Eccentricity based graph invariants of extremal graphs

By

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Dedicated

to

my mother (Late)

Acknowledgment

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Shehnaz Akhter

Abstract

Topological indices, sometimes also recognized as a graph-theoretic invariant, maintain the symmetry of the molecular structures and assign a mathematical language to predict features such as the radius of gyrations, viscosity, boiling points, etc. The topological invariant can be considered as a numeric amount which interconnected with a graph which captures the graph topology and is unchanged under graph automorphism. Nowadays, topological indices have been developing attention due to their significance in the domain of computational chemistry. There are certain crucial categories of topological indices with respect to their specific topological features, like degrees of vertices, distances between vertices, eccentricities of vertices, connectivity, matching number, etc.

The main focus of this dissertation is to derive extremal graphs with respect to some eccentricity based indices. We determine the extremal conjugated trees with respect to eccentric connectivity index and also eccentric adjacency index among all n-vertex conjugated trees. We focus on the unicyclic graphs with the largest unicyclic graph with respect to eccentric adjacency index with fixed order and girth. We determine the tree with the largest eccentric adjacency index among all the trees with a fixed diameter. Next we derive the extremal trees with the eccentric connectivity and the eccentric adjacency indices among the trees with a given bipartition size, fixed matching number, fixed independence number and fixed domination number. We obtain the graphs with fixed cut edges which have the largest eccentric adjacency index and characterized the extremal graphs. We determine the trees with the smallest and the largest total eccentricity index among the class of trees with p pendent vertices. Furthermore, we define a class of trees with a fixed diameter and investigate the trees with the smallest and the largest total eccentricity index in this class.

List of publications

(1) Shehnaz Akhter and Rashid Farooq, *Computing the eccentric connectivity index and eccentric adjacency index of conjugated trees*, Util. Math., (to appear)

(2) Shehnaz Akhter and Rashid Farooq, *On the eccentric adjacency index of unicyclic graphs and trees*, Asian-European Journal of Mathematics, 13(1) (2020), 205002.

(3) Shehnaz Akhter, *Two degree distance based topological indices of chemical trees*, IEEE Access, 7 (2019), 95653–95658.

(4) Shehnaz Akhter and Rashid Farooq, *Eccentric adjacency index of graphs with a given number of cut edges*, Bull. Malays. Math. Sci. Soc., (2019), 1–14, DOI: $10.1007/s40840-019-00820-x$.

(5) Rashid Farooq, Shehnaz Akhter and Juan Rada, *Total eccentricity index of trees with fixed pendent vertices and trees with fixed diameter*, (submitted).

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Chapter 1

An introduction to graph theory

In the first section of the chapter, we will come to know about a concise history and certain applications of graph theory in different dimensions. Section 1.2 contains some vital terminologies, notions and definitions of modern graph theory and these will be beneficial throughout this dissertation. Some widely known parameters of a graph like matching, domination number, independence number and vertex cover are discussed in Section 1.3. Section 1.4 incorporates a bit of discussions about trees and its related structures. In the last section of this chapter, we will give a short introduction and certain familiar outcomes of extremal graphs with respect to parameters. For other explanations of these concepts which are not explicitly given in this chapter, the reader is referred to [9, 14, 49, 64].

1.1 Historical background

In 1736, the city of Prussia named Königsberg was situated along the river which is familiar as Kaliningrad, Russia, in modern time. The river Pregel flowed through the city and partitioned it into four regions. These regions were joined by seven bridges. A well liked exercise among the residents of Königsberg was finding if it was possible to walk from island to island by crossing seven bridges exactly once and arrive back to the initial point. This challenge is labeled by the *Königsberg bridge* problem. The mayor of Prussia

"Carl Gottlieb Ehler" was concerned to this problem, and he wants to obtain the solution of it.

