EXTREMAL PROBLEMS RELATED TO THE STUDY OF GRAPH INDICES

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Declaration

I, Mesfin Masre Legese, with student ID number GSR/6619/09, hereby declare that this thesis is my own work and that it has not been previously submitted for assessment or completion of any post graduate qualification to another university or for another qualification.

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This is to certify that the thesis prepared by Mesfin Masre Legese, entitled: **Extremal Problems Related to the Study of Graph Indices** submitted in partial fulfillment of the requirements for the Degree of Doctor of Philosophy (in Mathematics) compiles with the regulations of the University and meets the accepted standards with respect to originality and quality.

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Abstract

Molecular descriptors called topological indices are graph invariants that play a significant role in chemistry, materials science, pharmaceutical sciences and engineering, since they can be correlated with a large number of physico-chemical properties of molecules. Topological indices are used in the process of correlating the chemical structures with various characteristics such as boiling points and molar heats of formation. Graph theory is used to characterize these chemical structures.

Binary and m-ary trees have extensive applications in chemistry and computer science, since these trees can represent chemical structures and various useful networks. In this thesis, we present exact values of all important distance-based indices for complete m-ary trees and we introduce the general eccentric connectivity index of a graph G which is defined as, $ECI_\alpha(G) = \sum_{v \in V(G)} ecc_G(v) d_G^\alpha(v)$ for $\alpha \in \mathbb{R}$, where $V(G)$ is the vertex set of G, $ecc_G(v)$ is the eccentricity of v and $d_G(v)$ is the degree of v in G.

The thesis consists of four chapters. In the first chapter we define the standard graph theory concepts, and introduce the distance-based graph invariants called topological indices. We give some background to these mathematical models, and show their applications, which are mainly in chemistry and pharmacology. To complete the chapter we present some known results

which will be relevant to our work.

Chapter 2 focuses on the most common distance-based indices of complete m-ary trees of a given height. We present exact values of all important distance-based indices for complete m-ary trees of a given height. We solve recurrence relations to obtain the value of the most well-known index called the Wiener index. New methods are used to express the other indices (the degree distance, the eccentric distance sum, the Gutman index, the edge-Wiener index, the hyper-Wiener index and the edge-hyper-Wiener index) as well. Values of distance-based indices for complete binary trees are corollaries of the main results.

Chapter 3 focuses on the general eccentric connectivity index of trees. We obtain lower and upper bounds on the general eccentric connectivity index for trees of given order, trees of given order and diameter, and trees of given order and number of pendant vertices. The upper bounds for trees of given order and diameter, and trees of given order and number of pendant vertices hold for $\alpha > 1$. All the other bounds are valid for $0 < \alpha \leq 1$ or $0 < \alpha < 1$. We present all the extremal graphs, which means that our bounds are best possible.

Chapter 4 focuses on the general eccentric connectivity index of unicyclic graphs. We obtain sharp lower and upper bounds on the general eccentric connectivity index for unicyclic graphs of given order, and unicyclic graphs of given order and girth. All the lower bounds are valid for $0 < \alpha < 1$ and all the upper bounds are valid for $0 < \alpha \leq 1$.

We use combinatorial methods, algebraic methods, analytic methods and various graph theoretical techniques, which, in combination with our ideas yield new results.

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Chapter 1

Introduction

In this chapter, we define the standard graph theoretical terms that will be used in the thesis, and introduce a mathematical model called a topological index. We then provide motivation for our work, and also present some relevant background results. Terms not defined in this chapter will be defined in subsequent chapters, as the need arises.

1.1 Graph theory terminology

Definition 1.1.1. A graph G consists of a finite, non-empty set, $V(G)$, of vertices, together with a (possibly empty) set, $E(G)$, of unordered pairs of vertices, called edges. The number of elements in the vertex set $V(G)$ is called the order of G, and the number of elements in the edge set $E(G)$ is called its size. If the order of G is 1, then we say G is trivial; otherwise G is called a nontrivial graph.

For $e \in E(G)$, if edge $e = \{u, v\}$ (or, simply $e = uv$), we say that u and v are adjacent vertices, whereas e is said to be incident with u (or v). We also say that e joins vertices u and v.

Definition 1.1.2. The line graph, $L(G)$, of a graph G is the graph with vertex set $E(G)$ in which $e, f \in E(G)$ are adjacent as vertices in $L(G)$ if and only if they are adjacent as edges in G.

Definition 1.1.3. The degree of a vertex $v \in V(G)$, $d_G(v)$, is the number of vertices (edges) adjacent (incident) to v. When it is obvious that we mean graph G, then we omit G and use $d(v)$. A vertex of degree 1 is called a pendant vertex.

A simple graph of order n in which all distinct pairs of vertices are adjacent is called complete graph and is denoted by K_n.

The neighbours of a vertex $v \in V(G)$ are the vertices adjacent to v. The neighbourhood of a vertex $v \in V(G)$, denoted as $N(v)$, is the set of all vertices which are adjacent to v. So, $d_G(v) = |N(v)|$.

Definition 1.1.4. A subgraph H of a graph G is a graph in which all its vertices belong to $V(G)$ and all its edges belong to $E(G)$. If a subgraph of G contains precisely all the vertices of G, it is called a spanning subgraph of G. For $U \subseteq V(G)$, the induced subgraph of G induced by U, $G[U]$ is the maximal subgraph of G which has vertex set U.

For $W \subseteq V(G), G - W$ denotes the graph obtained from G by deleting the vertices in W together with their incident edges. If $W = \{w\}$, we just write $G - w$ for $G - \{w\}$. For $E' \subseteq E(G), G - E'$ denotes the graph obtained from G by deleting the edges in E'. If $E' = \{uv\}$, we just write $G - uv$ for $G - \{uv\}$. $G + uv$ is obtained from G by adding an edge $uv \notin E(G)$.

A path of order n, $P_n : v_1v_2 \dots v_n$ is a graph with $V(P_n) = \{v_1, v_2, \dots, v_n\}$

and $E(P_n) = \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n\}$. For $n \geq 3$, adding an edge between v_1 and v_n in the path P_n yields a cycle graph of order n, denoted by C_n.

Definition 1.1.5. A graph G is connected if there is at least one path between every pair of vertices; otherwise it is disconnected. Disconnected graphs are thus split up into a number of connected subgraphs, called components. That is, a component of G is a maximal connected subgraph of G.

Definition 1.1.6. A tree is a connected graph with no cycles. In a rooted tree the level of a vertex is its distance from the root. The height of a rooted tree is the length of a longest path starting from the root. For an integer $m \geq 2$, an m-ary tree is a rooted tree in which every vertex has at most m children. A complete m-ary tree is an m-ary tree in which every internal vertex has exactly m children and all leaves have the same level. Note that if $m = 2$, then the complete m-ary tree is called complete binary tree.

Definition 1.1.7. A unicyclic graph is a connected graph containing exactly one cycle. The girth of a unicyclic graph is the length of its cycle.

Definition 1.1.8. The distance between u and v in $V(G)$, $d_G(u, v)$, is the length of a shortest $u - v$ path in G. The eccentricity, $ecc_G(u)$, of a vertex $u \in V(G)$ is the distance between u and a furthest vertex from u. When it is obvious that we mean graph G, then we omit G and use $d(u, v)$ and $ecc(u)$. The diameter of G, is defined as the maximum value of the eccentricities of the vertices of G.

A diametral path is a path between two vertices whose distance is the diameter.

For terms not defined here, the reader is referred to any introductory Graph Theory book, such as [15]. More specialized terminology not presented here will be defined as needed, in the relevant chapter. Throughout this thesis, we will consider a graph which is nontrivial, simple, undirected and connected.

1.2 Topological indices

Graph theory is largely applied to the characterization of chemical structures, as well as to qualitative and quantitative structure-property (QSPR) and structure-activity (QSAR) relations by means of certain numerical characteristics called topological indices.

In chemistry and biology, researchers study molecules with desired physicochemical properties, for example, boiling points, molecular volumes, flavor threshold concentration antiviral activity, energy levels, electronic populations, etc. And these properties can be quantitatively represented by some values of a certain index. The notion of a "topological index" appears first in a paper of the Japanese chemist Hosoya [45], who investigated the surprising relation between the physicochemical properties of a molecule and the number of its independant edge subsets (matchings). A topological index is a map from the set of chemical graphs to the set of real numbers. Therefore a topological index is a numeric quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. Since isomorphic graphs possess identical values for any given topological index, these indices are referred to as graph invariants. The advantage of topological indices is that they may be used directly as simple numerical descriptors in a comparison with physical, chemical, or biological parameters of molecules in quantitative structure-property relationships (QSPR) and in quantitative structure-activity relationships (QSAR).

Topological indices have been extensively studied due to their applications in chemistry, bioinformatics and network science. Over a hundred such distance-based and degree-based indices have been used in the literature [38, 43]. Let us present definitions of well-known distance-based topological indices of graphs.

The oldest of these topological indices, dating back to 1947, is the well-known Wiener index. It was originated by the chemist Harold Wiener [79] during the study on boiling points of paraffin (bi-product of petroleum) and he referred to it as path number, but afterwards the path number was assigned the name of its inventor and entitled as Wiener index or Wiener number.

Definition 1.2.1. The Wiener index of a graph G is defined as,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u,v)$$

and the edge-Wiener index

$$W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d(e,f),$$

where the distance between two edges in a graph G is defined as the distance between their corresponding vertices in the line graph $L(G)$ of G. Thus $W_e(G) = W(L(G))$.

Note that the factor of $\frac{1}{2}$ is required in the second definition of $W(G)$ since each unordered pair $\{u,v\}, u \neq v$, appears twice in $\sum_{u \in V(G)} \sum_{v \in V(G)} d(u,v)$. This pioneering, eminent and well studied index of graph G is a distance-based index. It deserves high rank in theoretical chemistry and chemical graph theory due to its theoretical as well as applicable nature.

A modification of this index is the generalized Wiener index defined as (see [43])

$$W_k(G) = \sum_{\{u,v\} \subseteq V(G)} d^k(u,v),$$

where k is a real number. In particular, for $k = -1$ it is called the reciprocal Wiener index and for $k = -2$ it is the Harary index or Harary number.

With Wiener's discovery of a close correlation between the boiling points of certain alkanes and the sum of the distances between vertices in the graphs representing their molecular structures [79], it became apparent that graph parameters, or topological indices, can potentially be used to predict properties of chemical compounds.

The Wiener index has been investigated in the mathematical, chemical and computer science literature under many different names and with slight differences in the definition, it is sometimes also called the distance or the total distance of a graph.

Definition 1.2.2. The hyper-Wiener index of a graph G is defined as

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

the edge-hyper-Wiener index is

$$WW_e(G) = \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d(e,f) + \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d^2(e,f).$$

The Schultz index includes both distance and degree in its definition. Described as a weighted version of the Wiener index, it was introduced independantly by Dobrynin and Kochetova [27], and Gutman [42], in 1994.

Definition 1.2.3. The Schultz index or degree distance of a graph G is defined as

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} (d(u) + d(v))d(u, v).$$

A related index, which uses the product, rather than the sum of the degrees, is called the Schultz index of the second kind [42], but for which the name Gutman index has also been used [74]. Throughout this thesis, the latter name is used.

Definition 1.2.4. The Gutman index of a graph G is defined as

$$Gut(G) = \sum_{\{u,v\} \subseteq V(G)} d(u)d(v)d(u, v).$$

Recently, some other indices based on eccentricity have been introduced and investigated by mathematicians, chemists and biologists. Here we list the most commonly used eccentricity-based topological indices. We begin with the eccentric connectivity index (ECI), which was put forward by Sharma, Goswami and Madan [70] in 1997. It has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature.

Definition 1.2.5. The eccentric connectivity index of a graph G is defined as

$$ECI(G) = \sum_{v \in V(G)} ecc(v)d(v).$$

Definition 1.2.6. The total eccentricity (see [20]) of a graph G is defined as

$$\zeta(G) = \sum_{v \in V(G)} ecc(v).$$

Definition 1.2.7. The eccentric distance sum (see [40]) of a graph G is defined as

$$EDS(G) = \sum_{v \in V(G)} ecc(v)D(v)$$

where $D(v) = \sum_{u \in V(G)} d(u, v)$.

In this thesis, we introduce the general eccentric connectivity index $ECI_\alpha(G)$ of a graph G.

Definition 1.2.8. The general eccentric connectivity index of a graph G is defined as

$$ECI_\alpha(G) = \sum_{v \in V(G)} ecc(v)d^\alpha(v)$$

for $\alpha \in \mathbb{R}$.

If $\alpha = 1$, we obtain the classical eccentric connectivity index and if $\alpha = 0$ we obtain the total eccentricity index of a graph G.

1.3 Literature review

1.3.1 Motivation

Topological indices have important use in medical, industrial and environmental research. Here we present some background material and give various applications, with emphasis on the Wiener index, eccentric connectivity index, eccentric distance sum, Gutman index and degree distance of a graph.

In chemistry, a molecular graph represents the topology of a molecule, by considering how the atoms are connected. This can be modelled by a graph, where the vertices represent the atoms, and the edges symbolize the covalent bonds between the atoms. Double and triple bonds, if any, are approximated by a single edge in forming the molecular graph. In many studies it is also assumed that, the molecular graphs are hydrogen-suppressed; that is, there will be no vertices corresponding to H-atoms and no edges corresponding to bonds between H-atoms to other atoms. For example, chemists often represent the benzene ring as a simple hexagon.

Chemical graph theory uses topological indices as a powerful tool for establishing relationships between the structure of the molecular graph, and its properties or activities. For instance, structural features such as size, shape, branching, symmetry, bonding patterns and the neighbourhood patterns of atoms in the molecules can be measured by a topological index [12, 14, 30]. The Wiener index has successfully characterized properties such as the boiling point, density, critical pressure, refractive indices, heats of isomerizaton and vaporization of various hydrocarbons [27]. This quantitative relationship between the structure of a molecule and its properties (or activities) is the basis of the so-called quantitative structure versus property (activity) relationship (QSPR, QSAR) studies. Here the term 'property' means physicochemical properties, whereas 'activity' refers to biological and pharmacological activities of the chemical compound [75].

Much recent work in pharmaceutical drug design has focused on identifying properties of chemicals directly from their molecular structure. In pharmaceutical research, both trial and error syntheses of compounds and their random screening for activity are time consuming and uneconomical [38]. So, preliminary investigations using QSAR and QSPR are done to select the most promising compounds for a desired property, and hence decrease the number of compounds which need to be synthesized during the process of designing new drugs [6, 38, 56]. Topological indices are 'one of the oldest and most widely used descriptors in QSAR' [34]. They have many advantages over other descriptors used in QSAR, such as geometrical, electrostatic, steric, electronic and quantum descriptors [38]. Topological indices can be computed easily and rapidly for any known compound, or even one not yet synthesized. Many software programs, such as CODES SA, SciQSAR and POLLY are readily available for both the calculation of the descriptor values, and subsequent multivariate statistical analysis [38, 66]. Furthermore, not only are they powerful tools for drug design and environmental toxicology assessment, but they are also being used for virtual screening, lead optimization, isomer discrimination, chemical documentation and combinatorial library design [30].

Therefore, one of the most interesting problems on topological indices is to study the extremal properties of topological indices and characterize the extremal structures. Another direction is to study the relation between topological indices and some other graph invariant, which helps researchers to know the indices better and find more internal information. The quantification of chemical structures is a basic problem in structure-activity relationships (SAR) which is an important tool for developing safer and potent drugs. The procedure for quantification of chemical structures is by translation of chemical structures into characteristic numerical descriptors (topological indices) [7, 13]. This procedure provides a correlation between quantitative biological activity and qualitative chemical structures.

Another active area of chemical research deals with nanotubes, nanotori, nanostars and other dendrimers. These polymeric materials are of major chemical importance as they are finding applications in a variety of high technology uses, both biomedical (such as MRI diagnostics, coating agents to protect or deliver drugs to specific parts of the body, as anti-bacterial and anti-viral agents, as vectors in gene therapy) and industrial [53]. Explicit values for various topological indices, and in particular, the eccentric connectivity index and eccentric distance sum, are being calculated for these classes of compounds (see, for example [4, 5, 68]).

In the second chapter of this thesis, we find the explicit values for various topological indices of dendrimers called complete m-ary trees. To compute our results, we use the method of combinatorial computing, graph theoretical tools and analytic techniques.

1.3.2 Relevant background results

Let us present some basic results on distance-based indices of a graph. Many researchers are interested in finding bounds for graph invariants and the related problem of figuring out the graphs achieving the maximum and minimum values of corresponding indices.

The minimum value of the Wiener index of a graph of given order is attained by the complete graph and the maximum value is attained by the path. A lower bound on the Wiener index of a graph of given order and size can be found in [29] and Plesník [65] pointed out that the bound is sharp for several graph classes, for example for trees, and planar graphs. An upper bound in terms of order and size was determined by Šolteś [72]. Liu and Pan [59] gave a lower bound on the Wiener index of trees in terms of its order and diameter and they showed that the bound is sharp by giving an extremal graph on the class. But the problem of finding an upper bound on the Wiener index of a tree in terms of order and diameter is quite challenging. This long-standing open problem of finding an upper bound for the Wiener index of a tree in terms of its order and diameter is addressed by Mukewumbi and Vetrík [64] for diameter at most 6. Alhevaz and Baghipur [1] gave upper and lower bounds for the (first) edge-hyper Wiener index of a graph in terms of its size and Gutman index by using a method, which applies group theory to graph theory.

The degree distance has recently been investigated in more detail in the mathematical literature. For trees of given order, Wiener index and degree distance have a linear relationship [42, 54]. Dankelmann, Gutman, Mukwembi and Swart [21] gave an upper bound on the degree distance in terms of order and diameter. The degree distance of unicyclic graphs of given order and girth was considered in [49]. Further results on the degree distance are given in [44].

Dankelmann et al. [22] gave a bound on the Gutman index of a connected graph in terms of its order. Mukwembi [63] improved this bound and he also gave an upper bound on the Gutman index of graphs of given order and diameter. An upper bound on the Gutman index of a graph in terms of its order, diameter and minimum degree, where diameter is not a constant, was given in [60] and the Gutman index of a graph in terms of its order, diameter and vertex-connectivity was studied in [61]. Gutman [42] revealed that, in the case of acyclic structures, the index is closely related to the Wiener index and reflects precisely the same structured features of a molecular graph as the Wiener index does. Dankelmann et al. [23] presented an upper bound for the Gutman index and also established the relation between the edge-Wiener index and Gutman index of graphs. Chen and Liu [18] studied the maximal and minimal Gutman index of unicyclic graphs, and they also determined the minimal Gutman index of bicyclic graphs [19]. Gutman [42] remarked that theoretical investigations on the Gutman index focusing on polycyclic molecules is more difficult. Since then, several authors [18, 36, 42] have studied the index and also its relationship with other graph parameters. In [60] the authors proved an asymptotic upper bound for any connected graph G of order n and minimum degree δ.

The eccentric distance sum was conceptualized by Gupta, Singh and Madan [40]. The investigation of the mathematical properties of eccentric distance sum started only recently [46, 48, 80]. First observe that removing an edge from a graph does not decrease distances. It follows that, as in the case of the Wiener index, for every spanning tree T of G, $EDS(G) \leq EDS(T)$. Thus the problem of finding an upper bound on the eccentric distance sum of a graph can now be restricted to finding an upper bound on the eccentric distance sum of trees. Ilić, Yu and Feng [40] proved that path graph has the maximum eccentric distance sum among connected graphs of a given order. Further, in the same paper, they established bounds on the eccentric distance sum in terms of other graph invariants, such as the Wiener index, degree distance, eccentric connectivity index, independence number, connectivity, matching number, chromatic number and clique number. Turning to lower bounds, clearly the complete graph minimizes the eccentric distance sum among all graphs of given order. This simple bound on the index was improved for trees and for unicyclic graphs. Among trees of a given order the star was identified to be the unique graph which minimizes the index [80]. In the same paper, Yu, Feng and Ilić established the lower bound for eccentric distance sum for trees of a given order and diameter.

One of the newest distance-based topological indices, the eccentric connectivity index was conceptualized in 1997 by Sharma, Goswami and Madan [70]. This index belongs to well-known topological indices. The eccentric connectivity index provides very good correlations with respect to both biological and physical properties of chemical substances [55]. This index has shown an excellent predictive power in pharmaceutical properties, for instance, it is useful for predicting anti-HIV activity of chemical substances [30]. Experiments reveal that prediction using eccentric connectivity index, of analgesic activity [70] and of anti-inflammatory activity [41] is more accurate than prediction using the Wiener index. Mathematical properties of the eccentric connectivity index have been extensively studied. We explore most of the known mathematical results to date.

