_{n,d}),$$

the equality holds if and only if T is in $\mathbb{L}_{n,d}$.

Proof. Let T' be a tree having the smallest general eccentric connectivity coindex among trees with n vertices and diameter d, we will prove by contradiction that T' is the tree $V_{n,d}$.

Consider a tree $T'_{n,d}$ with order n and diameter d and assume that for certain values of n and d, the condition $ECCI_a(T'_{n,d}) \leq ECCI_a(V_{n,d})$ holds , where $T'_{n,d}$ is not $V_{n,d}$. Let $T'_{n^*,d}$ be a tree with the smallest possible order n^* such that $ECCI_a(T'_{n^*,d}) \leq ECCI_a(V_{n^*,d})$.

Let $u_0u_1\dots u_d$ be a diametral path in $T'_{n^*,d}$. Then $T'_{n^*,d}$ contain a pendant vertex, say v such that $v \notin \{u_0, u_d\}$. We refer to the vertex connected to v in $T'_{n^*,d}$ as z.

Let $V(T'_{n^*-1,d}) = V(T'_{n^*,d})\backslash\{v\}$ and $E(T'_{n^*-1,d}) = E(T'_{n^*,d})\backslash\{vz\}$. Then $T'_{n^*-1,d}$ is a tree order n^*-1 and diameter d. Let $d_{T'_{n^*,d}}(z) = p$, $2 \le p \le n^*-d+1$. We have $d_{T'_{n^*-1,d}}(z) = p-1$, $d_{T'_{n^*,d}}(v) = 1$ and $d_{T'_{n^*,d}}(x) = d_{T'_{n^*-1,d}}(x)$ for all $x \in V(T'_{n^*,d})\backslash\{v,z\}$ we also know that $ecc_{T'_{n^*,d}}(v) \ge \lceil \frac{d}{2} \rceil + 1, ecc_{T'_{n^*-1,d}}(z) = ecc_{T'_{n^*,d}}(z) \ge \lceil \frac{d}{2} \rceil$ and $ecc_{T'_{n^*-1,d}}(x) = ecc_{T'_{n^*,d}}(x)$ for $x \in V(T'_{n^*,d})\backslash\{v,z\}$.

Thus

$$\begin{aligned}
ECCI_a(T'_{n^*,d}) - ECCI_a(T'_{n^*-1,d}) &\ge ecc^a_{T'_{n^*,d}}(v)(n^*-1-d_{T'_{n^*,d}}(v)) + ecc^a_{T'_{n^*,d}}(z)(n^*-1-d_{T'_{n^*,d}}(z)) \\
&\quad - ecc^a_{T'_{n^*-1,d}}(z)((n^*-1)-1-d_{T'_{n^*-1,d}}(z)) \\
&\ge \left(\left\lceil \frac{d}{2} \right\rceil + 1\right)^a (n^*-2) + \left\lceil \frac{d}{2} \right\rceil^a (n^*-1-p) - \left\lceil \frac{d}{2} \right\rceil^a ((n^*-1)-1-p+1) \\
&\ge \left(\left\lceil \frac{d}{2} \right\rceil + 1\right)^a (n^*-2) + \left\lceil \frac{d}{2} \right\rceil^a (n^*-1-p-n^*+1+p) \\
&\ge \left(\left\lceil \frac{d}{2} \right\rceil + 1\right)^a (n^*-2).
\end{aligned}$$

Since $T'_{n^*,d}$ is a tree with the smallest possible order n^* such that $ECCI_a(T'_{n^*,d}) \le ECCI_a(V_{n^*,d})$, we obtain $ECCI_a(T'_{n^*-1,d}) > ECCI_a(V_{n^*-1,d})$ which implies that

$$ECCI_a(T'_{n^*,d}) - ECCI_a(T'_{n^*-1,d}) < ECCI_a(V_{n^*,d}) - ECCI_a(V_{n^*-1,d}).$$

Let's calculate the value of, $ECCI_a(V_{n^*,d}) - ECCI_a(V_{n^*-1,d})$.