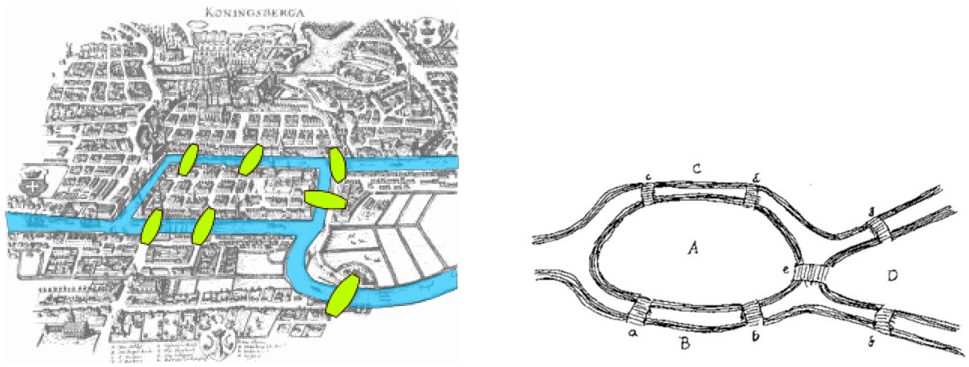

Figure 1.1: Königsberg bridge problem and Euler's sketches.

Therefore, he discussed it with a Swiss mathematician Leonhard Euler in 1735. At that time, Euler concluded that the solution of Königsberg bridge problem was impossible. Also he wrote a research paper on it and presented it in front of his teammates at the Academy of Sciences at St. Petersburg. Moreover, Euler gave justification on it in his research paper in 1736, see [33]. In coming to this consequence, Euler figure out the problem in the form of graph theory, but he does not design any graph model of it; he only sketches it. Later in 1789, Higgins [52] designed the first graph, when he presented a chemical structure in the form of vertices and edges.

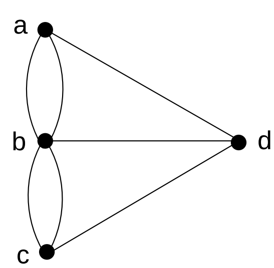

Figure 1.2: Graphical form of Königsberg bridge problem.

For further study on the historical aspects and the solution of Königsberg bridge problem, see [7, 41, 53]. The first concise book related to graph theory was composed in 1936 by Könic [63]. Since then the Euler's explanation of Königsberg bridge problem and the first book on graph theory, the area of graph theory developed. Afterwards, it became the renowned and one of the most significant branch of applied mathematics. Usually known that graph theory has implementations in combinatorics, but it has also beneficial applications in chemistry, optimization theory, biology, applied mathematics, electrical engineering, computer science, bioinformatics, network analysis, sociology, business administration, economics and other scientific and not-so-scientific areas.

1.2 Basic notations and some well known families of graphs

A graph $\mathcal{H}$ consists of a non-empty set of vertices $\mathcal{V}_{\mathcal{H}}$ and a set of edges $\mathcal{E}_{\mathcal{H}}$, and it is represented by $\mathcal{H} = (\mathcal{V}_{\mathcal{H}}, \mathcal{E}_{\mathcal{H}})$. The vertices in $\mathcal{H}$ are specified by points, and they may represent some objects, for example, cities, people, atoms, etc. The edges in $\mathcal{H}$ are indicated by lines or curves connecting the vertices of $\mathcal{H}$. The order $n_{\mathcal{H}}$ and the size $e_{\mathcal{H}}$ of $\mathcal{H}$ are the cardinalities of $\mathcal{V}_{\mathcal{H}}$ and $\mathcal{E}_{\mathcal{H}}$, respectively, and $\mathcal{H}$ is known as a $(n_{\mathcal{H}}, e_{\mathcal{H}})$-graph. A graph with a finite set of vertices and edges is characterized as a finite graph, on the other hand, it is recognized as an infinite graph. Two or more edges that join the same pair of vertices are described as multiple edges, and a loop is an edge that joins a vertex with itself. A graph $\mathcal{H}$ is recognized as a simple graph if it has no multiple edges and loops. Throughout this dissertation, every examined graph is undirected, simple and finite.