It was proved independantly by Morgan, Mukwembi and Swart [62], as well as by Zhou and Du [84], that the minimum eccentric connectivity index for a graph of order n is attained by the star S_n. An asymptotic maximum of the eccentric connectivity index was independantly determined by Morgan, Mukwembi and Swart [62], and by Došlić, Saheli and Vukičević [28]. For trees, the maximum eccentric connectivity index value among trees of order n is attained by the path P_n [28, 62]. Morgan, Mukwembi and Swart [62] obtained the sharp lower bound on the eccentric connectivity index for graphs with given order and diameter. They also proved an asymptotic upper bound on the eccentric connectivity index for graphs with given order and diameter. Morgan, Mukwembi and Swart [62] obtained the sharp lower and upper bounds on the eccentric connectivity index for trees with given order and diameter. The lower bound was given also in [84]. Zhou and Du [84] found the sharp upper bound and Ilić [47] gave the sharp lower bound for trees with given order and number of pendant vertices. The tight lower and upper bounds for trees of given order were given in [84]. Trees with given degree sequence were investigated in [77], Ilić [47] gave the sharp lower and upper bounds for unicyclic graphs with given order and girth. Zhang and Hua [81] obtained the tight upper bound, and Zhou and Du [84] stated the tight lower bound for unicyclic graphs of given order. General graphs of diameter 2 were studied in [82] and bipartite graphs in [83].

Chapter 2

Distance-based indices of complete m-ary trees

2.1 Preliminary results

In this section we express the hyper-Wiener index of a graph and the edge-hyper-Wiener index of a tree with the help of the second derivative of the Wiener polynomial. The Wiener polynomial of a connected graph G is defined as

$$W(G,x) = \sum_{\{u,v\} \subseteq V(G)} x^{d(u,v)}$$

and the Hosoya polynomial is

$$H(G,x) = \sum_{k \geq 0} n(G,k)x^k$$

where $n(G,k)$ is the number of pairs of vertices that have distance k. The edge-Hosoya polynomial of G is defined as

$$H_e(G,x) = \sum_{k\geq 0} n_e(G,k)x^k$$

where $n_e(G,k)$ is the number of pairs of edges of distance k.

Cash [17] proved the following result on the hyper-Wiener index.

Theorem 2.1.1. *For a connected graph G we have $WW(G) = H'(G,1) + \frac{1}{2}H''(G,1)$, where $H'(G,1)$ is the first derivative and $H''(G,1)$ is the second derivative of the Hosoya polynomial, evaluated at $x=1$.*

Tratnik and Pleteršek [73] obtained results on the edge-hyper-Wiener index, the Hosoya polynomial and the edge-Hosoya polynomial.

Theorem 2.1.2. *Let G be a connected graph and let T be a tree. Then*

(i) $WW_e(G) = H_e'(G,1) + \frac{1}{2}H_e''(G,1)$,

(ii) $H(G,x) = W(G,x) + |V(G)|$,

(iii) $H_e(T,x) = \frac{W(T,x)}{x}$.

From the second equation we have

$$H'(G,x) = W'(G,x) \quad \text{and} \quad H''(G,x) = W''(G,x). \tag{2.1}$$

Then we can express the hyper-Wiener index of a graph in terms of the Wiener index and the second derivative of the Wiener polynomial.

Theorem 2.1.3. *For a connected graph G we have $WW(G) = W(G) + \frac{1}{2}W''(G,1)$.*

Proof. Clearly, $W(G) = W'(G,1)$ so from (2.1) we obtain $H'(G,1) = W(G)$ and $H''(G,1) = W''(G,1)$, thus by Theorem 2.1.1, we get $WW(G) = W(G) + \frac{1}{2}W''(G,1)$. $\square$

Let us differentiate the third equation of Theorem 2.1.2. We obtain

$$H_e'(T,x) = \frac{xW'(T,x) - W(T,x)}{x^2}. \tag{2.2}$$

Similarly, we differentiate (2.2) to get $H_e''(T,x)$

$$\begin{aligned} &= \frac{x^2(W'(T,x) + xW''(T,x) - W'(T,x)) - 2x(xW'(T,x) - W(T,x))}{x^4} \\ &= \frac{W''(T,x)}{x} - \frac{2W'(T,x)}{x^2} + \frac{2W(T,x)}{x^3}. \end{aligned} \tag{2.3}$$

Now we express the edge-hyper-Wiener index of a tree in terms of the second derivative of the Wiener polynomial.

Theorem 2.1.4. *Let T be a tree. Then $WW_e(T) = \frac{1}{2}W''(T,1)$.*

Proof. By (2.2), we have $H_e'(T,1) = W'(T,1) - W(T,1)$ and by (2.3), we get $H_e''(T,1) = W''(T,1) - 2W'(T,1) + 2W(T,1)$. Hence, from Theorem 2.1.2 we obtain

$$WW_e(T) = H_e'(T,1) + \frac{1}{2}H_e''(T,1) = \frac{1}{2}W''(T,1).$$

$\square$

2.2 Wiener index

We present a few lemmas and use them to obtain the Wiener index of complete m-ary trees, which is the main result of this chapter. Let $N_i(v)$ be the set of vertices at distance i from v and let $N_{\leq i}(v)$ be the set of vertices at distance at most i from v in G.

Lemma 2.2.1. *Let $T_{h,m}$ be a complete m-ary tree of height h with the root vertex v_0. The number of vertices at distance i from v_0 is m^i, where $0 \leq i \leq h$.*

Proof. Clearly, $|N_0(v_0)| = 1$ and $|N_1(v_0)| = d(v_0) = m$. Since every vertex in $N_{i-1}(v_0)$ is adjacent to m vertices in $N_i(v_0)$ for $i = 2, 3, \ldots h$, we obtain $|N_i(v_0)| = |N_{i-1}(v_0)|m = m^i$. □

The number of vertices in a complete m-ary tree of height h is given in Lemma 2.2.2.

Lemma 2.2.2. *We have $|V(T_{h,m})| = \frac{m^{h+1}-1}{m-1}$.*

Proof. We have

$$\begin{aligned} |V(T_{h,m})| &= |N_0(v_0)| + |N_1(v_0)| + |N_2(v_0)| + \cdots + |N_h(v_0)| \\ &= 1 + m + m^2 + \cdots + m^h \\ &= \frac{m^{h+1}-1}{m-1}. \end{aligned}$$

□

Since we know the distance between the root $v_0 \in V(T_{h,m})$ and any vertex of $T_{h,m}$, we obtain the following lemma.

Lemma 2.2.3. *Let $T_{h,m}$ be a complete m-ary tree of height h. Then*

$$\sum_{u \in V(T_{h,m})} d(v_0, u) = \frac{hm^{h+2} - (h+1)m^{h+1} + m}{(m-1)^2}.$$

Proof. For a vertex $u \in N_i(v_0)$ we have $d(v_0, u) = i$ and by Lemma 2.2.1, $|N_i(v_0)| = m^i$, where $i = 1, 2, \ldots, h$. Therefore

$$\begin{aligned}
& \sum_{u \in V(T_{h,m})} d(v_0, u) \\
= & \sum_{u \in N_1(v_0)} d(v_0, u) + \sum_{u \in N_2(v_0)} d(v_0, u) + \cdots + \sum_{u \in N_h(v_0)} d(v_0, u) \\
= & \; m + 2m^2 + 3m^3 + \cdots + hm^h.
\end{aligned}$$

Then

$$\begin{aligned}
(1-m) \sum_{u \in V(T_{h,m})} d(v_0, u) &= m + m^2 + m^3 + \cdots + m^h - hm^{h+1} \\
&= \frac{m(1-m^h)}{1-m} - hm^{h+1}
\end{aligned}$$

and

$$\sum_{u \in V(T_{h,m})} d(v_0, u) = \frac{m(1-m^h)}{(1-m)^2} - \frac{hm^{h+1}}{1-m} = \frac{hm^{h+2} - (h+1)m^{h+1} + m}{(m-1)^2}.$$

□

For any rooted tree T with root vertex v_0, we denote by $l(T)$ the sum of the distances from the root v_0 of T to all its vertices. That is, $l(T) = \sum_{u \in V(T)} d(u, v_0)$.

Lemma 2.2.4. *Let T be any rooted tree with the root vertex v_0 such that $d_T(v_0) = m$. Let T_1, T_2, ..., T_m be the rooted trees with root vertices v_{r_1}, $v_{r_2}, \ldots, v_{r_m}$ respectively obtained by removing the root vertex v_0 from T. Let*

n_i be the number of vertices in T_i, where $1 \leq i \leq m$. Then

$$W(T) = \sum_{i=1}^{m} W(T_i) + \sum_{i=1}^{m}(n_i + l(T_i)) + \sum_{1\leq i<j\leq m} (n_j l(T_i) + 2n_i n_j + n_i l(T_j)).$$

Proof.

$$\begin{aligned}
W(T) &= \sum_{u,v\in V(T)} d(u,v) \\
&= \sum_{i=1}^{m} \sum_{u,v\in V(T_i)} d(u,v) + \sum_{i=1}^{m} \sum_{u\in V(T_i)} d(v_0,u) + \sum_{1\leq i<j\leq m} \sum_{v\in V(T_j)} \sum_{u\in V(T_i)} d(u,v) \\
&= \sum_{i=1}^{m} W(T_i) + \sum_{i=1}^{m} \sum_{u\in V(T_i)} (d(v_0,v_{r_i}) + d(v_{r_i},u)) + \\
&\quad \sum_{1\leq i<j\leq m} \sum_{v\in V(T_j)} \sum_{u\in V(T_i)} (d(u,v_{r_i}) + d(v_{r_i},v_0) + d(v_0,v_{r_j}) + d(v_{r_j},v)) \\
&= \sum_{i=1}^{m} W(T_i) + \sum_{i=1}^{m} \sum_{u\in V(T_i)} (1 + d(v_{r_i},u)) \\
&\quad + \sum_{1\leq i<j\leq m} \sum_{u\in V(T_i)} \sum_{v\in V(T_j)} (d(u,v_{r_i}) + 2 + d(v_{r_j},v)) \\
&= \sum_{i=1}^{m} W(T_i) + \sum_{i=1}^{m}(n_i + l(T_i)) \\
&\quad + \sum_{1\leq i<j\leq m} \left(\sum_{v\in V(T_j)} \sum_{u\in V(T_i)} d(u,v_{r_i}) + \sum_{u\in V(T_i)} \sum_{v\in V(T_j)} 2 + \sum_{u\in V(T_i)} \sum_{v\in V(T_j)} d(v_{r_j},v) \right) \\
&= \sum_{i=1}^{m} W(T_i) + \sum_{i=1}^{m}(n_i + l(T_i)) + \sum_{1\leq i<j\leq m} (n_j l(T_i) + 2n_i n_j + n_i l(T_j)).
\end{aligned}$$

$\square$

Since every complete m-ary tree is a rooted tree, we use Lemma 2.2.4 to study the Wiener index of complete m-ary trees. We replace all trees $T_1, T_2, \ldots, T_m$ by $T_{h-1,m}$ and we get

Lemma 2.2.5.

$$W(T_{h,m}) = mW(T_{h-1,m}) + \left(\frac{hm^{h+1} - (h+1)m^h + 1}{(m-1)^2}\right) m^{h+1}, \ h \geq 1$$

with initial value $W(T_{0,m}) = 0$.

Proof. By Lemma 2.2.4, we have

$$\begin{aligned}
& W(T_{h,m}) \\
= \ & mW(T_{h-1,m}) + m(|V(T_{h-1,m})| + l(T_{h-1,m})) \\
& + \binom{m}{2}(2|V(T_{h-1,m})|l(T_{h-1,m}) + 2|V(T_{h-1,m})|^2) \\
= \ & mW(T_{h-1,m}) + m(|V(T_{h-1,m})| + l(T_{h-1,m}))((m-1)|V(T_{h-1,m})| + 1).
\end{aligned}$$

From Lemmas 2.2.2 and 2.2.3 we obtain

$$|V(T_{h-1,m})| = \frac{m^h - 1}{m-1} \quad \text{and} \quad l(T_{h-1,m}) = \frac{(h-1)m^{h+1} - hm^h + m}{(m-1)^2},$$

thus

$$\begin{aligned}
W(T_{h,m}) &= mW(T_{h-1,m}) + m\left(\frac{m^h - 1}{m-1} + \frac{(h-1)m^{h+1} - hm^h + m}{(m-1)^2}\right) m^h \\
&= mW(T_{h-1,m}) + \left(\frac{hm^{h+1} - (h+1)m^h + 1}{(m-1)^2}\right) m^{h+1}.
\end{aligned}$$

□

We solve this recurrence relation and get an explicit formula for $W(T_{h,m})$.

Theorem 2.2.6. *Let $T_{h,m}$ be a complete m-ary tree of height h. Then*

$$W(T_{h,m}) = \frac{(hm - h - 2)m^{2h+2} + (hm + 2m - h)m^{h+1}}{(m-1)^3}.$$

Proof. By Lemma 2.2.5 we have

$$W(T_{h,m}) = mW(T_{h-1,m}) + \left(\frac{hm^{h+1} - (h+1)m^h + 1}{(m-1)^2}\right) m^{h+1}, \ h \geq 1$$

with initial value $W(T_{0,m}) = 0$. The homogeneous part of the recurrence relation is

$$W^g(T_{h,m}) = mW^g(T_{h-1,m})$$

and the general solution of the homogeneous part is

$$W^g(T_{h,m}) = km^h \tag{2.4}$$

where k is a constant to be calculated. The non-homogeneous part of the recurrence relation is

$$\begin{aligned} f(h) &= \left(\frac{hm^{h+1} - (h+1)m^h + 1}{(m-1)^2}\right) m^{h+1} \\ &= \left(\frac{hm}{m-1} - \frac{m}{(m-1)^2}\right) m^{2h} + \frac{mm^h}{(m-1)^2}. \end{aligned}$$

The particular solution is

$$W^p(T_{h,m}) = (Ah + B)m^{2h} + Chm^h,$$

where A, B and C are constants to be calculated. To find the values of A, B and C we substitute $W^p(T_{h,m})$ into the recurrence relation. That is,

$$\begin{aligned} W^p(T_{h,m}) &= mW^p(T_{h-1,m}) + \left(\frac{hm^{h+1} - (h+1)m^h + 1}{(m-1)^2}\right) m^{h+1} \\ &= m((A(h-1) + B)m^{2(h-1)} + C(h-1)m^{h-1}) \\ &\quad + \left(\frac{hm}{m-1} - \frac{m}{(m-1)^2}\right) m^{2h} + \frac{mm^h}{(m-1)^2}. \end{aligned}$$

This implies that

$$\begin{aligned}
& (Ah+B)m^{2h} + Chm^h \\
= \; & (Ah-A+B)m^{2h-1} + (Ch-C)m^h + \left(\frac{hm}{m-1} - \frac{m}{(m-1)^2}\right)m^{2h} \\
& + \frac{mm^h}{(m-1)^2}.
\end{aligned}$$

Thus

$$\begin{aligned}
& \left(\frac{(m-1)Ah + (m-1)B + A}{m}\right)m^{2h} + Cm^h \\
= \; & \left(\frac{hm}{m-1} - \frac{m}{(m-1)^2}\right)m^{2h} + \frac{mm^h}{(m-1)^2}.
\end{aligned}$$

Consequently,

$$\frac{(m-1)Ah + (m-1)B + A}{m} = \frac{hm}{m-1} - \frac{m}{(m-1)^2}$$

and

$$C = \frac{m}{(m-1)^2}.$$

This implies that A and B satisfy

$$\begin{aligned}
(m-1)A &= \frac{m^2}{m-1} \\
(m-1)B + A &= -\frac{m^2}{(m-1)^2}.
\end{aligned}$$

Solving this system for A and B gives

$$A = \frac{m^2}{(m-1)^2}, \quad B = \frac{-2m^2}{(m-1)^3}.$$

Thus the particular solution is

$$W^p(T_{h,m}) = \left(\frac{hm^2}{(m-1)^2} - \frac{2m^2}{(m-1)^3}\right) m^{2h} + \frac{hm^{h+1}}{(m-1)^2}. \tag{2.5}$$

The general solution of our recurrence relation is the sum of the general solution of the homogeneous part and the particular solution. That is,

$$W(T_{h,m}) = W^g(T_{h,m}) + W^p(T_{h,m}). \tag{2.6}$$

From (2.4), (2.5) and (2.6) we have

$$W(T_{h,m}) = km^h + \left(\frac{hm^2}{(m-1)^2} - \frac{2m^2}{(m-1)^3}\right) m^{2h} + \frac{hm^{h+1}}{(m-1)^2}.$$

Using the initial value $W(T_{0,m}) = 0$ we get

$$k = \frac{2m^2}{(m-1)^3}.$$

Therefore

$$\begin{aligned} W(T_{h,m}) &= \left(\frac{2m^2}{(m-1)^3} + \frac{mh}{(m-1)^2}\right) m^h + \left(h\left(\frac{m}{m-1}\right)^2 - \frac{2m^2}{(m-1)^3}\right) m^{2h} \\ &= \frac{(hm-h-2)m^{2h+2} + (hm+2m-h)m^{h+1}}{(m-1)^3}. \end{aligned}$$

□

2.3 Distance-based indices

In this section we study the edge-Wiener index, the hyper-Wiener index, the edge-hyper-Wiener index, the degree distance, the Gutman index and the eccentric distance sum.

An ancestor of a vertex $v_i \in N_i(v_0)$ for $1 \leq i \leq h$ is any vertex, say v_{i-p} where $0 \leq p \leq i$, which belongs to the path connecting v_i and the root v_0 in $T_{h,m}$. Then v_i is called a descendant of v_{i-p}.

Theorem 2.3.1. *Let $T_{h,m}$ be a complete m-ary tree of height h. Then*

$$EDS(T_{h,m}) = \frac{4h^2m^{2h+4} - am^{2h+3} + bm^{2h+2} + cm^{h+3} - dm^{h+2} + em^{h+1} - m}{(m-1)^4},$$

where $a = 8h^2+10h-1$, $b = 4h^2+10h+4$, $c = 4h^2+7h-1$, $d = 8h^2+10h+4$ and $e = 4h^2+3h+1$.