$$\begin{aligned}
ECCI_a(V_{n^*,d}) - ECCI_a(V_{n^*-1,d}) &= \left\lceil \frac{d}{2} \right\rceil^a (n^*-1-(n^*-d+1)) - \left\lceil \frac{d}{2} \right\rceil^a ((n^*-1)-1-(n^*+d)) \\
&\quad + \left(\left\lceil \frac{d}{2} \right\rceil + 1\right)^a (n^*-2) \\
&= \left\lceil \frac{d}{2} \right\rceil^a (d-2) - \left\lceil \frac{d}{2} \right\rceil^a (d-2) + \left(\left\lceil \frac{d}{2} \right\rceil + 1\right)^a (n^*-2) \\
&= \left(\left\lceil \frac{d}{2} \right\rceil + 1\right)^a (n^*-2).
\end{aligned}$$

Since $ECCI_a(T'_{n^*,d}) - ECCI_a(T'_{n^*-1,d}) < ECCI_a(V_{n^*,d}) - ECCI_a(V_{n^*-1,d})$, we have $\left(\lceil \frac{d}{2} \rceil + 1\right)^a (n^*-2) < \left(\lceil \frac{d}{2} \rceil + 1\right)^a (n^*-2)$, which is contradiction. Hence the proof is done. Thus the extremal tree is in $\mathbb{L}_{n,d}$.

□

4.3 Trees of given order and number of pendant vertices

In section, we examine the limits on the general eccentric connectivity index for trees with n vertices and p pendant vertices. Obviously, $2 \leq p \leq n-1$.

Let $\mathbb{K}_{n,p}$ be set of trees of order n and p pendant vertices obtaining from the path $u_0u_1u_2\ldots u_{n-p+1}$ by attaching all the other $p-2$ pendant vertices at u_{n-p} or u_1. We can easily show that all the trees in $\mathbb{K}_{n,p}$ have the same general eccentric connectivity coindex. Let $X_{n,p}$ be a tree in $\mathbb{K}_{n,p}$.

Theorem 4.4. *Let T be any tree having order $n \geq 4$ and p pendant vertices. Then for $a > 1$,*

$$ECCI_a(T) \leq ECCI_a(X_{n,p}),$$

the equality holds if and only if T is in $\mathbb{K}_{n,p}$.

Proof. We are aware that P_n is the only tree with 2 pendant vertices, and S_n is the only tree with $n-1$ pendant vertices. Consequently, $3 \leq p \leq n-2$ can be assumed.

Let T be a tree with the largest $ECCI_a$ among trees with a given order n and p pendant vertices we want to show that T is $X_{n,p}$. Let $P = u_0u_1\ldots u_d$ be a diametral path in T. Assume that T is not the graph $X_{n,p}$, then there exist a vertex $w \in \{u_2, u_3, \ldots, u_{n-p-1}\}$ of T such that $d(w) \geq 3$. Let $\{w_1, w_2, \ldots, w_k\}$ be the set of vertices not on P which are adjacent to w.

Let $V(T') = V(T)$ and $E(T') = \{u_{d-1}w_1, u_{d-1}w_2, \ldots, u_{d-1}w_k\} \bigcup E(T) \backslash \{ww_1, ww_2, \ldots, ww_k\}$. The number of pendant vertices is the same in both T and T'. We have $d_T(u_{d-1}) = t \geq 2$, $d_T(w) = r = k+2$, for $k \geq 1$. Then $d_{T'}(u_{d-1}) = t+k$, $d_{T'}(w) = 2$ and $d_{T'}(y) = d_T(y)$ for all $y \in V(T) \backslash \{u_{d-1}, w\}$, $d_T(w_i) = d_{T'}(w_i) = 1$, $(i = 1, 2, \ldots, k)$, $ecc_{T'}(w_i) > ecc_T(w_i)$, $ecc_{T'}(w) = ecc_T(w) < ecc_{T'}(u_{d-1}) = ecc_T(u_{d-1})$. It is obvious that $ecc_{T'}(y) \geq ecc_T(y)$ for all $y \in V(T)\backslash\{u_{d-1}, w\}$. Thus