If $h_l, h_m \in \mathcal{V}_{\mathcal{H}}$, then $h_l h_m$ is an edge among h_l and h_m, and these are said to be end vertices of $h_l h_m$. So the vertices h_l and h_m are linked or neighbors to each other and $h_l h_m$ is incident on both vertices h_l and h_m. The set of neighbors of $h_l \in \mathcal{V}_{\mathcal{H}}$ is recognized as *neighborhood* of h_l and is written by $\Gamma_{\mathcal{H}}(h_l)$. For a given vertex $h_l \in \mathcal{V}_{\mathcal{H}}$, the *degree* of h_l, represented by $\deg_{\mathcal{H}}(h_l)$, is the number of its linked edges in $\mathcal{H}$. The degree of a given vertex having loop is two. A vertex with degree "0" is recognized as an *isolated* vertex and a degree "1" vertex is specified as a *pendent* vertex. The set of pendent vertices of $\mathcal{H}$ is represented by $P_{\mathcal{H}}$ and the set of pendent vertices linked to a specific vertex $h_l \in \mathcal{V}_{\mathcal{H}}$ is written by $P_{\mathcal{H}}(h_l)$. The sum of the degrees of linked vertices of $h_l \in \mathcal{V}_{\mathcal{H}}$ is described as $S_{\mathcal{H}}(h_l) = \sum\limits_{h_m \in \Gamma_{\mathcal{H}}(h_l)} \deg_{\mathcal{H}}(h_m)$.

The smallest (respectively, largest) degree of $\mathcal{H}$ is the smallest (respectively, largest) degree among all vertices of $\mathcal{H}$ and is represented as $\delta_{\mathcal{H}}$ ($\triangle_{\mathcal{H}}$). For a vertex $h_l \in \mathcal{V}_{\mathcal{H}}$, we have

$$0 \leq \delta_{\mathcal{H}} \leq \deg_{\mathcal{H}}(h_l) \leq \triangle_{\mathcal{H}} \leq n_H - 1.$$

If the degree of every vertex in $\mathcal{H}$ is same, then $\mathcal{H}$ is a *regular* graph. The *complement* of $\mathcal{H}$, written by $\overline{\mathcal{H}}$, is a graph having $\mathcal{V}_{\overline{\mathcal{H}}} = \mathcal{V}_{\mathcal{H}}$ and $h_l h_m \in \mathcal{E}_{\overline{\mathcal{H}}}$ if and only if $h_l h_m \notin \mathcal{E}_{\mathcal{H}}$. Therefore, the order and size of $\overline{\mathcal{H}}$ are $n_{\mathcal{H}}$ and $\binom{n_{\mathcal{H}}}{2} - e_{\mathcal{H}}$, respectively. For a vertex $h_l \in \mathcal{V}_{\overline{\mathcal{H}}}$, we have $\deg_{\overline{\mathcal{H}}}(h_l) = n_{\mathcal{H}} - 1 - \deg_{\mathcal{H}}(h_l)$.

A *path* P_n on n vertices $h_1, h_2, \ldots, h_n$ is written as $h_1 h_2 \ldots h_n$ and is represented by h_1, h_n-path. The vertices h_1 and h_n are the end vertices and $h_2, \ldots, h_{n-1}$ are the internal vertices of the path $P_n = h_1 h_2 \ldots h_n$. Two paths P and P' with no common internal vertices are called internally disjoint paths. If paths P and P' share no common edge, then they are called an edge-disjoint paths. An n-vertex *cycle* with vertices $h_1, \ldots, h_n$ is represented by $C_n = h_1 h_2 \ldots h_n h_1$ and is named as a cycle of length n. In a connected simple graph $\mathcal{H}$, a cycle containing s vertices is called an s-cycle in $\mathcal{H}$. The shortest (respectively, largest) length of a cycle in $\mathcal{H}$ is described as the girth (respectively, circumference) of $\mathcal{H}$.

A simple graph is a complete graph, written as K_n, if each pair of vertices is linked. The graph K_1 is represented as a trivial graph. Since every pair of vertices is linked in K_n, therefore, it has the largest possible size as compared to any other simple n-vertex graph. A *clique* of $\mathcal{H}$ is a complete graph contained in $\mathcal{H}$, and the largest clique of $\mathcal{H}$ is a clique with largest size among all cliques contained in $\mathcal{H}$. The cardinality of largest clique of $\mathcal{H}$ is known as the clique number of $\mathcal{H}$ and is written as $\omega_{\mathcal{H}}$.