Proof. For the root vertex $v_0 \in V(T_{h,m})$ we get

$$D(v_0) = m + 2m^2 + 3m^3 + \cdots + hm^h = \frac{hm^{h+2} - (h+1)m^{h+1} + m}{(m-1)^2}$$

(see the proof of Lemma 2.2.3 for detailed computation). Now we obtain $D(v_i)$ for any vertex $v_i \in N_i(v_0)$ where $1 \leq i \leq h$. In the following computation, one line corresponds to a vertex, say v_{i-p} in $N_{i-p}(v_0)$ for $p = 0, 1, 2, \ldots, i$, which is a ancestor of v_i and those descendants of v_{i-p} that were not considered before.

$$\begin{aligned} D(v_i) \;&= m + 2m^2 + 3m^3 + \cdots + (h-i)m^{h-i} \\ &+1 + 2(m-1) + 3(m-1)m + \cdots + (h-i+2)(m-1)m^{h-i} \\ &+2 + 3(m-1) + 4(m-1)m + \cdots + (h-i+4)(m-1)m^{h-i+1} + \\ &\vdots \\ &+i + (i+1)(m-1) + (i+2)(m-1)m + \cdots + (i+h)(m-1)m^{h-1}. \end{aligned}$$

Thus $D(v_i)$

$$
\begin{aligned}
&= \frac{(h-i)m^{h-i+2}-(h-i+1)m^{h-i+1}+m}{(m-1)^2} \\
&\quad +\frac{(h-i+2)m^{h-i+2}-(h-i+3)m^{h-i+1}+1}{m-1} \\
&\quad +\frac{(h-i+4)m^{h-i+3}-(h-i+5)m^{h-i+2}+1}{m-1}+ \\
&\quad \vdots \\
&\quad +\frac{(h+i)m^{h+1}-(h+i+1)m^{h}+1}{m-1} \\
&= \frac{(h-i)m^{h-i+2}-(h-i+1)m^{h-i+1}+m}{(m-1)^2} \\
&\quad +\sum_{p=1}^{i}\frac{(h-i+2p)m^{h-i+p+1}-(h-i+2p+1)m^{h-i+p}+1}{m-1} \\
&= \frac{(h-i)m^{h-i+2}-(h-i+1)m^{h-i+1}+m}{(m-1)^2}+\frac{(h-i)m^{h-i+1}}{m-1}\sum_{p=1}^{i}m^p \\
&\quad +\frac{2m^{h-i+1}}{m-1}\sum_{p=1}^{i}pm^p-\frac{(h-i+1)m^{h-i}}{m-1}\sum_{p=1}^{i}m^p-\frac{2m^{h-i}}{m-1}\sum_{p=1}^{i}pm^p \\
&\quad +\frac{1}{m-1}\sum_{p=1}^{i}1 \\
&= \frac{(h-i)m^{h-i+2}-(h-i+1)m^{h-i+1}+m}{(m-1)^2} \\
&\quad +\frac{(h-i)m^{h-i+1}-(h-i+1)m^{h-i}}{m-1}\sum_{p=1}^{i}m^p+2m^{h-i}\sum_{p=1}^{i}pm^p \\
&\quad +\frac{i}{m-1} \\
&= \frac{(h-i)m^{h-i+2}-(h-i+1)m^{h-i+1}+m}{(m-1)^2} \\
&\quad +\frac{(h-i)m^{h-i+1}-(h-i+1)m^{h-i}}{m-1}\cdot\frac{m^{i+1}-m}{m-1} \\
&\quad +2m^{h-i}\ \frac{m^{i+2}-(i+1)m^{i+1}+m}{(m-1)^2}+\frac{i}{m-1} \\
&= \frac{(h+i)m^{h+2}-(h+i+3)m^{h+1}+2m^{h-i+1}+(i+1)m-i}{(m-1)^2}.
\end{aligned}
$$

Hence we obtain

$$EDS(T_{h,m}) = \sum_{v\in V(T_{h,m})} ecc(v)D(v) = \sum_{i=0}^{h}\sum_{v\in N_i(v_0)} ecc(v)D(v)$$

$$= \sum_{i=0}^{h} m^i(h+i)\ \frac{(h+i)m^{h+2}-(h+i+3)m^{h+1}+2m^{h-i+1}+(i+1)m-i}{(m-1)^2}$$

since there are m^i vertices in $N_i(v_0)$ and $ecc(v_i) = h+i$ for any vertex $v_i \in N_i(v_0)$ where $0 \le i \le h$. Thus $EDS(T_{h,m})$

$$\begin{aligned}
= \ & \frac{1}{(m-1)^2}\Bigg(m^{h+2}\sum_{i=0}^{h}(i^2+2hi+h^2)m^i - m^{h+1}\sum_{i=0}^{h}(i^2+2hi+3i+h^2+3h)m^i \\
& +2m^{h+1}\sum_{i=0}^{h}(i+h) + m\sum_{i=0}^{h}(i^2+hi+i+h)m^i - \sum_{i=0}^{h}(i^2+hi)m^i\Bigg) \\
= \ & \frac{1}{(m-1)^2}\Bigg((m^{h+2}-m^{h+1}+m-1)\sum_{i=0}^{h} i^2m^i \\
& +(2hm^{h+2}-(2h+3)m^{h+1}+(h+1)m-h)\sum_{i=0}^{h} im^i \\
& +(h^2m^{h+2}-(h^2+3h)m^{h+1}+hm)\sum_{i=0}^{h} m^i + 2m^{h+1}\Bigg(h(h+1)+\frac{h(h+1)}{2}\Bigg)\Bigg).
\end{aligned}$$

We know that

$$\sum_{i=0}^{h} m^i = \frac{m^{h+1}-1}{m-1} \quad \text{and} \quad \sum_{i=0}^{h} im^i = \frac{hm^{h+2}-(h+1)m^{h+1}+m}{(m-1)^2}. \tag{2.7}$$

Since $(m-1)^2\sum_{i=0}^{h} i^2m^i$

$$\begin{aligned}
= \ & m+2m^2+2m^3+2m^4+\cdots+2m^h-(h^2+2h-1)m^{h+1}+h^2m^{h+2} \\
= \ & m+2m^2(1+m+m^2+\cdots+m^{h-2})-(h^2+2h-1)m^{h+1}+h^2m^{h+2} \\
= \ & \frac{2m^2(m^{h-1}-1)}{m-1}+m-(h^2+2h-1)m^{h+1}+h^2m^{h+2},
\end{aligned}$$

we obtain

$$\sum_{i=0}^{h} i^2 m^i = \frac{2(m^{h+1}-m^2)}{(m-1)^3} + \frac{m-(h^2+2h-1)m^{h+1}+h^2m^{h+2}}{(m-1)^2}. \tag{2.8}$$

We use (2.7) and (2.8) and simplify the expression to get

$$EDS(T_{h,m}) = \frac{4h^2m^{2h+4} - am^{2h+3} + bm^{2h+2} + cm^{h+3} - dm^{h+2} + em^{h+1} - m}{(m-1)^4},$$

where $a = 8h^2+10h-1$, $b = 4h^2+10h+4$, $c = 4h^2+7h-1$, $d = 8h^2+10h+4$ and $e = 4h^2+3h+1$. □

We use Lemmas 2.3.2, 2.3.3 and 2.3.4 to obtain the Wiener polynomial of complete m-ary trees.

Lemma 2.3.2. *Let u be any leaf of $T_{h,m}$. Then*

$$\sum_{v \in N_{\leq h-1}(v_0)} x^{d(u,v)} = \frac{x^2(m-1)((mx^2)^h-1)}{(mx-1)(mx^2-1)} + \frac{x^{h+1}-x}{mx-1}.$$

Proof. In the following computation, one line corresponds to a vertex, say v_{h-i} in $N_{h-i}(v_0)$ for $i = 1, 2, \ldots, h$, which is an ancestor of u and those descendants of v_{h-i} that were not considered before. We have

$$\begin{aligned}\sum_{v \in N_{\leq h-1}(v_0)} x^{d(u,v)} &= x \\ &\quad +x^2+(m-1)x^3 \\ &\quad +x^3+(m-1)x^4+m(m-1)x^5 \\ &\quad +x^4+(m-1)x^5+m(m-1)x^6+m^2(m-1)x^7+ \\ &\quad \vdots\end{aligned}$$

$$+x^h + (m-1)x^{h+1} + m(m-1)x^{h+2}$$
$$+m^2(m-1)x^{h+3} + \cdots + m^{h-2}(m-1)x^{2h-1}$$

which is equal to

$$
\begin{aligned}
& x + x^2 + x^3 + \cdots + x^h \\
& +(m-1)x^3(1 + x + x^2 + \cdots + x^{h-2}) \\
& +m(m-1)x^5(1 + x + x^2 + \cdots + x^{h-3}) \\
& +m^2(m-1)x^7(1 + x + x^2 + \cdots + x^{h-4}) + \\
& \vdots \\
& +m^{h-3}(m-1)x^{2h-3}(1+x) \\
& +m^{h-2}(m-1)x^{2h-1} \\
= \; & x\left(\frac{x^h - 1}{x-1}\right) + (m-1)x^3\left(\frac{x^{h-1}-1}{x-1}\right) + m(m-1)x^5\left(\frac{x^{h-2}-1}{x-1}\right) \\
& +m^2(m-1)x^7\left(\frac{x^{h-3}-1}{x-1}\right) + \cdots + m^{h-2}(m-1)x^{2h-1}\left(\frac{x-1}{x-1}\right) \\
= \; & \frac{x^{h+1}-x}{x-1} + \frac{(m-1)x^3}{x-1}(x^{h-1} - 1 + mx^2(x^{h-2}-1) \\
& +m^2x^4(x^{h-3}-1) + \cdots + m^{h-2}x^{2(h-2)}(x-1)) \\
= \; & \frac{x^{h+1}-x}{x-1} + \frac{(m-1)x^3}{x-1}(x^{h-1} + mx^h + m^2x^{h+1} + \cdots + m^{h-2}x^{2h-3}) \\
& -\frac{(m-1)x^3}{x-1}(1 + mx^2 + m^2x^4 + \cdots + m^{h-2}x^{2(h-2)}) \\
= \; & \frac{x^{h+1}-x}{x-1} + \frac{(m-1)x^3}{x-1}(x^{h-1}(1 + mx + (mx)^2 + \cdots + (mx)^{h-2)}) \\
& -\frac{(m-1)x^3}{x-1}\left(1 + mx^2 + (mx^2)^2 + \cdots + (mx^2)^{h-2}\right) \\
= \; & \frac{x^{h+1}-x}{x-1} + \frac{(m-1)x^{h+2}}{x-1}\left(\frac{(mx)^{h-1}-1}{mx-1}\right) - \frac{(m-1)x^3}{x-1}\left(\frac{(mx^2)^{h-1}-1}{mx^2-1}\right)
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{(x^{h+1}-x)(mx-1)(mx^2-1)}{(x-1)(mx-1)(mx^2-1)} + \frac{(m-1)x^{h+2}(mx^2-1)((mx)^{h-1}-1)}{(x-1)(mx-1)(mx^2-1)} \\
&\quad - \frac{(m-1)x^3(mx-1)((mx^2)^{h-1}-1)}{(x-1)(mx-1)(mx^2-1)} \\
&= \frac{m^{h+1}x^{2h+3} - m^h x^{2h+3} - m^{h+1}x^{2h+2} + m^h x^{2h+2}}{(x-1)(mx-1)(mx^2-1)} \\
&\quad + \frac{mx^{h+4} - mx^{h+3} - x^{h+2} + x^{h+1} - mx^4 + mx^2}{(x-1)(mx-1)(mx^2-1)} \\
&\quad + \frac{x^3-x}{(x-1)(mx-1)(mx^2-1)} \\
&= \frac{m^{h+1}x^{2h+2}(x-1) - m^h x^{2h+2}(x-1)}{(x-1)(mx-1)(mx^2-1)} \\
&\quad + \frac{mx^{h+3}(x-1) - x^{h+1}(x-1) - mx^2(x^2-1) + x(x^2-1)}{(x-1)(mx-1)(mx^2-1)} \\
&= \frac{(mx^2)^{h+1} - x^2(mx^2)^h + mx^{h+3} - x^{h+1} - mx^3 - mx^2 + x^2 + x}{(mx-1)(mx^2-1)} \\
&= \frac{mx^2((mx^2)^h-1) - x^2((mx^2)^h-1) + x^{h+1}(mx^2-1) - x(mx^2-1)}{(mx-1)(mx^2-1)} \\
&= \frac{x^2(m-1)((mx^2)^h-1)}{(mx-1)(mx^2-1)} + \frac{x^{h+1}-x}{mx-1}.
\end{aligned}
$$

□

Since there are m^h leaves in $T_{h,m}$, we have

$$\sum_{u \in N_h(v_0)} \sum_{v \in N_{\leq h-1}(v_0)} x^{d(u,v)} = m^h \left(\frac{x^2(m-1)((mx^2)^h-1)}{(mx-1)(mx^2-1)} + \frac{x^{h+1}-x}{mx-1} \right).$$

Lemma 2.3.3. *Let u be any leaf of $T_{h,m}$. Then*

$$\sum_{v \in N_h(v_0)} x^{d(u,v)} = \frac{x^2(m-1)((mx^2)^h-1)}{mx^2-1}.$$

Proof. Let u be any leaf of $T_{h,m}$. Since there are $m-1$ leaves at distance 2 from u, $m(m-1)$ leaves at distance 4 from u, $\ldots$, $m^{h-1}(m-1)$ leaves at distance $2h$ from u, we obtain

$$\begin{aligned}
\sum_{v\in N_h(v_0)} x^{d(u,v)} &= (m-1)x^2 + m(m-1)x^4 + m^2(m-1)x^6 + ... \\
&= +m^{h-1}(m-1)x^{2h} \\
&= (m-1)x^2(1 + mx^2 + m^2x^4 + ... + m^{h-1}x^{2(h-1)}) \\
&= (m-1)x^2(1 + mx^2 + (mx^2)^2 + ... + (mx^2)^{h-1}) \\
&= x^2(m-1)\left(\frac{(mx^2)^h - 1}{mx^2 - 1}\right) = \frac{x^2(m-1)((mx^2)^h - 1)}{mx^2 - 1}.
\end{aligned}$$

□

Considering all pairs of leaves of $T_{h,m}$, we have

$$\begin{aligned}
\sum_{\{u,v\}\subseteq N_h(v_0)} x^{d(u,v)} &= \frac{1}{2}\sum_{u\in N_h(v_0)}\sum_{v\in N_h(v_0)} x^{d(u,v)} = \frac{m^h}{2}\,\frac{x^2(m-1)((mx^2)^h - 1)}{mx^2 - 1} \\
&= \frac{x^2m^h(m-1)((mx^2)^h - 1)}{2(mx^2 - 1)}.
\end{aligned}$$

In Lemmas 2.3.2 and 2.3.3 we presented results involving leaves of $T_{h,m}$. Similarly, it can be proved that for any vertex $u \in N_k(v_0)$, where $k = 2, 3, \ldots, h$,

$$\sum_{v\in N_{\leq k-1}(v_0)} x^{d(u,v)} = \frac{x^2(m-1)((mx^2)^k - 1)}{(mx-1)(mx^2-1)} + \frac{x^{k+1} - x}{mx - 1}$$

and

$$\sum_{v\in N_k(v_0)} x^{d(u,v)} = \frac{x^2(m-1)((mx^2)^k - 1)}{mx^2 - 1}$$

and consequently we obtain

$$\sum_{u\in N_k(v_0)}\sum_{v\in N_{\le k-1}(v_0)} x^{d(u,v)} = m^k\left(\frac{x^2(m-1)((mx^2)^k-1)}{(mx-1)(mx^2-1)}+\frac{x^{k+1}-x}{mx-1}\right)$$

and

$$\sum_{\{u,v\}\subseteq N_k(v_0)} x^{d(u,v)} = \frac{x^2m^k(m-1)((mx^2)^k-1)}{2(mx^2-1)}.$$

Lemma 2.3.4. *For $k = 2, 3, \ldots, h$, we have*

$$W(T_{k,m},x)-W(T_{k-1,m},x) = \frac{x^2m^k(m-1)((mx^2)^k-1)(mx+1)}{2(mx^2-1)(mx-1)}+\frac{m^k(x^{k+1}-x)}{mx-1}.$$

Proof. $W(T_{k,m},x)$

$$\begin{aligned}
&= \sum_{\{u,v\}\subseteq V(T_{k,m})} x^{d(u,v)}\\
&= \sum_{\{u,v\}\subseteq V(T_{k-1,m})} x^{d(u,v)} + \sum_{\{u,v\}\subseteq N_k(v_0)} x^{d(u,v)} + \sum_{u\in N_k(v_0),v\in N_{\le k-1}(v_0)} x^{d(u,v)}\\
&= W(T_{k-1,m},x) + \frac{x^2m^k(m-1)((mx^2)^k-1)}{2(mx^2-1)}\\
&\quad +m^k\left(\frac{x^2(m-1)((mx^2)^k-1)}{(mx-1)(mx^2-1)}+\frac{x^{k+1}-x}{mx-1}\right)\\
&= W(T_{k-1,m},x) + \frac{x^2m^k(m-1)((mx^2)^k-1)}{mx^2-1}\left(\frac{1}{2}+\frac{1}{mx-1}\right)+\frac{m^k(x^{k+1}-x)}{mx-1}\\
&= W(T_{k-1,m},x) + \frac{x^2m^k(m-1)((mx^2)^k-1)}{mx^2-1}\cdot\frac{mx-1+2}{2(mx-1)}+\frac{m^k(x^{k+1}-x)}{mx-1}.
\end{aligned}$$

This implies that

$$W(T_{k,m},x)-W(T_{k-1,m},x) = \frac{x^2m^k(m-1)((mx^2)^k-1)(mx+1)}{2(mx^2-1)(mx-1)}+\frac{m^k(x^{k+1}-x)}{mx-1}.$$

□

Let us present the Wiener polynomial of complete m-ary trees.

Theorem 2.3.5. *Let $T_{h,m}$ be a complete m-ary tree of height h. Then*

$$\begin{aligned} W(T_{h,m},x) &= \frac{x^2(m-1)(mx+1)}{2(mx^2-1)(mx-1)}\left(\frac{(mx)^{2h+2}-(mx)^4}{(mx)^2-1}-\frac{m^{h+1}-m^2}{m-1}\right) \\ &\quad +\frac{x}{mx-1}\left(\frac{(mx)^{h+1}-(mx)^2}{mx-1}-\frac{m^{h+1}-m^2}{m-1}\right)+\binom{m}{2}x^2 \\ &\quad +mx. \end{aligned}$$

Proof. From Lemma 2.3.4 we obtain $\sum_{k=2}^{h}\left(W(T_{k,m},x)-W(T_{k-1,m},x)\right)$

$$\begin{aligned} &= \sum_{k=2}^{h}\frac{x^2m^k(m-1)((mx^2)^k-1)(mx+1)}{2(mx^2-1)(mx-1)}+\sum_{k=2}^{h}\frac{m^k(x^{k+1}-x)}{mx-1} \\ &= \frac{x^2(m-1)(mx+1)}{2(mx^2-1)(mx-1)}\sum_{k=2}^{h}((mx)^{2k}-m^k)+\frac{x}{mx-1}\sum_{k=2}^{h}((mx)^k-m^k) \\ &= \frac{x^2(m-1)(mx+1)}{2(mx^2-1)(mx-1)}\left(\frac{(mx)^{2h+2}-(mx)^4}{(mx)^2-1}-\frac{m^{h+1}-m^2}{m-1}\right) \\ &\quad +\frac{x}{mx-1}\left(\frac{(mx)^{h+1}-(mx)^2}{mx-1}-\frac{m^{h+1}-m^2}{m-1}\right). \end{aligned}$$

Since $\sum_{k=2}^{h}\left(W(T_{k,m},x)-W(T_{k-1,m},x)\right)=W(T_{h,m},x)-W(T_{1,m},x)$ and $W(T_{1,m},x)=\binom{m}{2}x^2+mx$, we obtain

$$\begin{aligned} W(T_{h,m},x) &= \frac{x^2(m-1)(mx+1)}{2(mx^2-1)(mx-1)}\left(\frac{(mx)^{2h+2}-(mx)^4}{(mx)^2-1}-\frac{m^{h+1}-m^2}{m-1}\right) \\ &\quad +\frac{x}{mx-1}\left(\frac{(mx)^{h+1}-(mx)^2}{mx-1}-\frac{m^{h+1}-m^2}{m-1}\right)+\binom{m}{2}x^2 \\ &\quad +mx. \end{aligned}$$

$\square$

We differentiate $W(T_{h,m},x)$ to obtain the first derivative of the Wiener polynomial of $T_{h,m}$. We have $W'(T_{h,m},x)$

$$\begin{aligned}
= \quad & \frac{x(m-1)(h(mx)^{2h+2}-(mx)^4)}{(mx-1)^2(mx^2-1)} \\
& + \frac{(m-1)((x^2+x)mx-2x)((mx)^4-(mx)^{2h+2})}{(mx-1)^3(mx^2-1)^2} \\
& + \frac{h(mx)^{h+2}-(h+2)(mx)^{h+1}-(mx)^3+3(mx)^2}{(mx-1)^3} \\
& + \frac{(m^h-m)((x+1)(mx)^3-2(mx)^2)}{(mx-1)^2(mx^2-1)^2} + \frac{m^{h+1}-m^2}{(m-1)(mx-1)^2} \\
& + (m-1)mx+m.
\end{aligned}$$

Note that substituting $x=1$ into this function and simplifying gives the Wiener index of $T_{h,m}$. That is,

$$W'(T_{h,m},1) = \frac{m^{2h+2}(hm-h-2)+m^{h+1}((h+2)m-h)}{(m-1)^3} = W(T_{h,m}).$$

Similarly, taking the derivative of $W'(T_{h,m},x)$ gives the second derivative of $W(T_{h,m},x)$. So $W''(T_{h,m},x)$ is

$$\begin{aligned}
& \frac{(m-1)a}{(mx-1)^2(mx^2-1)^2((mx)^2-1)^2} + \frac{(m-1)b}{(mx-1)^4(mx^2-1)^3(mx+1)} \\
& + \frac{c}{(mx-1)^4} - \frac{(m^{h+1}-m^2)d}{(mx-1)^3(mx^2-1)^3} - \frac{2m^{h+2}-2m^3}{(mx-1)^3(m-1)} + m(m-1),
\end{aligned}$$

where

$$
\begin{aligned}
a &= (2xh^2+xh)(mx)^{2h+7}-(2h^2+8xh+2mh+3h)(mx)^{2h+6}\\
&\quad -(4xh^2+2xh-4hm-4h-x)(mx)^{2h+5}\\
&\quad +(4h^2+8xh+8x+10h+2m+1)(mx)^{2h+4}\\
&\quad +(2xh^2+xh-4mh-4h-4m-x-4)(mx)^{2h+3}\\
&\quad +(2hm-2h^2-7h+2m-5)(mx)^{2h+2}\\
&\quad -3x(mx)^9+(8x+2m+5)(mx)^8+(5x-4m-4)(mx)^7\\
&\quad -(16x+2m+15)(mx)^6-(2x-8m-8)(mx)^5-(4m-14)(mx)^4,\\
b &= (2x^2+3x)(mx)^{2h+6}-(3x-1)(mx)^{2h+5}-(7x+3)(mx)^{2h+4}\\
&\quad +(3x+3)(mx)^{2h+3}+(mx)^{2h+2}-(2x^2+3x)(mx)^8\\
&\quad +(3x-1)(mx)^7+(7x+3)(mx)^6-(3x+3)(mx)^5-(mx)^4,\\
c &= m(h^2-h)(mx)^{h+2}-2m(h^2+h-2)(mx)^{h+1}\\
&\quad +m(h^2+3h+2)(mx)^h-6m(mx),\\
d &= (3x+2x^2)(mx)^4-(3x-1)(mx)^3-(7x+3)(mx)^2+(3x+3)(mx)+1.
\end{aligned}
$$

We substitute $x=1$ to the equation for $W''(T_{h,m},x)$ and after simplifying we obtain

$$
W''(T_{h,m},1)=\frac{a}{(m+1)^2(m-1)^4}+\frac{b}{(m-1)^4}+m(m-1), \tag{2.9}
$$

where

$$
\begin{aligned}
a &= (2h^2-h)m^{2h+6}-(8h-5)m^{2h+5}-(4h^2+6h-16)m^{2h+4}\\
&\quad +(8h+17)m^{2h+3}+(2h^2+7h+6)m^{2h+2},
\end{aligned}
$$

$$\begin{aligned} b &= (h^2-h-5)m^{h+3} - (2h^2+2h+6)m^{h+2} + (h^2+3h+1)m^{h+1} \\ &\quad -m^6 + 5m^5 - 10m^4 + 10m^3 - 5m^2. \end{aligned}$$

By Theorem 2.1.3 we have $WW(T_{h,m}) = W(T_{h,m}) + \frac{1}{2}W''(T_{h,m}, 1)$, therefore we use (2.9) and Theorem 2.2.6 to obtain the hyper-Wiener index of $T_{h,m}$.