$$
\begin{aligned}
ECCI_a(T') - ECCI_a(T) &= \sum_{i=1}^{k} ecc^a_{T'}(w_i)(n-1-d_{T'}(w_i)) - \sum_{i=1}^{k} ecc^a_T(w_i)(n-1-d_T(w_i)) \\
&+ ecc^a_{T'}(w)(n-1-d_{T'}(w)) - ecc^a_T(w)(n-1-d_T(w)) \\
&+ ecc^a_{T'}(u_{d-1})(n-1-d_{T'}(u_{d-1})) - ecc^a_T(u_{d-1})(n-1-d_T(u_{d-1})) \\
&= k(n-2)(ecc^a_{T'}(w_i) - ecc^a_T(w_i)) + ecc^a_{T'}(w)(n-1-2) \\
&- ecc^a_T(w)(n-1-(k+2)) + ecc^a_{T'}(u_{d-1})(n-1-(t+k)) \\
&- ecc^a_T(u_{d-1})(n-1-t) \\
&= k(n-2)(ecc^a_{T'}(w_i) - ecc^a_T(w_i)) + ecc^a_T(w)(n-3-n+3+k) \\
&+ ecc^a_{T'}(u_{d-1})(n-1-t-k-n+1+t) \\
&> k(ecc^a_{T'}(w_i) - ecc^a_T(w_i)) - k(ecc^a_{T'}(u_{d-1}) - ecc^a_T(w)) \\
&= k((ecc_{T'}(u_{d-1})+1)^a - (ecc_T(w)+1)^a - k(ecc^a_{T'}(u_{d-1}) - ecc^a_T(w)) \\
&= k[(ecc_T(u_{d-1})+1)^a - (ecc_T(w)+1)^a - ecc^a_T(u_{d-1}) + ecc^a_T(w)]. \\
&= k[(ecc_T(u_{d-1})+1)^a - ecc^a_T(u_{d-1}) + ecc^a_T(w) - (ecc_T(w)+1)^a].
\end{aligned}
$$

Since $ecc^a_T(u_{d-1}) > ecc^a_T(w)$ by Lemma 4.1, we have $(ecc_T(u_{d-1})+1)^a - ecc^a_T(u_{d-1}) + ecc^a_T(w) - (ecc_T(w)+1)^a > 0$. This implies that, $ECCI_a(T') > ECCI_a(T)$, which is a contradiction. Therefore, the graphs in $\mathbb{K}_{n,p}$ are trees with the largest general *ECCI* among trees of a given order n and p pendant vertices. □

Let $\mathbb{R}_{n,p}$ be the set of trees of order n and p pendant vertices obtaining from the path $u_0u_1u_2\ldots u_{n-p+1}$ by attaching all the other $p-2$ pendant vertices at $u_{\lfloor \frac{n-p+1}{2} \rfloor}$ or $u_{\lceil \frac{n-p+1}{2} \rceil}$. If $n-p+1$ is even, then $\mathbb{R}_{n,p}$ has only one element. We can easily show that all the trees in $\mathbb{R}_{n,p}$ have the same general eccentric connectivity coindex. Let $Y_{n,p}$ be a tree in $\mathbb{R}_{n,p}$.

Theorem 4.5. *Let T be any tree having order $n \geq 4$ and p pendant vertices. Then for $a > 1$, we have*

$$ECCI_a(T) \geq ECCI_a(Y_{n,p}),$$

equality holds if and only if T is in $\mathbb{R}_{n,p}$.

Proof. P_n is the only tree having 2 pendant vertices, while S_n is the only tree having $n-1$ pendant vertices. Thus, $3 \leq p \leq n-2$ can be assumed.

Let T be a tree with the smallest $ECCI_a$ among trees with a given order n and p pendant vertices we want to show that T is $Y_{n,p}$. Let $P = u_0u_1\ldots u_d$ be diametral path in T. Assume that T is not the graph $Y_{n,p}$, then there exist a vertex $z \in \{u_1, u_2, \dots, u_{d-1}\} - \{u_{\lfloor \frac{d}{2} \rfloor}, u_{\lceil \frac{d}{2} \rceil}\}$ such that $d(z) \geq 3$. Let $\{z_1, z_2, \dots, z_k\}$ be the set of neighbors of z that are not on P.

Let $V(T') = V(T)$ and $E(T') = \{z_1 u_{\lceil \frac{d}{2} \rceil}, z_2 u_{\lceil \frac{d}{2} \rceil} \dots, z_k u_{\lceil \frac{d}{2} \rceil}\} \bigcup E(T) \backslash \{zz_1, zz_2, \dots, zz_k\}$. It is evident that T and T' have the same number of vertices and the same number of pendant vertices. Let $d_T(u_{\lceil \frac{d}{2} \rceil}) = s \geq 2$ and $d_T(z) = k+2 \geq 3$. Then $d_{T'}(u_{\lceil \frac{d}{2} \rceil}) = s+k$, $d_{T'}(z) = 2$ and $d_T(x) = d_{T'}(x)$ for $x \in V(T) \backslash \{u_{\lceil \frac{d}{2} \rceil}, z\}$. $ecc_{T'}(z_i) < ecc_T(z_i)$, $ecc_{T'}(z) = ecc_T(z) > ecc_{T'}(u_{\lceil \frac{d}{2} \rceil}) = ecc_T(u_{\lceil \frac{d}{2} \rceil})$. It is obvious that $ecc_{T'}(x) \leq ecc_T(x)$ for all $x \in V(T) \backslash \{u_{\lceil \frac{d}{2} \rceil}, z\}$. Thus