A graph $\mathcal{H}$ is known as a *bipartite* graph if $\mathcal{V}_{\mathcal{H}}$ can be converted into two independent sets $\mathcal{V}_l$ and $\mathcal{V}_m$ of vertices such that no single edge has two end points in a similar V_p,

$p = l$ or m. A bipartite graph is known as a *complete bipartite* graph if every pair of vertices in $\mathcal{V}_l$ and $\mathcal{V}_m$ are linked and is represented by $K_{l,m}$. If the two disjoint sets have cardinality l and m, respectively, then (l, m) is a bipartition size of $\mathcal{H}$, where $l+m = n_{\mathcal{H}}$.

A graph $\mathcal{H}$ is known as a j*-partite* graph if there exists a decomposition $\mathcal{V}_1, \mathcal{V}_2, \ldots, \mathcal{V}_j$ of $\mathcal{V}_{\mathcal{H}}$ such that every $\mathcal{V}_l$ is an independent set, $l = 1, 2, \ldots, j$. Moreover, $\mathcal{H}$ is a *complete* j*-partite* graph such that $h_1h_2 \in \mathcal{E}_{\mathcal{H}}$ if and only if $h_1 \in \mathcal{V}_r$ and $h_2 \in \mathcal{V}_s$, where $r \neq s$, and is written by $K_{n_1,n_2,\ldots,n_j}$, where $|\mathcal{V}_l| = n_l$ for $l = 1, 2, \ldots, j$.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be graphs with disjoint-vertex sets. The union of $\mathcal{H}_1$ and $\mathcal{H}_2$, signified by $\mathcal{H}_1 \cup \mathcal{H}_2$, is a graph whose vertex set $\mathcal{V}_{\mathcal{H}_1 \cup \mathcal{H}_2} = \mathcal{V}_{\mathcal{H}_1} \cup \mathcal{V}_{\mathcal{H}_2}$ and edge set $\mathcal{E}_{\mathcal{H} \cup \mathcal{H}_2} = \mathcal{E}_{\mathcal{H}_1} \cup \mathcal{E}_{\mathcal{H}_2}$. The order and size of $\mathcal{H}_1 \cup \mathcal{H}_2$ are $n_{\mathcal{H}_1} + n_{\mathcal{H}_2}$ and $e_{\mathcal{H}_1} + e_{\mathcal{H}_2}$, respectively. Similarly, the intersection of $\mathcal{H}_1$ and $\mathcal{H}_2$, represented by $\mathcal{H}_1 \cap \mathcal{H}_2$, is a graph with $\mathcal{V}_{\mathcal{H}_1} \cap \mathcal{V}_{\mathcal{H}_2}$ vertex set and $\mathcal{E}_{\mathcal{H}_1} \cap \mathcal{E}_{\mathcal{H}_2}$ edge set. If $\mathcal{H}$ is a graph and $h_1, h_2 \in \mathcal{V}_{\mathcal{H}}$ are non-linked vertices of $\mathcal{H}$, then the graph constructed by joining h_1 and h_2 is written by $\mathcal{H} \cup \{h_1h_2\}$. The subdivision graph, represented by $S(\mathcal{H})$, is the graph constructed from a graph $\mathcal{H}$ by replacing each of edge $h_1h_2 \in \mathcal{E}_{\mathcal{H}}$ by a length two h_1uh_2 path, where $u \notin \mathcal{V}_{\mathcal{H}}$.