Theorem 2.3.6. *Let $T_{h,m}$ be a complete m-ary tree of height h. Then*

$$WW(T_{h,m}) = \frac{a}{2(m+1)^2(m-1)^4} + \frac{b}{2(m-1)^4} + \binom{m}{2},$$

where

$$\begin{aligned} a &= (2h^2+h)m^{2h+6} - (8h-1)m^{2h+5} - (4h^2+10h-12)m^{2h+4} \\ &\quad +(8h+21)m^{2h+3} + (2h^2+9h+10)m^{2h+2}, \\ b &= (h^2+h-1)m^{h+3} - (2h^2+6h+10)m^{h+2} + (h^2+5h+1)m^{h+1} \\ &\quad -m^6 + 5m^5 - 10m^4 + 10m^3 - 5m^2. \end{aligned}$$

Since by Theorem 2.10 we have $WW_e(T_{h,m}) = \frac{1}{2}W''(T_{h,m}, 1)$, we can use (2.9) to get the edge-hyper-Wiener index of $T_{h,m}$.

Theorem 2.3.7. *Let $T_{h,m}$ be a complete m-ary tree of height h. Then*

$$WW_e(T_{h,m}) = \frac{a}{2(m+1)^2(m-1)^4} + \frac{b}{2(m-1)^4} + \binom{m}{2},$$

where

$$\begin{aligned} a &= (2h^2-h)m^{2h+6}-(8h-5)m^{2h+5}-(4h^2+6h-16)m^{2h+4} \\ &\quad +(8h+17)m^{2h+3}+(2h^2+7h+6)m^{2h+2}, \\ b &= (h^2-h-5)m^{h+3}-(2h^2+2h+6)m^{h+2}+(h^2+3h+1)m^{h+1} \\ &\quad -m^6+5m^5-10m^4+10m^3-5m^2. \end{aligned}$$

Let us consider the degree distance, the Gutman index and the edge-Wiener index, Klein et al. [54] showed that for every tree T of order n,

$$DD(T) = 4W(T) - n(n-1). \tag{2.10}$$

Gutman [42] showed that

$$Gut(T) = 4W(T) - (2n-1)(n-1) \tag{2.11}$$

and from [16] we have

$$W_e(T) = W(T) - \binom{n}{2}. \tag{2.12}$$

Thus we can easily obtain the degree-distance, the Gutman index and the edge-Wiener index of complete m-ary trees.

Theorem 2.3.8. *Let $T_{h,m}$ be a complete m-ary tree of height h. Then $DD(T_{h,m})$ is*

$$\frac{(4hm-m-4h-7)m^{2h+2}+(m^2+4hm+8m-4h-1)m^{h+1}-m^2+m}{(m-1)^3}.$$

Proof. From (2.10) we have $DD(T_{h,m}) = 4W(T_{h,m}) - n(n-1)$ and Lemma

2.2.2 gives $n = \frac{m^{h+1}-1}{m-1}$. So using Theorem 2.2.6, we obtain $DD(T_{h,m})$

$$
\begin{aligned}
&= \frac{4(hm-h-2)m^{2h+2}+4(hm+2m-h)m^{h+1}}{(m-1)^3} - \frac{m^{h+1}-1}{m-1}\left(\frac{m^{h+1}-1}{m-1}-1\right) \\
&= \frac{(4hm-m-4h-7)m^{2h+2}+(m^2+4hm+8m-4h-1)m^{h+1}-m^2+m}{(m-1)^3}.
\end{aligned}
$$

□

Theorem 2.3.9. *Let $T_{h,m}$ be a complete m-ary tree of height h. Then $Gut(T_{h,m})$ is*

$$\frac{(4hm-2m-4h-6)m^{2h+2}+(3m^2+4hm+6m-4h-1)m^{h+1}-m^3+m}{(m-1)^3}.$$

Proof. From (2.11) we have $Gut(T_{h,m}) = 4W(T_{h,m}) - (2n-1)(n-1)$ and Lemma 2.2.2 gives $n = \frac{m^{h+1}-1}{m-1}$. Therefore $Gut(T_{h,m})$

$$
\begin{aligned}
&= \frac{4(hm-h-2)m^{2h+2}+4(hm+2m-h)m^{h+1}}{(m-1)^3} \\
&\quad - \left(\frac{2m^{h+1}-2}{m-1}-1\right)\left(\frac{m^{h+1}-1}{m-1}-1\right) \\
&= \frac{(4hm-2m-4h-6)m^{2h+2}+(3m^2+4hm+6m-4h-1)m^{h+1}-m^3+m}{(m-1)^3}.
\end{aligned}
$$

□

Theorem 2.3.10. *Let $T_{h,m}$ be a complete m-ary tree of height h. Then $W_e(T_{h,m})$ is*

$$\frac{(2hm-m-2h-3)m^{2h+2}+(m^2+2hm+4m-2h-1)m^{h+1}-m^2+m}{2(m-1)^3}.$$

Proof. From (2.12) we have $W_e(T_{h,m}) = W(T_{h,m}) - \binom{n}{2}$ and Lemma 2.2.2

gives $n = \frac{m^{h+1}-1}{m-1}$. Thus using Theorem 2.2.6, we get $W_e(T_{h,m})$

$$
\begin{aligned}
&= \frac{(hm-h-2)m^{2h+2}+m^{h+1}((h+2)m-h)}{(m-1)^3} - \frac{m^{h+1}-1}{2(m-1)}\left(\frac{m^{h+1}-1}{m-1}-1\right) \\
&= \frac{(2hm-m-2h-3)m^{2h+2}+(m^2+2hm+4m-2h-1)m^{h+1}-m^2+m}{2(m-1)^3}.
\end{aligned}
$$

□

We obtain values of distance-based indices for complete binary trees when using $m = 2$ in Theorems 2.2.6, 2.3.1 and Theorems 2.3.6 – 2.3.10.

Corollary 2.3.11. *For a complete binary tree $T_{h,2}$ of height h we have*

$$
\begin{aligned}
W(T_{h,2}) &= (h-2)2^{2h+2}+(h+4)2^{h+1}, \\
EDS(T_{h,2}) &= (4h^2-10h+6)2^{2h+2}+(4h^2+11h-11)2^{h+1}-2, \\
WW(T_{h,2}) &= (4h^2-14h+24)2^{2h}+(h^2-3h-23)2^h-1, \\
WW_e(T_{h,2}) &= (4h^2-18h+32)2^{2h}+(h^2-5h-31)2^h-1, \\
DD(T_{h,2}) &= (4h-9)2^{2h+2}+(4h+19)2^{h+1}-2, \\
Gut(T_{h,2}) &= (4h-10)2^{2h+2}+(4h+23)2^{h+1}-6, \\
W_e(T_{h,2}) &= (4h-10)2^{2h}+(2h+11)2^h-1.
\end{aligned}
$$

Chapter 3

General eccentric connectivity index of trees

In this chapter, we present lower and upper bounds on the general eccentric connectivity index for trees of given order, trees of given order and diameter, and trees of given order and number of pendant vertices. The upper bounds for trees of given order and diameter, and trees of given order and number of pendant vertices hold for $\alpha > 1$. All the other bounds are valid for $0 < \alpha \leq 1$ or $0 < \alpha < 1$. We present all the extremal graphs, which means that our bounds are best possible.

Note that the general eccentric connectivity index of a graph G defined as

$$ECI_\alpha(G) = \sum_{v \in V(G)} ecc(v) d^\alpha(v).$$

If $\alpha = 1$, we obtain the classical eccentric connectivity index.

Proofs of known results for the classical eccentric connectivity index do not work for the general eccentric connectivity index, therefore we use new different techniques. We use the following lemma in the proofs of our next main results.

Lemma 3.0.12. *Let* $1 \le x < y$ *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*

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

Proof. We consider the function

$$f(x) = (x+c)^a - x^a$$

for $x \ge 1$. The derivative of $f(x)$ is

$$f'(x) = a[(x+c)^{a-1} - x^{a-1}].$$

If $a > 1$, then $(x+c)^{a-1} > x^{a-1}$, so $f'(x) > 0$ and $f(x)$ is strictly increasing. Let $a < 1$. Then $1 - a = b > 0$. We get

$$(x+c)^{a-1} - x^{a-1} = \left(\frac{1}{x+c}\right)^b - \left(\frac{1}{x}\right)^b < 0$$

since $0 < \frac{1}{x+c} < \frac{1}{x} \le 1$ and $\left(\frac{1}{x+c}\right)^b < \left(\frac{1}{x}\right)^b$. Therefore, if $a < 0$, we have $f'(x) > 0$ and $f(x)$ is a strictly increasing function. If $0 < a < 1$, we obtain $f'(x) < 0$ and $f(x)$ is strictly decreasing.

Thus for $a > 1$ or $a < 0$, if $x < y$, then $f(x) < f(y)$, so

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

For $0 < a < 1$, if $x < y$, then $f(x) > f(y)$ and

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

□

3.1 Trees of given order

We present bounds on the general eccentric connectivity index for trees having n vertices, where $0 < \alpha < 1$. In Theorem 3.1.2 we include also the case $\alpha = 1$. The only tree with three vertices is the path P_3, so we can assume that $n \geq 4$.

Theorem 3.1.1. *Let T be any tree of order $n \geq 4$. Then for $0 < \alpha < 1$ we have*

$$ECI_\alpha(T) \geq (n-1)^\alpha + 2(n-1)$$

with equality if and only if T is S_n.

Proof. The star S_n contains one vertex of eccentricity 1 and degree $n-1$, and $n-1$ vertices of eccentricity 2 and degree 1. Thus $ECI_\alpha(S_n) = (n-1)^\alpha + 2(n-1)$.

Let T' be a tree having the smallest ECI_α index among trees with n vertices. We prove that T' is the star S_n.

Assume to the contrary that T' is not S_n. Let $v_0v_1v_2\ldots v_d$ be a diametral path in T'. Clearly, $d \geq 3$. Let $d_{T'}(v_1) = p$ and $d_{T'}(v_{d-1}) = q$. We can assume that $p \geq q$. Let $V(T'') = V(T')$ and $E(T'') = \{v_1v_d\} \cup E(T') \setminus \{v_{d-1}v_d\}$. Then $d_{T''}(v_1) = p+1$ and $d_{T''}(v_{d-1}) = q-1$. We have $ecc_{T'}(v_{d-1}) = ecc_{T''}(v_{d-1}) =$

$ecc_{T'}(v_1) = d-1$ and $d-2 \leq ecc_{T''}(v_1) \leq d-1$. For all $x \in V(T) \setminus \{v_1, v_{d-1}\}$, $d_{T'}(x) = d_{T''}(x)$ and $ecc_{T'}(x) \geq ecc_{T''}(x)$. Thus

$$\begin{aligned} ECI_\alpha(T') - ECI_\alpha(T'') &\geq ecc_{T'}(v_1)d^\alpha_{T'}(v_1) - ecc_{T''}(v_1)d^\alpha_{T''}(v_1) \\ &\quad + ecc_{T'}(v_{d-1})d^\alpha_{T'}(v_{d-1}) - ecc_{T''}(v_{d-1})d^\alpha_{T''}(v_{d-1}) \\ &\geq (d-1)[p^\alpha - (p+1)^\alpha] + (d-1)[q^\alpha - (q-1)^\alpha]. \end{aligned}$$

By Lemma 3.0.12, $[p^\alpha - (p+1)^\alpha] + [q^\alpha - (q-1)^\alpha] > 0$, so $ECI_\alpha(T') > ECI_\alpha(T'')$, which is a contradiction. The proof is complete. □

Theorem 3.1.2. *Let T be any tree of order $n \geq 4$. Then for $0 < \alpha \leq 1$ we have*

$$ECI_\alpha(T) \leq \left\lfloor \frac{3n^2 - 10n + 8}{2} \right\rfloor 2^{\alpha-1} + 2(n-1)$$

with equality if and only if T is P_n.

Proof. Let T' be a tree having the largest ECI_α index among trees with n vertices. We prove by contradiction that T' is the path P_n.

Assume that T' is not P_n. Let $v_0v_1v_2\ldots v_d$ be a diametral path in T'. Clearly, T' contains a pendant vertex, say u, such that $u \notin \{v_0, v_d\}$. We denote the vertex adjacent to u in T' by w. We define a tree T'' with $V(T'') = V(T')$ and $E(T'') = \{uv_0\} \cup E(T') \setminus \{uw\}$.

For any vertex x in T', $ecc_{T'}(x) = d_{T'}(x, v_0)$ or $ecc_{T'}(x) = d_{T'}(x, v_d)$. Thus, without loss of generality, assume that $ecc_{T'}(w) = d_{T'}(w, v_0)$. Then $ecc_{T''}(w) = d_{T''}(w, u) = ecc_{T'}(w) + 1$. We get $ecc_{T'}(u) \leq d$, $ecc_{T''}(u) = d+1$ and $ecc_{T'}(v_0) = ecc_{T''}(v_0) = d$. Let $S = \{u, w, v_0\}$. For all $x \in V(T') \setminus S$, we have $ecc_{T''}(x) \geq ecc_{T'}(x)$.

Let $d_{T'}(w) = p \geq 2$. Then $d_{T''}(w) = p-1$, $d_{T'}(u) = d_{T''}(u) = 1$, $d_{T'}(v_0) = 1$,

$d_{T''}(v_0) = 2$, and $d_{T''}(x) = d_{T'}(x)$ for $x \in V(T') \setminus S$. Then

$$\begin{aligned}
ECI_\alpha(T'') - ECI_\alpha(T') &= \sum_{v \in V(T') \setminus S} [ecc_{T''}(v) d^\alpha_{T''}(v) - ecc_{T'}(v) d^\alpha_{T'}(v)] \\
&\quad + \sum_{v \in S} [ecc_{T''}(v) d^\alpha_{T''}(v) - ecc_{T'}(v) d^\alpha_{T'}(v)] \\
&\geq \sum_{v \in S} [ecc_{T''}(v) d^\alpha_{T''}(v) - ecc_{T'}(v) d^\alpha_{T'}(v)] \\
&\geq [ecc_{T'}(w) + 1](p-1)^\alpha - ecc_{T'}(w) p^\alpha \\
&\quad + (d+1)1^\alpha - d \cdot 1^\alpha + d \cdot 2^\alpha - d \cdot 1^\alpha \\
&= ecc_{T'}(w)[(p-1)^\alpha - p^\alpha] \\
&\quad + (p-1)^\alpha + 1 + d(2^\alpha - 1) \\
&\geq ecc_{T'}(w)[(p-1)^\alpha - p^\alpha] \\
&\quad + (p-1)^\alpha + 1 + ecc_{T'}(w)(2^\alpha - 1)
\end{aligned}$$

Let $f(p) = ecc_{T'}(w)[(p-1)^\alpha - p^\alpha + 2^\alpha - 1] + (p-1)^\alpha + 1$. Then $f'(p) = \alpha\left[(ecc_{T'}(w)+1)(p-1)^{\alpha-1} - ecc_{T'}(w) p^{\alpha-1}\right]$. For $0 < \alpha \leq 1$ we have $(p-1)^{\alpha-1} \geq p^{\alpha-1}$, thus $f'(p) > 0$ which means that $f(p)$ is increasing. So $f(p) \geq f(2) = 2 > 0$. This implies that $ECI_\alpha(T'') - ECI_\alpha(T') > 0$ and $ECI_\alpha(T'') > ECI_\alpha(T')$, a contradiction.

Hence P_n is the tree with the largest ECI_α index. If n is even, then

$$ECI_\alpha(P_n) = \left(\frac{3n^2 - 10n + 8}{4}\right) 2^\alpha + 2(n-1).$$

If n is odd, then

$$ECI_\alpha(P_n) = \left(\frac{3n^2 - 10n + 7}{4}\right) 2^\alpha + 2(n-1).$$

This implies that for any $n \geq 4$,

$$ECI_\alpha(P_n) = \left\lfloor \frac{3n^2 - 10n + 8}{2} \right\rfloor 2^{\alpha-1} + 2(n-1).$$

□

3.2 Trees of given order and diameter

Let us investigate bounds on the general eccentric connectivity index for trees with n vertices and diameter d. We know that $2 \leq d \leq n-1$.

Let $V_{n,d}$ be a tree which consists of the path of length d and all the other $n-d-1$ vertices are adjacent to one central vertex of that path. We prove that $V_{n,d}$ is the unique tree having the smallest general eccentric connectivity index among trees with n vertices and diameter d.

Theorem 3.2.1. *Let T be any tree of order $n \geq 4$ and diameter d. Then for $0 < \alpha \leq 1$ we have*

$$ECI_\alpha(T) \;\geq\; \begin{cases} (3d^2-6d)2^{\alpha-2} + \frac{d(n-d+1)^\alpha}{2} + \frac{dn+2n-d^2+d-2}{2} & \text{if } d \text{ is even,} \\ (3d^2-6d-1)2^{\alpha-2} + \frac{(d+1)(n-d+1)^\alpha}{2} + \frac{dn+3n-d^2-3}{2} & \text{if } d \text{ is odd,} \end{cases}$$

with equality if and only if T is $V_{n,d}$.

Proof. Note that the only tree of diameter 2 is $S_n \cong V_{n,2}$ and the only tree of diameter $n-1$ is $P_n \cong V_{n,n-1}$. So we can assume that $3 \leq d \leq n-2$.

Let T' be a tree having the smallest ECI_α index among trees with n vertices and diameter d. We prove by contradiction that T' is $V_{n,d}$.