$$
\begin{aligned}
ECCI_a(T') - ECCI_a(T) = & \sum_{i=1}^{k} ecc^a_{T'}(z_i)(n-1-d_{T'}(z_i)) - \sum_{i=1}^{k} ecc^a_T(z_i)(n-1-d_T(z_i)) \\
& + ecc^a_{T'}(z)(n-1-d_{T'}(z)) - ecc^a_T(z)(n-1-d_T(z)) \\
& + ecc^a_{T'}(u_{\lceil \frac{d}{2} \rceil})(n-1-d_{T'}(u_{\lceil \frac{d}{2} \rceil})) - ecc^a_T(u_{\lceil \frac{d}{2} \rceil})(n-1-d_T(u_{\lceil \frac{d}{2} \rceil})) \\
& = k(n-1-d_T(z_1))(ecc^a_{T'}(z_i) - ecc^a_T(z_i)) + ecc^a_{T'}(z)(n-3) - ecc^a_T(z)(n-1-(k+2) \\
& + ecc^a_{T'}(u_{\lceil \frac{d}{2} \rceil})(n-1-(s+k)) - ecc^a_T(u_{\lceil \frac{d}{2} \rceil})(n-1-s) \\
& < k(n-2)(ecc^a_{T'}(z_i) - ecc^a_T(z_i)) + k(n-2)(ecc^a_T(z) - ecc^a_{T'}(u_{\lceil \frac{d}{2} \rceil})) \\
& = k(n-2)[ecc^a_{T'}(z_i) - ecc^a_T(z_i) + ecc^a_T(z) - ecc^a_{T'}(u_{\lceil \frac{d}{2} \rceil})] \\
& = k(n-2)[(ecc_{T'}(u_{\lceil \frac{d}{2}) \rceil}) + 1)^a - (ecc_T(z)+1)^a + ecc^a_T(z) - ecc^a_{T'}(u_{\lceil \frac{d}{2} \rceil})] \\
& = k(n-2)[(ecc_T(u_{\lceil \frac{d}{2}) \rceil}) + 1)^a - ecc^a_T(u_{\lceil \frac{d}{2} \rceil}) + ecc^a_T(z) - (ecc_T(z)+1)^a].
\end{aligned}
$$

Since $ecc_T(z) > ecc_T(u_{\lceil \frac{d}{2}) \rceil})$, by Lemma 4.1 we have $(ecc_T(u_{\lceil \frac{d}{2} \rceil} + 1)^a - ecc^a_T(u_{\lceil \frac{d}{2} \rceil}) + ecc^a_T(z) - (ecc^a_T(z)+1)^a < 0$. This implies that, $ECCI_a(T') < ECCI_a(T)$, which is a contradiction. Therefore, the graphs in $\mathbb{R}_{n,p}$ are trees with the smallest general $ECCI$ among trees of a given order n and p pendant vertices. □

Chapter 5

Conclusion and Future Work

5.1 Conclusion

In this thesis, we introduced the general eccentric connectivity coindex, $ECCI_a$ of connected graphs. We studied the general eccentric connectivity coindex of tree graphs of given graph parameters. We obtained a lower bound of the general eccentric connectivity coindex of trees of a given order. We obtained also upper and lower bounds of the general eccentric connectivity coindex of trees of a given order and diameter, order and number of pendant vertices for $a > 1$. We determined the extremal graphs which attained the extremal values.

5.2 Future Work

We present many difficult unresolved problems concerning the general eccentric connectivity coindex for general graphs and trees.

1. Find upper bound on $ECCI_a(T)$ for trees T of given order, where $a > 1$.
2. Find lower and upper bounds on $ECCI_a(T)$ for trees T of given order, where $a < 1$.
3. Find lower and upper bounds on $ECCI_a(T)$ for trees T of given order and diameter, where $a < 1$.
4. Find lower and upper bounds on $ECCI_a(G)$ for general connected graphs G of given order and other parameters like diameter, number of pendant vertices for $a \in \mathbb{R}$.

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