Let us assume that for some n and d, there exists a tree $T'_{n,d}$ of order n and diameter d with $ECI_\alpha(T'_{n,d}) \leq ECI_\alpha(V_{n,d})$ (where $T'_{n,d}$ is not $V_{n,d}$). Let $T'_{n^*,d}$ be a tree with the smallest possible order n^* such that $ECI_\alpha(T'_{n^*,d}) \leq ECI_\alpha(V_{n^*,d})$.

Let $v_0v_1v_2\ldots v_d$ be a diametral path in $T'_{n^*,d}$. Then $T'_{n^*,d}$ contains a pendant vertex, say u, such that $u \notin \{v_0, v_d\}$. We denote the vertex adjacent to u in $T'_{n^*,d}$ by w. Let $V(T'_{n^*-1,d}) = V(T'_{n^*,d})\setminus\{u\}$ and $E(T'_{n^*-1,d}) = E(T'_{n^*,d})\setminus\{uw\}$. Then $T'_{n^*-1,d}$ is a tree of order n^*-1 and diameter d.

Let $d_{T'_{n^*,d}}(w) = p$. Then $2 \leq p \leq n^* - d + 1$. We have $d_{T'_{n^*-1,d}}(w) = p - 1$, $d_{T'_{n^*,d}}(u) = 1$ and $d_{T'_{n^*-1,d}}(x) = d_{T'_{n^*,d}}(x)$ for all $x \in V(T'_{n^*,d}) \setminus \{u, w\}$. We also know that $ecc_{T'_{n^*,d}}(u) \geq \lceil \frac{d}{2} \rceil + 1$, $ecc_{T'_{n^*-1,d}}(w) = ecc_{T'_{n^*,d}}(w) \geq \lceil \frac{d}{2} \rceil$ and $ecc_{T'_{n^*-1,d}}(x) = ecc_{T'_{n^*,d}}(x)$ for $x \in V(T'_{n^*,d}) \setminus \{u, w\}$. Thus

$$\begin{aligned}
ECI_\alpha(T'_{n^*,d}) - ECI_\alpha(T'_{n^*-1,d}) &\geq ecc_{T'_{n^*,d}}(u)d^\alpha_{T'_{n^*,d}}(u) + ecc_{T'_{n^*,d}}(w)d^\alpha_{T'_{n^*,d}}(w) \\
&\quad - ecc_{T'_{n^*-1,d}}(w)d^\alpha_{T'_{n^*-1,d}}(w) \\
&= ecc_{T'_{n^*,d}}(u) + ecc_{T'_{n^*,d}}(w)p^\alpha \\
&\quad - ecc_{T'_{n^*,d}}(w)(p-1)^\alpha \\
&\geq \left\lceil \frac{d}{2} \right\rceil + 1 + \left\lceil \frac{d}{2} \right\rceil (p^\alpha - (p-1)^\alpha) \\
&= \left\lceil \frac{d}{2} \right\rceil (p^\alpha - (p-1)^\alpha + 1) + 1.
\end{aligned}$$

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

$$\begin{aligned} ECI_\alpha(T'_{n^*,d}) - ECI_\alpha(T'_{n^*-1,d}) &< ECI_\alpha(V_{n^*,d}) - ECI_\alpha(V_{n^*-1,d}) \\ &= \left\lceil \frac{d}{2} \right\rceil ((n^* - d + 1)^\alpha - (n^* - d)^\alpha + 1) + 1. \end{aligned}$$

So

$$\left\lceil \frac{d}{2} \right\rceil (p^\alpha - (p-1)^\alpha + 1) + 1 < \left\lceil \frac{d}{2} \right\rceil ((n^* - d + 1)^\alpha - (n^* - d)^\alpha + 1) + 1$$

and

$$p^\alpha - (p-1)^\alpha < (n^* - d + 1)^\alpha - (n^* - d)^\alpha,$$

which is a contradiction, since $2 \le p \le n^* - d + 1$ (see Lemma 3.0.12).

Thus T' is $V_{n,d}$. It remains to find $ECI_\alpha(V_{n,d})$. We have

$$ECI_\alpha(V_{n,d}) = (3d^2 - 6d)2^{\alpha-2} + \frac{d(n-d+1)^\alpha}{2} + \frac{dn + 2n - d^2 + d - 2}{2}$$

for even d, and

$$ECI_\alpha(V_{n,d}) = (3d^2 - 6d - 1)2^{\alpha-2} + \frac{(d+1)(n-d+1)^\alpha}{2} + \frac{dn + 3n - d^2 - 3}{2}$$

for odd d, hence the proof is complete. □

Let $B_{n,d}$ be a tree which consists of the path $v_0 v_1 v_2 \ldots v_d$ and all the other $n - d - 1$ vertices are attached to v_1. We present the sharp upper bound on the general eccentric connectivity index for trees with n vertices and diameter d.

Theorem 3.2.2. *Let T be any tree of order $n \ge 4$ and diameter d. Then* *for $\alpha > 1$ we have*

$$ECI_\alpha(T) \leq \left\lfloor \frac{3d^2 - 8d + 5}{2} \right\rfloor 2^{\alpha-1} + (d-1)(n-d+1)^\alpha + d(n-d+1)$$

with equality if and only if T is $B_{n,d}$.

Proof. Note that the only tree of diameter 2 is $S_n \cong B_{n,2}$ and the only tree of diameter $n-1$ is $P_n \cong B_{n,n-1}$. So we can assume that $3 \leq d \leq n-2$.

Let T' be a tree having the largest ECI_α index among trees with n vertices and diameter d. We prove by contradiction that T' is $B_{n,d}$.

Let us assume that T' is not $B_{n,d}$. Let $D = v_0v_1v_2 \ldots v_d$ be a diametral path in T'. Without loss of generality, we assume that $d_{T'}(v_1) \geq d_{T'}(v_{d-1})$.

Then there exists a nonpendant vertex $w \notin V(D)$ whose all neighbors except for one are pendant vertices or a nonpendant vertex $w \in V(D) \setminus \{v_1\}$ whose all neighbors which are not in D are pendant vertices. Note that if $V(T') \setminus V(D)$ contains a nonpenadnt vertex, then w can be any nonpendant vertex furthest from D. If all nonpendant vertices are in D, then w is any vertex in $V(D) \setminus \{v_1\}$ having degree at least 3 (since T' is not $B_{n,d}$, such a vertex does exist). We denote the pendant vertices adjacent to w in T' by $w_1, w_2, \ldots, w_p$, where $p \geq 1$. It follows that $d_{T'}(w) = p + \epsilon$, where $\epsilon = 1$ or 2.

Let T'' be a tree with $V(T'') = V(T')$ and $E(T'') = \{v_1w_1, v_1w_2, \ldots, v_1w_p\}$ $\cup E(T') \setminus \{ww_1, ww_2, \ldots, ww_p\}$. Then T'' has order n and diameter d. We have $d_{T'}(v_1) = q \geq 2$. Then $d_{T''}(v_1) = q + p$ and $d_{T''}(w) = \epsilon$. We obtain $ecc_{T'}(v_1) = ecc_{T''}(v_1) = d - 1$, $ecc_{T'}(w) = ecc_{T''}(w) \leq d - 1$, $ecc_{T'}(w_i) \leq d$ and $ecc_{T''}(w_i) = d$, where $i = 1, 2, \ldots, p$. For all $x \in V(T') \setminus \{v_1, w\}$, $d_{T'}(x) = d_{T''}(x)$ and for $x \in V(T') \setminus \{w_1, w_2, \ldots, w_p\}$, $ecc_{T'}(x) = ecc_{T''}(x)$.

Thus

$$\begin{aligned}
ECI_\alpha(T'')-ECI_\alpha(T') &= ecc_{T''}(v_1)d^\alpha_{T''}(v_1) - ecc_{T'}(v_1)d^\alpha_{T'}(v_1) \\
&\quad + ecc_{T''}(w)d^\alpha_{T''}(w) - ecc_{T'}(w)d^\alpha_{T'}(w) \\
&\quad + \sum_{i=1}^{p}(ecc_{T''}(w_i)d^\alpha_{T''}(w_i) - ecc_{T'}(w_i)d^\alpha_{T'}(w_i)) \\
&= (d-1)[(q+p)^\alpha - q^\alpha] + ecc_{T'}(w)[\epsilon^\alpha - (p+\epsilon)^\alpha] \\
&\quad + p[d - ecc_{T'}(w_1)] \\
&\geq (d-1)[(q+p)^\alpha - q^\alpha] + (d-1)[\epsilon^\alpha - (p+\epsilon)^\alpha] \quad (3.1)
\end{aligned}$$

If $q > 2$, then by Lemma 3.0.12,

$$(q+p)^\alpha - q^\alpha > (p+\epsilon)^\alpha - \epsilon^\alpha,$$

which implies that $ECI_\alpha(T'') - ECI_\alpha(T') > 0$ and $ECI_\alpha(T'') > ECI_\alpha(T')$.

If $q = 2$, then by Lemma 3.0.12, $(q+p)^\alpha - q^\alpha \geq (p+\epsilon)^\alpha - \epsilon^\alpha$ with equality if and only if $\epsilon = 2$, which means that $w \in V(D)$. Then the equality in (3.1) occurs only if $ecc_{T''}(w) = d-1$, which implies that $w = v_{d-1}$. But we assumed that $d_{T'}(v_1) \geq d_{T'}(v_{d-1})$ which means that $d_{T'}(v_{d-1}) = 2$, so $p = 0$ and v_{d-1} is not adjacent to pendant vertices not in D. This is not possible, therefore we again get $ECI_\alpha(T'') > ECI_\alpha(T')$, which is a contradiction.

So T' is $B_{n,d}$. We get

$$ECI_\alpha(B_{n,d}) = \left(\frac{3d^2-8d+4}{4}\right)2^\alpha + (d-1)(n-d+1)^\alpha + d(n-d+1)$$

for even d, and

$$ECI_\alpha(B_{n,d}) = \left(\frac{3d^2-8d+5}{4}\right)2^\alpha + (d-1)(n-d+1)^\alpha + d(n-d+1)$$

for odd d. This implies that for any $n \geq 4$,

$$ECI_\alpha(B_{n,d}) = \left\lfloor \frac{3d^2 - 8d + 5}{2} \right\rfloor 2^{\alpha-1} + (d-1)(n-d+1)^\alpha + d(n-d+1),$$

hence the proof is complete. □

3.3 Trees of given order and number of pendant vertices

In this section we study trees with n vertices and p pendant vertices. Clearly, $2 \leq p \leq n-1$. Let $X_{n,p}$ be a tree which consists of p paths attached to one vertex, such that the lengths of any two paths differ by at most one. We obtain the sharp lower bounds on the general eccentric connectivity index for trees with n vertices and p pendant vertices.

Theorem 3.3.1. *Let T be any tree having order $n \geq 4$ and p pendant vertices. Let $k = \lfloor \frac{n-1}{p} \rfloor$. Then for $0 < \alpha < 1$ we have*

$$ECI_\alpha(T) \geq \left\lceil \frac{3(n-1)(n-p-1)}{p} \right\rceil 2^{\alpha-1} + (n-1)p^{\alpha-1} + 2(n-1)$$

if $n \equiv 1$ (mod p),

$$ECI_\alpha(T) \geq (3pk^2 - pk - 2p + 2k + 2)2^{\alpha-1} + (k+1)p^\alpha + (2k+1)p$$

if $n \equiv 2$ (mod p),

$$ECI_\alpha(T) \geq [(4k+2)(n-1) - (k^2+3k+2)p]2^{\alpha-1} + (k+1)p^\alpha + (k+1)p + n - 1$$

otherwise, with equalities if and only if T is $X_{n,p}$.

Proof. The only tree with 2 pendant vertices is P_n and the only tree with $n-1$ pendant vertices is S_n, so we can assume that $3 \leq p \leq n-2$.

Let T' be a tree having the smallest ECI_α index among trees with n vertices and p pendant vertices. We prove that T' is $X_{n,p}$.

Let $D = v_0v_1v_2 \dots v_d$ be a diametral path in T'. We know that every tree has at most 2 central vertices. Let u be a central vertex with maximum degree, say $d_{T'}(u) = q \geq 2$. Clearly, $u = v_{\lfloor \frac{d}{2} \rfloor}$ or $v_{\lceil \frac{d}{2} \rceil}$. Note that $ecc_{T'}(u) = \lceil \frac{d}{2} \rceil$.

Claim 3.3.1. *The degree of every vertex in $V(T') \setminus \{u\}$ is at most 2.*

Assume to the contrary that there exists a vertex w ($\neq u$) such that $d_{T'}(w) = r \geq 3$. Let $w_1, w_2, \dots, w_{r-2}$ be any $r-2$ neighbors of w not in D and not on the path between u and w.

Let T'' be a tree with $V(T'') = V(T')$ and $E(T'') = \{uw_1, uw_2, \dots, uw_{r-2}\} \cup E(T') \setminus \{ww_1, ww_2, \dots, ww_{r-2}\}$. Clearly, T'' has p pendant vertices. We have $d_{T''}(u) = q + r - 2$, $d_{T''}(w) = 2$ and $d_{T'}(x) = d_{T''}(x)$ for all $x \in V(T') \setminus \{u, w\}$.

For each $i = 1, 2, \dots, r-2$, there is no path in T' with the first vertex w and the second vertex w_i which is longer than $\lceil \frac{d}{2} \rceil$. We also know that for every vertex x in T', $ecc_{T'}(x) = d_{T'}(x, v_0)$ or $d_{T'}(x, v_d)$ (which is at least $\lceil \frac{d}{2} \rceil$). Thus $ecc_{T''}(x) \leq ecc_{T'}(x)$ for all $x \in V(T')$. It follows that

$$\begin{aligned} ECI_\alpha(T'') - ECI_\alpha(T') &\leq ecc_{T''}(u)d^\alpha_{T''}(u) - ecc_{T'}(u)d^\alpha_{T'}(u) \\ &\quad + ecc_{T''}(w)d^\alpha_{T''}(w) - ecc_{T'}(w)d^\alpha_{T'}(w) \end{aligned}$$

$$
\begin{aligned}
&\leq \; ecc_{T'}(u)[d^{\alpha}_{T''}(u) - d^{\alpha}_{T'}(u)] \\
&\quad - ecc_{T'}(w)[d^{\alpha}_{T'}(w) - d^{\alpha}_{T''}(w)] \\
&= \; ecc_{T'}(u)[(q+r-2)^{\alpha} - q^{\alpha}] - ecc_{T'}(w)[r^{\alpha} - 2^{\alpha}] \\
&\leq \; ecc_{T'}(w)[(q+r-2)^{\alpha} - q^{\alpha} - (r^{\alpha} - 2^{\alpha})].
\end{aligned}
$$

If $q \geq 3$, then by Lemma 3.0.12,

$$(q+r-2)^{\alpha} - q^{\alpha} < r^{\alpha} - 2^{\alpha},$$

which gives $ECI_{\alpha}(T'') - ECI_{\alpha}(T') < 0$ and $ECI_{\alpha}(T'') < ECI_{\alpha}(T')$.

Let $q = 2$. Since u is a central vertex with maximum degree and $d_{T'}(u) = 2$, it follows that w is not a central vertex, so $ecc_{T'}(w) \geq ecc_{T'}(u) + 1 = \lceil \frac{d}{2} \rceil + 1$. Then

$$
\begin{aligned}
ECI_{\alpha}(T'') - ECI_{\alpha}(T') &\leq ecc_{T'}(u)[(q+r-2)^{\alpha} - q^{\alpha}] - ecc_{T'}(w)[r^{\alpha} - 2^{\alpha}] \\
&\leq ecc_{T'}(u)[(q+r-2)^{\alpha} - q^{\alpha}] - (ecc_{T'}(u)+1)[r^{\alpha} - 2^{\alpha}] \\
&= ecc_{T'}(u)[(q+r-2)^{\alpha} - q^{\alpha} - (r^{\alpha} - 2^{\alpha})] - (r^{\alpha} - 2^{\alpha}) \\
&= 2^{\alpha} - r^{\alpha} < 0.
\end{aligned}
$$

Hence, $ECI_{\alpha}(T'') < ECI_{\alpha}(T')$, which is a contradiction.

Thus $d_{T'}(x) \leq 2$ for each $x \in V(T') \setminus \{u\}$. So T' consists of p paths attached to u. Since u is a central vertex of T', two longest paths attached to u differ by at most 1. Let $uu_1u_2 \ldots u_t$ and $uu'_1u'_2 \ldots u'_{t-\epsilon}$, where $\epsilon = 0$ or 1, be those two paths.

We prove that the lengths of any two paths starting at u differ by at most one. Assume to the contrary that there are two paths, whose lengths differ by at least 2. It means that there is a path $uu''_1u''_2\dots u''_s$ in T', such that $1 \le s \le t-2$ and $d_{T'}(u''_s) = 1$.

Let $V(T'') = V(T')$ and $E(T'') = \{u_{t-1}u''_{s-1}, u_{t-1}u''_s, u_{t-2}u_t\} \cup E(T') \setminus \{u''_{s-1}u''_s, u_{t-2}u_{t-1}, u_{t-1}u_t\}$. Then T' is a tree with the same pendant vertices. Note that if $s = 1$, then $u''_{s-1} = u$. We have $d_{T'}(u''_s) = d_{T''}(u''_s) = d_{T'}(u_t) = d_{T''}(u_t) = 1$ and $d_{T'}(u_{t-1}) = d_{T''}(u_{t-1}) = 2$. Moreover, $d_{T'}(x) = d_{T''}(x)$ for all $x \in V(T')$. We also know that $ecc_{T'}(u''_s) = s+t$, $ecc_{T''}(u''_s) = (s+1)+t-\epsilon$, $ecc_{T'}(u_t) = 2t-\epsilon$, $ecc_{T''}(u_t) = (t-1)+(t-\epsilon)$, $ecc_{T'}(u_{t-1}) = (t-1)+(t-\epsilon)$ and $ecc_{T''}(u_{t-1}) = s+(t-\epsilon)$. Note that $ecc_{T''}(x) \le ecc_{T'}(x)$ for all $x \in V(T') \setminus \{u''_s\}$. Then

$$\begin{aligned} ECI_\alpha(T') - ECI_\alpha(T'') &\ge ecc_{T'}(u''_s)d^\alpha_{T'}(u''_s) - ecc_{T''}(u''_s)d^\alpha_{T''}(u''_s) \\ &\quad + ecc_{T'}(u_t)d^\alpha_{T'}(u_t) - ecc_{T''}(u_t)d^\alpha_{T''}(u_t) \\ &\quad + ecc_{T'}(u_{t-1})d^\alpha_{T'}(u_{t-1}) - ecc_{T''}(u_{t-1})d^\alpha_{T''}(u_{t-1}) \\ &= (s+t) - (s+t-\epsilon+1) + (2t-\epsilon) - (2t-\epsilon-1) \\ &\quad + [(2t-\epsilon-1) - (s+t-\epsilon)]2^\alpha \\ &= (t-s-1)2^\alpha + \epsilon > 0, \end{aligned}$$

so $ECI_\alpha(T') > ECI_\alpha(T'')$, a contradiction.

Thus T' is $X_{n,p}$. It remains to find $ECI_\alpha(X_{n,p})$. We write $d^\alpha(u)$ and $ecc(u)$ instead of $d^\alpha_{X_{n,p}}(u)$ and $ecc_{X_{n,p}}(u)$, respectively. Since the lengths of any two paths with the first vertex u differ by at most one, the lengths of any path that starts at u is $\lfloor \frac{n-1}{p} \rfloor$ or $\lceil \frac{n-1}{p} \rceil$. Let $k = \lfloor \frac{n-1}{p} \rfloor$. So $X_{n,p}$ has $(n-1)-kp$ paths of length $k+1$ and $(k+1)p-n+1$ paths of length k.

Let $n \equiv 1 \pmod p$. Then each path with the first vertex u (say $Q =$

$uu_1u_2\dots u_k$) has length $\frac{n-1}{p}$. Then

$$\begin{aligned}\sum_{i=1}^{k} ecc(u_i)d^\alpha(u_i) &= 1^\alpha 2k + [(2k-1)+(2k-2)+\cdots+(k+1)]2^\alpha \\ &= 3k(k-1)2^{\alpha-1}+2k\end{aligned}$$

and

$$\begin{aligned}ECI_\alpha(X_{n,p}) &= ecc(u)d^\alpha(u) + p\sum_{i=1}^{k} ecc(u_i)d^\alpha(u_i) \\ &= kp^\alpha + p[3k(k-1)2^{\alpha-1}+2k] \\ &= \left[\frac{3(n-1)(n-p-1)}{p}\right]2^{\alpha-1} + (n-1)p^{\alpha-1} + 2(n-1).\end{aligned}$$

Let $n \equiv 2 \pmod{p}$. Then we have $p-1$ paths of length k and one path of length $k+1$ starting at u. Let $Q = uu_1u_2\dots u_k$ be a path of length k. Then

$$\begin{aligned}\sum_{i=1}^{k} ecc(u_i)d^\alpha(u_i) &= (2k+1)1^\alpha + [(2k)+(2k-1)+\cdots+(k+2)]2^\alpha \\ &= (3k^2-k-2)2^{\alpha-1}+2k+1.\end{aligned}$$

Let $Q' = uu'_1u'_2\dots u'_{k+1}$ be the path of length $k+1$. Then

$$\begin{aligned}\sum_{i=1}^{k+1} ecc(u'_i)d^\alpha(u'_i) &= (2k+1)1^\alpha + [(2k)+(2k-1)+\cdots+(k+1)]2^\alpha \\ &= (3k^2+k)2^{\alpha-1}+2k+1.\end{aligned}$$

Consequently, we obtain

$$ECI_\alpha(X_{n,p}) = ecc(u)d^\alpha(u) + (p-1)\sum_{i=1}^{k} ecc(u_i)d^\alpha(u_i) + \sum_{i=1}^{k+1} ecc(u'_i)d^\alpha(u'_i)$$

$$
\begin{aligned}
&= (k+1)p^\alpha + (p-1)[(3k^2-k-2)2^{\alpha-1} + 2k+1] \\
&\quad + (3k^2+k)2^{\alpha-1} + 2k+1 \\
&= (3pk^2 - pk - 2p + 2k + 2)2^{\alpha-1} + (k+1)p^\alpha + (2k+1)p.
\end{aligned}
$$

Let $n \not\equiv 1 \pmod{p}$ and $n \not\equiv 2 \pmod{p}$. Then there are $(n-1)-kp$ paths of length $k+1$ and $(k+1)p-n+1$ paths of length k starting at u. Let $Q = uu_1u_2\dots u_k$ be a path of length k. Then

$$
\begin{aligned}
\sum_{i=1}^{k} ecc(u_i)d^\alpha(u_i) &= (2k+1)1^\alpha + [(2k)+(2k-1)+\cdots+(k+2)]2^\alpha \\
&= (3k^2-k-2)2^{\alpha-1} + 2k+1.
\end{aligned}
$$

Let $Q' = uu'_1u'_2\dots u'_{k+1}$ be a path of length $k+1$. Then

$$
\begin{aligned}
\sum_{i=1}^{k+1} d^\alpha(u'_i)ecc(u'_i) &= (2k+2)1^\alpha + [(2k+1)+(2k)+\cdots+(k+2)]2^\alpha \\
&= (3k^2+3k)2^{\alpha-1} + 2k+2.
\end{aligned}
$$

Then

$$
\begin{aligned}
ECI_\alpha(X_{n,p}) &= ecc(u)d^\alpha(u) + [(k+1)p-n+1]\sum_{i=1}^{k} ecc(u_i)d^\alpha(u_i) \\
&\quad + [(n-1)-kp]\sum_{i=1}^{k+1} d^\alpha(u'_i)ecc(u'_i) \\
&= (k+1)p^\alpha + [(k+1)p-n+1][(3k^2-k-2)2^{\alpha-1}+2k+1] \\
&\quad + (n-1-kp)[(3k^2+3k)2^{\alpha-1}+2k+2] \\
&= [(4k+2)(n-1)-(k^2+3k+2)p]2^{\alpha-1} \\
&\quad + (k+1)p^\alpha + (k+1)p + n - 1.
\end{aligned}
$$

□

Let $B'_{n,p}$ be a tree which consists of the path $v_1v_2\ldots v_{n-p+1}$ and all the other $p-1$ vertices are attached to v_1. It is easy to see that $B'_{n,p} \cong B_{n,n-p+1}$. We show that $ECI_\alpha(T) \leq ECI_\alpha(B'_{n,p})$ for every tree having n vertices and p pendant vertices.

Theorem 3.3.2. *Let T be any tree having order $n \geq 4$ and p pendant vertices. Then for $\alpha > 1$ we have*

$$ECI_\alpha(T) \leq \left\lfloor \frac{3(n-p)^2 - 2(n-p)}{2} \right\rfloor 2^{\alpha-1} + (n-p)p^\alpha + (n-p+1)p$$

with equality if and only if T is $B'_{n,p}$.

Proof. The only tree with 2 pendant vertices is $P_n \cong B'_{n,2}$ and the only tree with $n-1$ pendant vertices is $S_n \cong B'_{n,n-1}$, thus we can assume that $3 \leq p \leq n-2$.

Let T' be a tree having the largest ECI_α index among trees with n vertices and p pendant vertices. We prove by contradiction that T' is $B'_{n,p}$.

Assume that T' is not $B'_{n,p}$. Let $P : v_0v_1v_2\ldots v_d$ be a longest path in T'. We can assume that $d_{T'}(v_1) \geq d_{T'}(v_{d-1})$. Since T' is not $B'_{n,p}$, there exists a vertex $w \in \{v_2, v_3, \ldots, v_{d-1}\}$, where $d_{T'}(w) = r \geq 3$. Let $w_1, w_2, \ldots, w_{r-2}$ be vertices adjacent to w which are not in P.

Let $V(T'') = V(T')$ and $E(T'') = \{v_1w_1, v_1w_2, \ldots, v_1w_{r-2}\} \cup E(T') \setminus \{ww_1, ww_2, \ldots, ww_{r-2}\}$. We have $d_{T'}(v_1) = q \geq 2$. Then $d_{T''}(v_1) = q + r - 2$, $d_{T''}(w) = 2$ and $d_{T'}(x) = d_{T''}(x)$ for all $x \in V(T') \setminus \{v_1, w\}$. It is obvious that $ecc_{T'}(x) \leq$

$ecc_{T''}(x)$ for all $x \in V(T')$. Thus

$$\begin{aligned}
ECI_\alpha(T'') - ECI_\alpha(T') &\geq ecc_{T''}(v_1)d^\alpha_{T''}(v_1) - ecc_{T'}(v_1)d^\alpha_{T'}(v_1) \\
&\quad + ecc_{T''}(w)d^\alpha_{T''}(w) - ecc_{T'}(w)d^\alpha_{T'}(w) \\
&\geq ecc_{T'}(v_1)[d^\alpha_{T''}(v_1) - d^\alpha_{T'}(v_1)] \\
&\quad + ecc_{T'}(w)[d^\alpha_{T''}(w) - d^\alpha_{T'}(w)] \\
&= ecc_{T'}(v_1)[(q+r-2)^\alpha - q^\alpha] + ecc_{T'}(w)[2^\alpha - r^\alpha] \\
&\geq ecc_{T'}(w)[(q+r-2)^\alpha - q^\alpha + 2^\alpha - r^\alpha].
\end{aligned}$$

If $q \geq 3$, then by Lemma 3.0.12,

$$(q+r-2)^\alpha - q^\alpha > r^\alpha - 2^\alpha,$$

which gives $ECI_\alpha(T'') - ECI_\alpha(T') > 0$ and $ECI_\alpha(T'') > ECI_\alpha(T')$.

If $q = 2$, then $(q+r-2)^\alpha - q^\alpha + 2^\alpha - r^\alpha = 0$. We know that $d_{T'}(v_1) \geq d_{T'}(v_{d-1})$, so $w \neq v_{d-1}$ (since $d_{T'}(w) = r \geq 3$). Thus $w \in \{v_2, v_3, \ldots, v_{d-2}\}$, which means that $ecc_{T'}(w) \leq d-2$ and $ecc_{T'}(w_i) \leq d-1$ for $i = 1, 2, \ldots, r-2$. On the other hand, $ecc_{T''}(w_i) = d$. Since

$$ecc_{T''}(v_1)d^\alpha_{T''}(v_1) - ecc_{T'}(v_1)d^\alpha_{T'}(v_1) + ecc_{T''}(w)d^\alpha_{T''}(w) - ecc_{T'}(w)d^\alpha_{T'}(w) \geq 0,$$

we have

$$\begin{aligned}
ECI_\alpha(T'') - ECI_\alpha(T') &\geq \sum_{i=1}^{r-2}[ecc_{T''}(w_i)d^\alpha_{T''}(w_i) - ecc_{T'}(w_i)d^\alpha_{T'}(w_i)] \\
&\geq \sum_{i=1}^{r-2}[d \cdot d^\alpha_{T''}(w_i) - (d-1)d^\alpha_{T'}(w_i)].
\end{aligned}$$

We have $d^{\alpha}_{T''}(w_i) = d^{\alpha}_{T'}(w_i)$, thus $ECI_{\alpha}(T'') - ECI_{\alpha}(T') \geq \sum_{i=1}^{r-2} d^{\alpha}_{T''}(w_i) > 0$. Hence, $ECI_{\alpha}(T'') > ECI_{\alpha}(T')$, which is a contradiction.

Thus T' is $B'_{n,p}$. We have

$$ECI_{\alpha}(B'_{n,p}) = \left[\frac{3(n-p)^2 - 2(n-p)}{4}\right] 2^{\alpha} + (n-p)p^{\alpha} + (n-p+1)p$$

for even $n-p$, and

$$ECI_{\alpha}(B'_{n,p}) = \left[\frac{3(n-p)^2 - 2(n-p) - 1}{4}\right] 2^{\alpha} + (n-p)p^{\alpha} + (n-p+1)p$$

for odd $n-p$. This implies that for any $n \geq 4$,

$$ECI_{\alpha}(B'_{n,p}) = \left\lfloor \frac{3(n-p)^2 - 2(n-p)}{2} \right\rfloor 2^{\alpha-1} + (n-p)p^{\alpha} + (n-p+1)p.$$

$\square$

Chapter 4

General eccentric connectivity index of unicyclic graphs

In this chapter, we present lower and upper bounds on the general eccentric connectivity index for unicyclic graphs of given order, and unicyclic graphs of given order and girth. All the lower bounds are valid for $0 < \alpha < 1$, and the upper bounds are valid for $0 < \alpha \leq 1$. We present all the extremal graphs, which means that our bounds are best possible.

4.1 Unicyclic graphs of given order and girth

Bounds on the general eccentric connectivity index for unicyclic graphs of order n and girth k, where $0 < \alpha < 1$, are given in this section. Theorem 4.1.2 includes also the case $\alpha = 1$. For $k \geq 3$ let C_k be a cycle with $V(C_k) = \{c_0, c_1, \dots, c_{k-1}\}$ and $E(C_k) = \{c_0c_1, c_1c_2, \dots, c_{k-2}c_{k-1}, c_{k-1}c_0\}$. Let $C_k(n-k)$ be a unicyclic graph which consists of the cycle C_k, where $n-k$ pendant vertices are attached to one of the vertices of that cycle.

We show that $ECI_\alpha(U) > ECI_\alpha(C_k(n-k))$ for every unicyclic graph different from $C_k(n-k)$. If $n = k$, then C_n is the only unicyclic graph of order n and girth k, so we can assume that $3 \leq k \leq n-1$.

Theorem 4.1.1. *Let U be any unicyclic graph with n vertices and girth k, where $3 \leq k \leq n-1$. Then for $0 < \alpha < 1$ we have*

$$ECI_\alpha(U) \geq \begin{cases} (k^2-k+2)2^{\alpha-1} + \frac{k(n-k+2)^\alpha}{2} + \frac{(k+2)(n-k)}{2} & \text{if } k \text{ is even,} \\ (k^2-2k+5)2^{\alpha-1} + \frac{(k-1)(n-k+2)^\alpha}{2} + \frac{(k+1)(n-k)}{2} & \text{if } k \text{ is odd,} \end{cases}$$

with equalities if and only if U is $C_k(n-k)$.

Proof. Let U' be a unicyclic graph of order n and the cycle of length k with the minimum ECI_α index.

Claim 4.1.1. *Every vertex not in the cycle is a pendant vertex.*

Assume to the contrary that U' contains vertices not in the cycle having degree at least 2. Let w be one of them whose all neighbors except for one, say u, are leaves. Let $N_{U'}(w) = \{u, w_1, w_2, \ldots, w_{r-1}\}$, where $r \geq 2$. Let $V(U'') = V(U')$ and $E(U'') = \{uw_1, uw_2, \ldots, uw_{r-1}\} \cup E(U') \setminus \{ww_1, ww_2, \ldots, ww_{r-1}\}$. Then U'' is a unicyclic graph. We have $d_{U'}(u) = p \geq 2$, $d_{U''}(u) = p + r - 1$, $d_{U'}(w) = r \geq 2$, $d_{U''}(w) = 1$ and $d_{U'}(x) = d_{U''}(x)$ for all $x \in V(U') \setminus \{u, w\}$. We know that $ecc_{U'}(w) = ecc_{U''}(w)$ and $ecc_{U'}(y) \geq ecc_{U''}(y)$ for all $y \in V(U')$. Clearly, $ecc_{U''}(w) = ecc_{U''}(u) + 1$. Thus

$$
\begin{aligned}
ECI_\alpha(U') - ECI_\alpha(U'') &\geq ecc_{U'}(u)d^\alpha_{U'}(u) - ecc_{U''}(u)d^\alpha_{U''}(u) \\
&\quad + ecc_{U'}(w)d^\alpha_{U'}(w) - ecc_{U''}(w)d^\alpha_{U''}(w) \\
&\geq ecc_{U''}(u)[p^\alpha - (p+r-1)^\alpha] + ecc_{U''}(w)(r^\alpha - 1^\alpha) \\
&> ecc_{U''}(u)[p^\alpha - (p+r-1)^\alpha + r^\alpha - 1].
\end{aligned}
$$

By Lemma 3.0.12, $r^\alpha - 1 > (p+r-1)^\alpha - p^\alpha$. This implies that $ECI_\alpha(U') - ECI_\alpha(U'') > 0$ and hence $ECI_\alpha(U') > ECI_\alpha(U'')$, which is a contradiction.

Claim 4.1.2. *At most one vertex of the cycle is adjacent to pendant vertices.*

Assume to the contrary that U' contains at least 2 vertices, say c_l and c_j ($l, j \in \{0, 1, 2, \ldots, k-1\}$), such that each of them is adjacent to at least one pendant vertex. Without loss of generality we can assume that $ecc_{U'}(c_l) \leq ecc_{U'}(c_j)$. Note that for each $i = 0, 1, 2, \ldots, k-1$, we have $ecc_{U'}(c_i) = \lfloor \frac{k}{2} \rfloor$ or $\lfloor \frac{k}{2} \rfloor + 1$ and the eccentricity of pendant vertices adjacent to c_i in U' is $ecc_{U'}(c_i) + 1$. We know that $d_{U'}(c_l) = p \geq 3$ and $d_{U'}(c_j) = r \geq 3$. Let $w_1, w_2, \ldots, w_{r-2}$ be the pendant vertices adjacent to c_j. Let $V(U'') = V(U')$ and $E(U'') = \{c_l w_1, c_l w_2, \ldots, c_l w_{r-2}\} \cup E(U') \setminus \{c_j w_1, c_j w_2, \ldots, c_j w_{r-2}\}$. Then $d_{U''}(c_l) = p+r-2$, $d_{U''}(c_j) = 2$ and $d_{U'}(x) = d_{U''}(x)$ for all $x \in V(U') \setminus \{c_l, c_j\}$. It is easy to see that $ecc_{U'}(c_j) = ecc_{U''}(c_j)$ and $ecc_{U'}(y) \geq ecc_{U''}(y)$ for all $y \in V(U')$. Thus $ecc_{U''}(c_l) \leq ecc_{U'}(c_l) \leq ecc_{U'}(c_j) = ecc_{U''}(c_j)$ and

$$
\begin{aligned}
ECI_\alpha(U') - ECI_\alpha(U'') &\geq ecc_{U'}(c_l)d^\alpha_{U'}(c_l) - ecc_{U''}(c_l)d^\alpha_{U''}(c_l) \\
&\quad + ecc_{U'}(c_j)d^\alpha_{U'}(c_j) - ecc_{U''}(c_j)d^\alpha_{U''}(c_j) \\
&\geq ecc_{U''}(c_l)[p^\alpha - (p+r-2)^\alpha] + ecc_{U''}(c_j)(r^\alpha - 2^\alpha) \\
&\geq ecc_{U''}(c_l)[p^\alpha - (p+r-2)^\alpha + r^\alpha - 2^\alpha].
\end{aligned}
$$

By Lemma 3.0.12, we get $r^\alpha - 2^\alpha > (p+r-2)^\alpha - p^\alpha$. Hence $ECI_\alpha(U') - ECI_\alpha(U'') > 0$ and $ECI_\alpha(U') > ECI_\alpha(U'')$, which is a contradiction.

So U' is $C_k(n-k)$. If k is even, then $C_k(n-k)$ contains $k-2$ vertices of eccentricity $\frac{k}{2}$ and degree 2, one vertex of eccentricity $\frac{k}{2}+1$ and degree 2, one vertex of eccentricity $\frac{k}{2}$ and degree $n-k+2$, and $n-k$ pendant vertices of eccentricity $\frac{k}{2}+1$. Thus

$$ECI_\alpha(C_k(n-k)) = (k^2-k+2)2^{\alpha-1} + \frac{k(n-k+2)^\alpha}{2} + \frac{(k+2)(n-k)}{2}.$$

If k is odd, then $C_k(n-k)$ contains $k-3$ vertices of eccentricity $\frac{k-1}{2}$ and degree 2, two vertices of eccentricity $\frac{k+1}{2}$ and degree 2, one vertex of eccentricity $\frac{k-1}{2}$ and degree $n-k+2$, and $n-k$ pendant vertices of eccentricity $\frac{k+1}{2}$. Thus

$$ECI_\alpha(C_k(n-k)) = (k^2-2k+5)2^{\alpha-1} + \frac{(k-1)(n-k+2)^\alpha}{2} + \frac{(k+1)(n-k)}{2}.$$

□

We use $P_a = u_0u_1\ldots u_a$ and $P'_b = u'_0u'_1\ldots u'_b$ to define three sets of unicyclic graphs. For positive integers a and b, let $A_{a,b}(k)$ be the set of unicyclic graphs obtained from C_k by identifying c_0 with u_a and u'_b. For $a \geq 2$ and $b \geq 1$, let $B_{a,b}(k)$ be the set of unicyclic graphs obtained from C_k by identifying c_0 with u_a and by identifying u'_b with u_i, where $1 \leq i \leq a-1$. For $a \geq 1$ and $b \geq 0$, let $D_{a,b}(k)$ be the set of unicyclic graphs obtained from C_k by identifying c_0 with u_a and one of the other vertices of C_k, say c_i, with u'_b $(1 \leq i \leq k-1)$. The unique graph in $D_{n-k+1,0}(k)$ is denoted by $C_k \star P_{n-k+1}$. So $C_k \star P_{n-k+1}$ is the unicyclic graph obtained from the cycle C_k and the path P_{n-k+1} by identifying one vertex of the cycle with an end-vertex of the path.

Theorem 4.1.2. *Let U be any unicyclic graph with n vertices and girth k, where $3 \leq k \leq n-1$. Then for $0 < \alpha \leq 1$ we have $ECI_\alpha(U) \leq ECI_\alpha(C_k \star P_{n-k+1})$ with equality if and only if U is $C_k \star P_{n-k+1}$.*

Proof. Let U' be a unicyclic graph having the largest ECI_α index among unicyclic graphs with n vertices and girth k. We prove that U' is $C_k \star P_{n-k+1}$. Let $D = v_0v_1v_2\ldots v_d$ be a diametral path in U'. Since U' is not C_n, then v_0 or v_d is a pendant vertex. We can assume that $d_{U'}(v_0) = 1$.

Claim 4.1.3. *Every vertex not in D has degree at least 2.*

Assume to the contrary that there exists a vertex $u \notin D$ and $d_{U'}(u) = 1$. Let w be the unique neighbor of u in U'. We have $d_{U'}(w) = s \geq 2$. Let $V(U_1) = V(U')$ and $E(U_1) = \{uv_0\} \cup E(U') \setminus \{uw\}$. Then U_1 is a unicyclic graph. We have $d_{U'}(v_0) = 1$, $d_{U_1}(v_0) = 2$, $d_{U'}(w) = s$, $d_{U_1}(w) = s-1$ and $d_{U'}(x) = d_{U_1}(x)$ for all $x \in V(U') \setminus \{v_0, w\}$. We know that $ecc_{U'}(y) \leq ecc_{U_1}(y)$ for all $y \in V(U')$. Moreover, $ecc_{U'}(v_0) = ecc_{U_1}(v_0) = d$, $ecc_{U'}(u) \leq d$ $ecc_{U_1}(u) = d+1$, $ecc_{U'}(w) \leq d-1$ and $ecc_{U_1}(w) \leq d$. Thus

$$\begin{aligned}
ECI_\alpha(U') - ECI_\alpha(U_1) &\leq ecc_{U'}(v_0)d^\alpha_{U'}(v_0) - ecc_{U_1}(v_0)d^\alpha_{U_1}(v_0) \\
&\quad + ecc_{U'}(w)d^\alpha_{U'}(w) - ecc_{U_1}(w)d^\alpha_{U_1}(w) \\
&\quad + ecc_{U'}(u)d^\alpha_{U'}(u) - ecc_{U_1}(u)d^\alpha_{U_1}(u) \\
&\leq d(1^\alpha - 2^\alpha) + ecc_{U_1}(w)[s^\alpha - (s-1)^\alpha] \\
&\quad + d \cdot 1^\alpha - (d+1)1^\alpha \\
&\leq d[1 - 2^\alpha + s^\alpha - (s-1)^\alpha] - 1 \leq -1,
\end{aligned}$$

since by Lemma 3.0.12, $2^\alpha - 1 > s^\alpha - (s-1)^\alpha$ for $s \geq 3$ and $0 < \alpha < 1$, and $1 - 2^\alpha + s^\alpha - (s-1)^\alpha = 0$ if $s = 2$ or $\alpha = 1$. Hence $ECI_\alpha(U') < ECI_\alpha(U_1)$, a contradiction.

Claim 4.1.4. *$U' \notin A_{a,b}(k)$ and $U' \notin B_{a,b}(k)$.*

From Claim 4.1.3 we know that U' is in $A_{a,b}(k)$, $B_{a,b}(k)$ or $D_{a,b}(k)$. We show by contradiction that $U' \notin A_{a,b}(k)$ and $U' \notin B_{a,b}(k)$.

Assume that $U' \in A_{a,b}(k)$. Without loss of generality, suppose that $a \geq b$. Let $V(U_2) = V(U')$ and $E(U_2) = \{u_0c_1, u_0c_{k-1}\} \cup E(U') \setminus \{c_0c_1, c_0c_{k-1}\}$. We have $d_{U'}(u_0) = 1$, $d_{U_2}(u_0) = 3$, $d_{U'}(c_0) = 4$, $d_{U_2}(c_0) = 2$ and $d_{U'}(x) = d_{U_2}(x)$ for all $x \in V(U')\backslash\{c_0, u_0\}$. Note that by Claim 4.1.3, the diametral path of U' is $u_0u_1 \dots u_au'_{b-1} \dots u'_0$ and $ecc_{U'}(y) = d_{U'}(y, u_0)$ or $d_{U'}(y, u'_0)$ for any vertex $y \in V(U')$. Therefore $ecc_{U_2}(y) \geq ecc_{U'}(y)$ for all $y \in V(U')$. Moreover, we know that $ecc_{U'}(u_0) = ecc_{U_2}(u_0) = a + b$, $ecc_{U'}(c_0) = a$ and $ecc_{U_2}(c_0) = a + \lfloor \frac{k}{2} \rfloor \leq a+b$ (note that $\lfloor \frac{k}{2} \rfloor \leq b$ because $\lfloor \frac{k}{2} \rfloor = d_{U'}(c_0, c_{\lfloor k/2 \rfloor}) \leq d_{U'}(c_0, u'_0) = b$). Thus

$$\begin{aligned} ECI_\alpha(U') - ECI_\alpha(U_2) &\leq ecc_{U'}(u_0)d^\alpha_{U'}(u_0) - ecc_{U_2}(u_0)d^\alpha_{U_2}(u_0) \\ &\quad + ecc_{U'}(c_0)d^\alpha_{U'}(c_0) - ecc_{U_2}(c_0)d^\alpha_{U_2}(c_0) \\ &= (a+b)(1^\alpha - 3^\alpha) + a \cdot 4^\alpha - \left(a + \left\lfloor \frac{k}{2} \right\rfloor\right) 2^\alpha \\ &< (a+b)(1 - 3^\alpha) + \left(a + \left\lfloor \frac{k}{2} \right\rfloor\right)(4^\alpha - 2^\alpha) \\ &\leq (a+b)(1 - 3^\alpha + 4^\alpha - 2^\alpha) \leq 0, \end{aligned}$$

since by Lemma 3.0.12, $3^\alpha - 1 > 4^\alpha - 2^\alpha$ if $0 < \alpha < 1$, and $1 - 3^\alpha + 4^\alpha - 2^\alpha = 0$ if $\alpha = 1$. So $ECI_\alpha(U') - ECI_\alpha(U_2) < 0$ and $ECI_\alpha(U') < ECI_\alpha(U_2)$, which is a contradiction. Hence $U' \notin A_{a,b}(k)$.

Assume that $U' \in B_{a,b}(k)$. Without loss of generality, suppose that $i \geq b$ (where $u_i = u'_b$). Let $V(U_3) = V(U')$ and $E(U_3) = \{u_0u_{i+1}\} \cup E(U') \setminus$

$\{u_iu_{i+1}\}$. We have $d_{U'}(u_0) = 1$, $d_{U_3}(u_0) = 2$, $d_{U'}(u_i) = 3$, $d_{U_3}(u_i) = 2$ and $d_{U'}(x) = d_{U_3}(x)$ for all $x \in V(U') \setminus \{u_0, u_i\}$. By Claim 4.1.3, the diametral path of U' is $u_0u_1 \ldots u_iu'_{b-1} \ldots u'_0$ and $ecc_{U'}(y) = d_{U'}(y, u_0)$ or $d_{U'}(y, u'_0)$ for any vertex $y \in V(U')$. Thus $ecc_{U_3}(y) \geq ecc_{U'}(y)$ for all $y \in V(U')$. Note that $ecc_{U'}(u_0) = ecc_{U_3}(u_0) = i+b$, $ecc_{U'}(u_i) = i$ and $ecc_{U_3}(u_i) = a+\lfloor \frac{k}{2} \rfloor$. From the definition of $B_{a,b}(k)$ we know that $i \leq a-1 < a + \lfloor \frac{k}{2} \rfloor$, so $-i > -(a + \lfloor \frac{k}{2} \rfloor)$. Therefore

$$
\begin{aligned}
ECI_\alpha(U') - ECI_\alpha(U_3) &\leq ecc_{U'}(u_0)d^\alpha_{U'}(u_0) - ecc_{U_3}(u_0)d^\alpha_{U_3}(u_0) \\
&\quad + ecc_{U'}(u_i)d^\alpha_{U'}(u_i) - ecc_{U_3}(u_i)d^\alpha_{U_3}(u_i) \\
&= (i+b)(1^\alpha - 2^\alpha) + i \cdot 3^\alpha - \left(a + \left\lfloor \frac{k}{2} \right\rfloor\right) 2^\alpha \\
&< (i+b)(1-2^\alpha) + i(3^\alpha - 2^\alpha) \\
&< (i+b)(1 - 2^\alpha + 3^\alpha - 2^\alpha) \leq 0,
\end{aligned}
$$

since by Lemma 3.0.12, $2^\alpha - 1 > 3^\alpha - 2^\alpha$ if $0 < \alpha < 1$, and $1 + 3^\alpha - 2 \cdot 2^\alpha = 0$ if $\alpha = 1$. Hence $ECI_\alpha(U') < ECI_\alpha(U_3)$ and $U' \notin B_{a,b}(k)$.

Claim 4.1.5. *$U' \in D_{a,0}(k)$.*

From Claims 4.1.3 and 4.1.4 we know that $U' \in D_{a,b}(k)$. Without loss of generality, assume that $a \geq b$. We show that $b = 0$.

Assume to the contrary that $b \geq 1$. Without loss of generality, suppose that $u'_b = c_t$ for $t \leq \lfloor \frac{k}{2} \rfloor$. We distinguish two cases: $k \geq 4$ and $k = 3$.

Let $k \geq 4$. Let $V(U_4) = V(U')$ and $E(U_4) = \{c_1c_{k-1}, c_{t+1}u'_{b-1}\} \cup E(U') \setminus \{c_0c_{k-1}, c_tc_{t+1}\}$. Then U_4 is a unicyclic graph containing k-cycle, U' and U_4 have the same diametral path (connecting u_0 and u'_0) and $ecc_{U'}(w) = ecc_{U_4}(w)$ for all $w \in V(U') \setminus \{c_{t+1}, c_{t+2}, \ldots, c_{k-1}\}$.

Let us show that $\sum_{i=t+1}^{k-1}(ecc_{U'}(c_i) - ecc_{U_4}(c_i)) < 0$. Two vertices c_r and c_z, where $t < r \leq z < k$, are called twins if $r + z = k + t$. It suffices to show that there exists a pair of twins $c_{r'}, c_{z'}$, such that $[ecc_{U'}(c_{r'}) - ecc_{U_4}(c_{r'})] + [ecc_{U'}(c_{z'}) - ecc_{U_4}(c_{z'})] < 0$ and for all the other pairs of twins c_r, c_z, we have $[ecc_{U'}(c_r) - ecc_{U_4}(c_r)] + [ecc_{U'}(c_z) - ecc_{U_4}(c_z)] \leq 0$. It is important to note that by Claim 4.1.3, both vertices of degree one are in a diametral path of U', thus the vertex furthest from c_0 is u_0' and $ecc_{U'}(c_0) = t + b \geq \lfloor \frac{k}{2} \rfloor$. Similarly, the vertex furthest from c_t is u_0 and $ecc_{U'}(c_t) = t + a \geq \lfloor \frac{k}{2} \rfloor$.

If $a \leq \frac{t-1}{2}$ and $k + t$ is odd or if $a \leq \frac{t}{2} - 1$ and $k + t$ is even, then

$$ecc_{U'}(c_{\lceil \frac{k}{2} \rceil + a}) = \left\lfloor \frac{k}{2} \right\rfloor, \quad ecc_{U_4}(c_{\lceil \frac{k}{2} \rceil + a}) = \left\lfloor \frac{k}{2} \right\rfloor + 1,$$
$$ecc_{U'}(c_{\lfloor \frac{k}{2} \rfloor + t - a}) = ecc_{U_4}(c_{\lfloor \frac{k}{2} \rfloor + t - a}) = \left\lfloor \frac{k}{2} \right\rfloor$$

and

$$\left[ecc_{U'}(c_{\lceil \frac{k}{2} \rceil + a}) - ecc_{U_4}(c_{\lceil \frac{k}{2} \rceil + a})\right] + \left[ecc_{U'}(c_{\lfloor \frac{k}{2} \rfloor + t - a}) - ecc_{U_4}(c_{\lfloor \frac{k}{2} \rfloor + t - a})\right] = -1.$$

The furthest vertex from c_t is u_0 in U' and one of the furthest vertices from $c_{\lceil \frac{k}{2} \rceil + a}$ is u_0 in U', so the furthest vertex from each vertex c_r, where $r = t + 1, t + 2, \ldots, \lceil \frac{k}{2} \rceil + a - 1$, is u_0 in both graphs U' and U_4, which implies that $ecc_{U'}(c_r) - ecc_{U_4}(c_r) = -1$. For the twin c_z of c_r, where $z = \lfloor \frac{k}{2} \rfloor + t - a + 1, \lfloor \frac{k}{2} \rfloor + t - a + 2, \ldots, k - 1$, we have $ecc_{U'}(c_z) - ecc_{U_4}(c_z) \leq 1$. For each vertex c_f, where $f = \lceil \frac{k}{2} \rceil + a + 1, \lceil \frac{k}{2} \rceil + a + 2, \ldots, \lfloor \frac{k}{2} \rfloor + t - a - 1$, we obtain $ecc_{U'}(c_f) = ecc_{U_4}(c_f) = \lfloor \frac{k}{2} \rfloor$, hence $\sum_{i=t+1}^{k-1}(ecc_{U'}(c_i) - ecc_{U_4}(c_i)) \leq -1$.

If $a \geq \frac{t}{2}$ and $k+t$ is odd, then

$$\begin{aligned}
ecc_{U'}(c_{\frac{k+t-1}{2}}) &= \frac{k-t+1}{2} + a, \quad ecc_{U_4}(c_{\frac{k+t-1}{2}}) = \frac{k-t+1}{2} + a + 1,\\
ecc_{U'}(c_{\frac{k+t+1}{2}}) &= \frac{k-t-1}{2} + a \quad \text{for} \quad a > b,\\
ecc_{U'}(c_{\frac{k+t+1}{2}}) &= \frac{k-t-1}{2} + a + 1 \quad \text{for} \quad a = b,\\
ecc_{U_4}(c_{\frac{k+t+1}{2}}) &= \frac{k-t-1}{2} + a + 1,
\end{aligned}$$

and

$$\left[ecc_{U'}(c_{\frac{k+t-1}{2}}) - ecc_{U_4}(c_{\frac{k+t-1}{2}})\right] + \left[ecc_{U'}(c_{\frac{k+t+1}{2}}) - ecc_{U_4}(c_{\frac{k+t+1}{2}})\right] \leq -1.$$

If $a \geq \frac{t-1}{2}$ and $k+t$ is even, then

$$ecc_{U'}(c_{\frac{k+t}{2}}) = \frac{k-t}{2} + a \quad \text{and} \quad ecc_{U_4}(c_{\frac{k+t}{2}}) = \frac{k-t}{2} + a + 1$$

(note that $c_{\frac{k+t}{2}}$ is its own twin). In these cases the furthest vertex from c_t and $c_{\lfloor \frac{k+t}{2} \rfloor}$ is u_0 in U', so the furthest vertex from each vertex c_r, where $r = t+1, t+2, \ldots, \lfloor \frac{k+t}{2} \rfloor - 1$, is u_0 in both graphs U' and U_4, which implies that $ecc_{U'}(c_r) - ecc_{U_4}(c_r) = -1$. For the vertex c_z, where $z = \lceil \frac{k+t}{2} \rceil + 1, \lceil \frac{k+t}{2} \rceil + 2, \ldots, k-1$, we have $ecc_{U'}(c_z) - ecc_{U_4}(c_z) \leq 1$, hence $\sum_{i=t+1}^{k-1}(ecc_{U'}(c_i) - ecc_{U_4}(c_i)) \leq -1$.

If $t \neq 1$, then $d_{U'}(c_0) = d_{U'}(c_t) = 3$, $d_{U_4}(c_0) = d_{U_4}(c_t) = 2$, $d_{U'}(u'_{b-1}) = d_{U'}(c_1) = 2$, $d_{U_4}(u'_{b-1}) = d_{U_4}(c_1) = 3$ and $d_{U'}(x) = d_{U_4}(x)$ for all $x \in V(U') \setminus$

$\{c_0, c_1, c_t, u'_{b-1}\}$. Thus

$$\begin{aligned}
ECI_\alpha(U') - ECI_\alpha(U_4) &< ecc_{U'}(c_0)d^\alpha_{U'}(c_0) - ecc_{U_4}(c_0)d^\alpha_{U_4}(c_0) \\
&\quad + ecc_{U'}(c_1)d^\alpha_{U'}(c_1) - ecc_{U_4}(c_1)d^\alpha_{U_4}(c_1) \\
&\quad + ecc_{U'}(c_t)d^\alpha_{U'}(c_t) - ecc_{U_4}(c_t)d^\alpha_{U_4}(c_t) \\
&\quad + ecc_{U'}(u'_{b-1})d^\alpha_{U'}(u'_{b-1}) - ecc_{U_4}(u'_{b-1})d^\alpha_{U_4}(u'_{b-1}) \\
&= ecc_{U'}(c_0)(3^\alpha - 2^\alpha) + ecc_{U'}(c_1)(2^\alpha - 3^\alpha) \\
&\quad + ecc_{U_4}(c_t)(3^\alpha - 2^\alpha) + ecc_{U_4}(u'_{b-1})(2^\alpha - 3^\alpha) \\
&= [(ecc_{U'}(c_0) - ecc_{U'}(c_1) + ecc_{U'}(c_t) \\
&\quad - ecc_{U'}(u'_{b-1})](3^\alpha - 2^\alpha) \leq 0,
\end{aligned}$$

since $ecc_{U'}(u'_{b-1}) = ecc_{U'}(c_t)+1$ and $ecc_{U'}(c_0) \leq ecc_{U'}(c_1)+1$. Thus $ECI_\alpha(U')$ $< ECI_\alpha(U_4)$.

If $t = 1$, then $d_{U'}(c_0) = 3$, $d_{U_4}(c_0) = 2$, $d_{U'}(u'_{b-1}) = 2$, $d_{U_4}(u'_{b-1}) = 3$ and $d_{U'}(x) = d_{U_4}(x)$ for all $x \in V(U') \setminus \{c_0, u'_{b-1}\}$. Thus

$$\begin{aligned}
ECI_\alpha(U') - ECI_\alpha(U_4) &< ecc_{U'}(c_0)d^\alpha_{U'}(c_0) - ecc_{U_4}(c_0)d^\alpha_{U_4}(c_0) \\
&\quad + ecc_{U'}(u'_{b-1})d^\alpha_{U'}(u'_{b-1}) - ecc_{U_4}(u'_{b-1})d^\alpha_{U_4}(u'_{b-1}) \\
&= ecc_{U'}(c_0)(3^\alpha - 2^\alpha) + ecc_{U_4}(u'_{b-1})(2^\alpha - 3^\alpha) \\
&= [(ecc_{U'}(c_0) - ecc_{U'}(u'_{b-1})](3^\alpha - 2^\alpha) < 0,
\end{aligned}$$

since $ecc_{U'}(u'_{b-1}) = a + 2$ and $ecc_{U'}(c_0) = max\{a, b+1\} < a + 2$. Thus $ECI_\alpha(U') < ECI_\alpha(U_4)$, which is a contradiction.

Let $k = 3$. We use the same graph U_4. However, for $k = 3$, we have $c_1 = c_t$ and $c_2 = c_{t+1} = c_{k-1}$, thus $E(U_4) = \{c_2u'_{b-1}\} \cup E(U') \setminus \{c_0c_2\}$. Then $d_{U'}(c_0) = 3$, $d_{U_4}(c_0) = 2$, $d_{U'}(u'_{b-1}) = 2$, $d_{U_4}(u'_{b-1}) = 3$ and $d_{U'}(x) = d_{U_4}(x)$

for all $x \in V(U') \setminus \{c_0, u'_{b-1}\}$. We have $ecc_{U'}(c_2) = a+1$, $ecc_{U_4}(c_2) = a+2$ and $ecc_{U'}(w) = ecc_{U_4}(w)$ for all $w \in V(U') \setminus \{c_2\}$. Note that $ecc_{U'}(u'_{b-1}) = a+2$ and $ecc_{U'}(c_0) = max\{a, b+1\} < a+2$. Then

$$\begin{aligned}
ECI_\alpha(U') - ECI_\alpha(U_4) &= ecc_{U'}(c_0)d^\alpha_{U'}(c_0) - ecc_{U_4}(c_0)d^\alpha_{U_4}(c_0) \\
&\quad + ecc_{U'}(u'_{b-1})d^\alpha_{U'}(u'_{b-1}) - ecc_{U_4}(u'_{b-1})d^\alpha_{U_4}(u'_{b-1}) \\
&\quad + ecc_{U'}(c_2)d^\alpha_{U'}(c_2) - ecc_{U_4}(c_2)d^\alpha_{U_4}(c_2) \\
&= ecc_{U'}(c_0)(3^\alpha - 2^\alpha) + (a+2)(2^\alpha - 3^\alpha) \\
&\quad + (a+1)2^\alpha - (a+2)2^\alpha \\
&< (a+2)[(3^\alpha - 2^\alpha) + (2^\alpha - 3^\alpha)] - 2^\alpha < 0.
\end{aligned}$$

Therefore $ECI_\alpha(U') < ECI_\alpha(U_4)$. Hence, we have a contradiction. So U' is $C_k \star P_{n-k+1}$. □

Suppose $G = C_k \star P_{n-k+1}$ and $c_k = c_0$, where $3 \leq k \leq n-1$. We need to consider two cases to compute the value of $ECI_\alpha(G)$.

Case 1: $n \geq \lfloor \frac{3k}{2} \rfloor$. We have $ecc_G(c_i) = ecc_G(c_{k-i}) = n-k+i$ for $i = 0, 1, 2, \ldots, \lfloor \frac{k}{2} \rfloor$. The diametral path $D = u_0u_1 \ldots u_{n-k-1}c_0c_{k-1}c_{k-2} \ldots c_{\lceil \frac{k}{2} \rceil}$ contains $n+1-\lceil \frac{k}{2} \rceil$ vertices. We obtain

$$\begin{aligned}
ECI_\alpha(G) &= ECI_\alpha(D) + \sum_{i=1}^{\lceil \frac{k}{2} \rceil - 1} ecc_G(c_i)d^\alpha_G(c_i) + ecc_G(c_0)d^\alpha_G(c_0) \\
&\quad - ecc_D(c_0)d^\alpha_D(c_0) + ecc_G(c_{\lceil \frac{k}{2} \rceil})d^\alpha_G(c_{\lceil \frac{k}{2} \rceil}) - ecc_D(c_{\lceil \frac{k}{2} \rceil})d^\alpha_D(c_{\lceil \frac{k}{2} \rceil})
\end{aligned}$$

$$
\begin{aligned}
&= \left\lfloor \frac{3(n+1-\lceil\frac{k}{2}\rceil)^2 - 10(n+1-\lceil\frac{k}{2}\rceil)+8}{2} \right\rfloor 2^{\alpha-1} \\
&\quad + 2\left(n+1-\left\lceil\frac{k}{2}\right\rceil - 1\right) + \left(\left\lceil\frac{k}{2}\right\rceil - 1\right)(n-k)2^{\alpha} + 2^{\alpha}\sum_{i=1}^{\lceil\frac{k}{2}\rceil-1} i \\
&\quad + (n-k)(3^{\alpha}-2^{\alpha}) + \left(n-\left\lceil\frac{k}{2}\right\rceil\right)(2^{\alpha}-1).
\end{aligned}
$$

If k is even, then

$$
\begin{aligned}
ECI_{\alpha}(G) &= \left\lfloor \frac{12n^2+3k^2-12kn-16n+8k+4}{8} \right\rfloor 2^{\alpha-1} \\
&\quad + (4kn-3k^2-8n+10k)2^{\alpha-3} + (n-k)3^{\alpha} + n - \frac{k}{2}.
\end{aligned}
$$

If k is odd, we get

$$
\begin{aligned}
ECI_{\alpha}(G) &= \left\lfloor \frac{12n^2+3k^2-12kn-28n+14k+15}{8} \right\rfloor 2^{\alpha-1} \\
&\quad + (4kn-3k^2-4n+8k-5)2^{\alpha-3} + (n-k)3^{\alpha} + n - \frac{k+1}{2}.
\end{aligned}
$$

Case 2: $n < \lfloor\frac{3k}{2}\rfloor$. Then $ecc_G(c_i) = ecc_G(c_{k-i}) = \lfloor\frac{k}{2}\rfloor$ for $0 \le i \le \lfloor\frac{3k}{2}\rfloor - n$, $ecc_G(c_i) = ecc_G(c_{k-i}) = n-k+i$ for $\lfloor\frac{3k}{2}\rfloor - n+1 \le i \le \lfloor\frac{k}{2}\rfloor$ and $ecc_G(u_{n-k-i}) = \lfloor\frac{k}{2}\rfloor + i$ for $1 \le i \le n-k$. Let $\epsilon = 1$ if k is even and $\epsilon = 0$ if k is odd. Then

$$
\begin{aligned}
ECI_{\alpha}(G) &= 2\sum_{i=1}^{\lfloor\frac{3k}{2}\rfloor-n} ecc_G(c_i)d_G^{\alpha}(c_i) + 2\sum_{i=\lfloor\frac{3k}{2}\rfloor-n+1}^{\lceil\frac{k}{2}\rceil-1} ecc_G(c_i)d_G^{\alpha}(c_i) \\
&\quad + \sum_{i=1}^{n-k-1} ecc_G(u_i)d_G^{\alpha}(u_i) + ecc_G(c_0)d_G^{\alpha}(c_0) \\
&\quad + \epsilon \cdot ecc_G(c_{\lfloor\frac{k}{2}\rfloor})d_G^{\alpha}(c_{\lfloor\frac{k}{2}\rfloor}) + ecc_G(u_0)d_G^{\alpha}(u_0)
\end{aligned}
$$

$$
\begin{aligned}
= \quad & \left(\left\lfloor \frac{3k}{2} \right\rfloor - n\right) \left\lfloor \frac{k}{2} \right\rfloor 2^{\alpha+1} + 2^{\alpha+1} \sum_{i=\lfloor \frac{3k}{2} \rfloor - n+1}^{\lceil \frac{k}{2} \rceil - 1} (n-k+i) \\
& + 2^{\alpha} \sum_{i=1}^{n-k-1} \left(\left\lfloor \frac{k}{2} \right\rfloor + i\right) + \left\lfloor \frac{k}{2} \right\rfloor 3^{\alpha} + \epsilon \left(n - k + \left\lfloor \frac{k}{2} \right\rfloor\right) 2^{\alpha} \\
& + \left(n - k + \left\lfloor \frac{k}{2} \right\rfloor\right),
\end{aligned}
$$

which is

$$(3n^2 + 3k^2 - 5kn - k - n)2^{\alpha-1} + \frac{k \cdot 3^{\alpha}}{2} + n - \frac{k}{2}$$

if k is even, and

$$(3n^2 + 3k^2 - 5nk - 3k + 2)2^{\alpha-1} + \frac{(k-1)3^{\alpha}}{2} + n - \frac{k+1}{2}$$

if k is odd.

4.2 Unicyclic graphs of given order

We use the results from the previous section to obtain bounds on the general eccentric connectivity index for unicyclic graphs with n vertices. The only unicyclic graph with three vertices is C_3, so we can assume that $n \geq 4$.

Theorem 4.2.1. *Let U be any unicyclic graph of order $n \geq 4$. Then for $0 < \alpha < 1$ we have*

$$ECI_{\alpha}(U) \geq 2^{\alpha+2} + (n-1)^{\alpha} + 2n - 6$$

with equality if and only if U is $C_3(n-3)$.

Proof. Let U' be a unicyclic graph having the smallest ECI_{α} index among unicyclic graphs with n vertices. Then from Theorem 4.1.1 we know that U' is $C_k(n-k)$ for some $k \geq 3$. We prove that U' is $C_3(n-3)$ which means that $ECI_\alpha(C_3(n-3)) < ECI_\alpha(C_k(n-k))$ for $4 \leq k \leq n$. We distinguish two cases.

Case 1: $4 \leq k \leq n-1$. Assume to the contrary that U' is $C_k(n-k)$ for some k, where $4 \leq k \leq n-1$. Let $b = \lfloor \frac{k}{2} \rfloor$. Let $V(U'') = V(U')$ and $E(U'') = \{c_{b-1}c_{b+1}, c_0c_b\} \cup E(U') \setminus \{c_{b-1}c_b, c_bc_{b+1}\}$. Then U'' is a unicyclic graph. We have $d_{U'}(c_0) = n-k+2$, $d_{U''}(c_0) = n-k+3$, $d_{U'}(c_b) = 2$, $d_{U''}(c_b) = 1$ and $d_{U'}(x) = d_{U''}(x)$ for all $x \in V(U') \setminus \{c_0, c_b\}$. It is easy to see that $ecc_{U''}(y) \leq ecc_{U'}(y)$ for all $y \in V(U')$. Note that $ecc_{U'}(c_0) = b = \lfloor \frac{k}{2} \rfloor$, $ecc_{U''}(c_0) = \lceil \frac{k}{2} \rceil - 1$. $ecc_{U'}(c_b) = b + 1 = \lfloor \frac{k}{2} \rfloor + 1$ and $ecc_{U''}(c_b) = \lceil \frac{k}{2} \rceil$. Thus

$$\begin{aligned}
ECI_\alpha(U') - ECI_\alpha(U'') &\geq ecc_{U'}(c_0)d^\alpha_{U'}(c_0) - ecc_{U''}(c_0)d^\alpha_{U''}(c_0) \\
&\quad + ecc_{U'}(c_b)d^\alpha_{U'}(c_b) - ecc_{U''}(c_b)d^\alpha_{U''}(c_b) \\
&\geq ecc_{U''}(c_0)[d^\alpha_{U'}(c_0) - d^\alpha_{U''}(c_0)] \\
&\quad + ecc_{U''}(c_b)[d^\alpha_{U'}(c_b) - d^\alpha_{U''}(c_b)] \\
&= \left(\left\lceil \frac{k}{2} \right\rceil - 1\right)[(n-k+2)^\alpha - (n-k+3)^\alpha] \\
&\quad + \left\lceil \frac{k}{2} \right\rceil (2^\alpha - 1^\alpha) \\
&= \left\lceil \frac{k}{2} \right\rceil [(n-k+2)^\alpha - (n-k+3)^\alpha] + (2^\alpha - 1)] \\
&\quad - (n-k+2)^\alpha + (n-k+3)^\alpha \\
&> \left\lceil \frac{k}{2} \right\rceil [(n-k+2)^\alpha - (n-k+3)^\alpha] + (2^\alpha - 1)]
\end{aligned}$$

By Lemma 3.0.12, we have

$$2^\alpha - 1 > (n-k+3)^\alpha - (n-k+2)^\alpha,$$

which implies that $ECI_\alpha(U') - ECI_\alpha(U'') > 0$ and $ECI_\alpha(U') > ECI_\alpha(U'')$, so U' does not have the smallest ECI_α index. We have a contradiction. Therefore, U' is $C_3(n-3)$.

Case 2: $k = n$. It suffices to compare $ECI_\alpha(C_3(n-3))$ and $ECI_\alpha(C_n)$. Let $f(n) = ECI_\alpha(C_n) = n\lfloor \frac{n}{2} \rfloor 2^\alpha$ and $g(n) = ECI_\alpha(C_3(n-3)) = 2^{\alpha+2} + (n-1)^\alpha + 2n - 6$. We consider the function $h(n) = f(n) - g(n)$. If n is even, then the derivative $h'(n) = n2^\alpha - \alpha(n-1)^{\alpha-1} - 2$. If n is odd, then $h'(n) = (n - \frac{1}{2})2^\alpha - \alpha(n-1)^{\alpha-1} - 2$. Thus for any n,

$$h'(n) \geq \left(n - \frac{1}{2}\right) 2^\alpha - \alpha(n-1)^{\alpha-1} - 2.$$

Since $1 < 2^\alpha < 2$, we get $(n-\frac{1}{2})2^\alpha > n - \frac{1}{2}$. Since $\frac{1}{n-1} < (n-1)^{\alpha-1} < 1$, we have $-\alpha(n-1)^{\alpha-1} > -\alpha > -1$. Therefore $h'(n) \geq (n - \frac{1}{2}) - 1 - 2 > 0$ for $n \geq 4$, which means that $h(n)$ is increasing. Consequently, we obtain

$$h(n) \geq h(4) = 8(2^\alpha) - 2^{\alpha+2} - 3^\alpha - 2 > 2^\alpha - 3^\alpha + 2^\alpha - 1.$$

By Lemma 3.0.12, we have $2^\alpha - 1 > 3^\alpha - 2^\alpha$. This implies that $h(n) > 0$ for every $n \geq 4$. Hence $ECI_\alpha(C_n) = f(n) > g(n) = ECI_\alpha(C_3(n-3))$ and $C_3(n-3)$ is the only graph having the smallest ECI_α index. $\square$

There are only two different unicyclic graphs with four vertices, namely C_4 and $C_3(1)$. By Theorem 4.2.1, we have $ECI_\alpha(C_4) > ECI_\alpha(C_3(1))$ for $0 < \alpha < 1$ and it can be easily checked that $ECI_1(C_4) > ECI_1(C_3(1))$. This means that for $n = 4$, C_4 is the unicyclic graph having the largest general eccentric connectivity index, where $0 < \alpha \leq 1$.

Theorem 4.2.2. *Let U be any unicyclic graph of order $n \geq 5$. Then for $0 < \alpha \leq 1$ we have*

$$ECI_\alpha(U) \leq \left\lfloor \frac{3n^2 - 12n + 17}{2} \right\rfloor 2^{\alpha-1} + (n-3)3^\alpha + n - 2$$

with equality if and only if U is $C_3 \star P_{n-2}$.

Proof. Let U' be a unicyclic graph having the largest ECI_α index among unicyclic graphs with n vertices. Then from Theorem 4.1.2 we know that U' is $C_k \star P_{n-k+1}$ for some $3 \leq k \leq n$. We prove that U' is $C_3 \star P_{n-2}$ which means that $ECI_\alpha(C_3 \star P_{n-2}) > ECI_\alpha(C_k \star P_{n-k+1})$ for $4 \leq k \leq n$. We distinguish two cases.

Case 1: $4 \leq k \leq n-1$. Assume to the contrary that U' is $C_k \star P_{n-k+1}$ for some k, where $4 \leq k \leq n-1$. Let $V(U'') = V(U')$ and $E(U'') = \{c_1c_3\} \cup E(U') \setminus \{c_0c_1\}$. Then U'' is a unicyclic graph. We have $d_{U'}(c_0) = 3$, $d_{U''}(c_0) = 2$, $d_{U'}(c_3) = 2$, $d_{U''}(c_3) = 3$ and $d_{U'}(x) = d_{U''}(x)$ for all $x \in V(U') \setminus \{c_0, c_3\}$. For all $y \in V(U')$, we obtain $ecc_{U'}(y) \leq ecc_{U''}(y)$. Note that $ecc_{U''}(c_0) = max\{n-k, k-2\}$ and $ecc_{U''}(c_3) = n-3$, so $ecc_{U''}(c_0) \leq ecc_{U''}(c_3)$. Since $ecc_{U'}(c_1) = \max\{\lfloor \frac{k}{2} \rfloor, n-k+1\}$ and $ecc_{U''}(c_1) = n-2$, we get $ecc_{U'}(c_1) < ecc_{U''}(c_1)$. Then

$$\begin{aligned} ECI_\alpha(U') - ECI_\alpha(U'') \quad < \quad & ecc_{U'}(c_0)d^\alpha_{U'}(c_0) - ecc_{U''}(c_0)d^\alpha_{U''}(c_0) \\ & + ecc_{U'}(c_3)d^\alpha_{U'}(c_3) - ecc_{U''}(c_3)d^\alpha_{U''}(c_3) \end{aligned}$$

$$
\begin{aligned}
&\le ecc_{U''}(c_0)[d_{U'}^{\alpha}(c_0) - d_{U''}^{\alpha}(c_0)] \\
&\quad + ecc_{U''}(c_3)[d_{U'}^{\alpha}(c_3) - d_{U''}^{\alpha}(c_3)] \\
&= ecc_{U''}(c_0)(3^{\alpha} - 2^{\alpha}) + ecc_{U''}(c_3)(2^{\alpha} - 3^{\alpha}) \\
&= [ecc_{U''}(c_0) - ecc_{U''}(c_3)](3^{\alpha} - 2^{\alpha}) \le 0,
\end{aligned}
$$

which implies that $ECI_{\alpha}(U') < ECI_{\alpha}(U'')$, so U' does not have the largest ECI_{α} index. Thus, we have a contradiction.

Case 2: $k = n$. It suffices to compare $ECI_{\alpha}(C_3 \star P_{n-2})$ and $ECI_{\alpha}(C_n)$. If n is even, then

$$
ECI_{\alpha}(C_3 \star P_{n-2}) = \left(\frac{3n^2 - 12n + 16}{4}\right) 2^{\alpha} + (n-3)3^{\alpha} + n - 2 = g(n). \quad (4.1)
$$

If n is odd, then

$$
ECI_{\alpha}(C_3 \star P_{n-2}) = \left(\frac{3n^2 - 12n + 17}{4}\right) 2^{\alpha} + (n-3)3^{\alpha} + n - 2 = g(n). \quad (4.2)
$$

Then the derivative of $g(n)$ is $g'(n) = (3n-6)2^{\alpha-1} + 3^{\alpha} + 1$ for every $n \ge 5$. Let $f(n) = ECI_{\alpha}(C_n) = n\lfloor \frac{n}{2} \rfloor 2^{\alpha}$. We consider the function $h(n) = g(n) - f(n)$.

If n is odd, then $h'(n) = (n-5)2^{\alpha-1} + 3^{\alpha} + 1 > 0$ for all $n \ge 5$. So $h(n)$ is increasing and $h(n) \ge h(5) = 2(3^{\alpha} - 2^{\alpha}) + 3 > 0$, which implies that $g(n) > f(n)$.

If n is even, then the derivative $h'(n) = (n-6)2^{\alpha-1} + 3^{\alpha} + 1 > 0$ for all $n \ge 5$. This implies that $h(n)$ is increasing. Thus $h(n) \ge h(5) = 2(3^{\alpha} - 2^{\alpha}) + 3 > 0$. Therefore $g(n) > f(n)$, which means that $ECI_{\alpha}(C_3 \star P_{n-2}) > ECI_{\alpha}(C_n)$ for every $n \ge 5$.

Hence, for each $n \ge 5$, $C_3 \star P_{n-2}$ is the only graph having the largest ECI_{α}

index. By (4.1) and (4.2),

$$ECI_\alpha(C_3 \star P_{n-2}) = \left\lfloor \frac{3n^2 - 12n + 17}{2} \right\rfloor 2^{\alpha-1} + (n-3)3^\alpha + n - 2.$$

□

Chapter 5

Conclusion and future research

5.1 Conclusion

In the second chapter of the thesis, we presented exact values of all important distance-based indices for complete m-ary trees of a given height. We solved recurrence relations to obtain the value of the most well-known index called the Wiener index. New methods were used to express the other indices (the degree distance, the eccentric distance sum, the Gutman index, the edge-Wiener index, the hyper-Wiener index and the edge-hyper-Wiener index) as well. Values of distance-based indices for complete binary trees are corollaries of the main results of this chapter.

In the third chapter, we introduced the general eccentric connectivity index $ECI_\alpha(G)$ of a graph G. Bounds on $ECI_\alpha(T)$ for trees T of given order, lower bounds on $ECI_\alpha(T)$ for trees T of given order and diameter, and trees of given order and number of pendant vertices, where $0 < \alpha < 1$ were given. We also gave upper bounds on $ECI_\alpha(T)$ for trees T of given order and diameter, and trees of given order and number of pendant vertices, where $\alpha > 1$.

In the fourth chapter, we presented lower and upper bounds on $ECI_\alpha(U)$ for unicyclic graphs U of given order and girth, where $0 < \alpha < 1$. Bounds on $ECI_\alpha(U)$ for unicyclic graphs U of given order, where $0 < \alpha < 1$, were also stated. In some theorems we included also the case $\alpha = 1$. All the extremal graphs were presented, which means that our bounds are best possible.

Proofs for the classical eccentric connectivity index do not work for the general eccentric connectivity index, therefore we used new different techniques which generalize the classical eccentric connectivity index.

In conclusion, we wish to state that the main aim of this research is met; and all objectives that enhanced the establishment of the aim achieved.

5.2 Future research

Further work can be carried out on the general eccentric connectivity index for trees, unicyclic graphs and general graphs of given graph parameters. We state a few challenging open problems on the general eccentric connectivity index for trees, unicyclic graphs and general graphs.

Problem 5.2.1. *Find lower and upper bounds on $ECI_\alpha(T)$ for trees T of given order, where $\alpha < 0$ or $\alpha > 1$.*

Problem 5.2.2. *Find lower bounds on $ECI_\alpha(T)$ for trees T of given order and diameter/trees of given order and number of pendant vertices, where $\alpha < 0$ or $\alpha > 1$.*

Problem 5.2.3. *Find upper bounds on $ECI_\alpha(T)$ for trees T of given order and diameter/trees of given order and number of pendant vertices, where $\alpha < 1$.*

Problem 5.2.4. *Find lower and upper bounds on $ECI_\alpha(U)$ for unicyclic graphs U of given order/unicyclic graphs of given order and girth, where $\alpha < 0$ or $\alpha > 1$.*

Problem 5.2.5. *Find lower and upper bounds on $ECI_\alpha(G)$ for general graphs G of given order, graphs of given order and diameter, graphs of given order and number of pendant vertices, for $\alpha \in \mathbb{R}$.*

These problems remain open for future research.

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