1.2.1 Subgraphs and isomorphic graphs

A graph $\mathcal{H}_2 = (\mathcal{V}_{\mathcal{H}_2}, \mathcal{E}_{\mathcal{H}_2})$ is a *subgraph* of a $\mathcal{H}_1 = (\mathcal{V}_{\mathcal{H}_1}, \mathcal{E}_{\mathcal{H}_1})$ graph if $\mathcal{V}_{\mathcal{H}_2} \subseteq \mathcal{V}_{\mathcal{H}_1}$ and $\mathcal{E}_{\mathcal{H}_2} \subseteq \mathcal{E}_{\mathcal{H}_1}$, and is represented by $\mathcal{H}_2 \subseteq \mathcal{H}_1$. A subgraph $\mathcal{H}_2$ is an *induced subgraph* of $\mathcal{H}_1$ if edge set of $\mathcal{H}_2$ is $\{h_1h_2 \mid h_1, h_2 \in \mathcal{V}_{\mathcal{H}_2}$ and $h_1h_2 \in \mathcal{E}_{\mathcal{H}_1}\}$. If $\mathcal{V}_{\mathcal{H}_2} = \mathcal{V}_{\mathcal{H}_1}$, then $\mathcal{H}_2$ is known as a *spanning subgraph* of $\mathcal{H}_1$.

Since a graph can be constructed in miscellaneous ways in which the shape of edges are not significant. All such drawings of a graph refer to the same graph and are described as isomorphic graphs. Therefore, if there exists a bijection mapping π among vertex sets of two simple graphs $\mathcal{H}_1$ and $\mathcal{H}_2$, with the condition that for $h_1, h_2 \in \mathcal{V}_{\mathcal{H}_1}$, $h_1h_2 \in \mathcal{E}_{\mathcal{H}_1} \Leftrightarrow \pi(h_1)\pi(h_2) \in \mathcal{E}_{\mathcal{H}_2}$, then $\mathcal{H}_1$ and $\mathcal{H}_2$ are said to be *isomorphic graphs* [9] and is written as $\mathcal{H}_1 \cong \mathcal{H}_2$. In isomorphism, both graphs must have the same properties, for example, order, size, vertex degree sequence, girth, same number of equal length cycle, same complements, etc. However, these conditions are not adequate to justify that two graphs are isomorphic to each other for a large n.

1.2.2 Connectivity and distances

Any two vertices $h_1, h_2 \in \mathcal{V}_{\mathcal{H}}$ are *connected* in $\mathcal{H}$ if h_1 and h_2 are joined by a path. A graph $\mathcal{H}$ is recognized as a *connected graph*, if any two vertices are connected by a path in $\mathcal{H}$. A maximal connected subgraph of $\mathcal{H}$ is known to be a *component* of $\mathcal{H}$. A graph $\mathcal{H}$ is called a 2-connected (respectively, 2-edge-connected), if $\mathcal{H} - h$ (respectively, $\mathcal{H} - h_1h_2$) is connected, for every $h \in \mathcal{V}_{\mathcal{H}}$ (respectively, $h_1h_2 \in \mathcal{E}_{\mathcal{H}}$).

A vertex set $\mathcal{U} \subset \mathcal{V}_{\mathcal{H}}$ is a *vertex-cut*, if deletion of vertices of $\mathcal{U}$ increases the components of $\mathcal{H}$. A *cut-vertex* is a vertex whose deletion from $\mathcal{H}$ form more components than the original graph. The cardinality of smallest vertex-cut is named as connectivity number of $\mathcal{H}$ and is written by $\kappa_{\mathcal{H}}$. A maximal connected graph is recognized as a block if it does not have any cut-vertex. An edge set $\mathcal{E}_1 \subset \mathcal{E}_{\mathcal{H}}$ is an *edge-cut* of $\mathcal{H}$, if deletion of edges of $\mathcal{E}_1$ increases the components of $\mathcal{H}$. If $|\mathcal{E}_1| = 1$ then $\mathcal{E}_1$ is known as a *bridge* or cut-edge, and it does not lie on a cycle [10]. A *cut-edge* is recognized as an internal cut edge if it is not a pendent edge. The cardinality of a smallest edge-cut is said to be edge-connectivity number of $\mathcal{H}$ and is represented as $\lambda_{\mathcal{H}}$.

For $h_1, h_2 \in \mathcal{V}_{\mathcal{H}}$, the distance between h_1 and h_2, represented by $d_{\mathcal{H}}(h_1, h_2)$, is described as the path of smallest length between h_1 and h_2 in $\mathcal{H}$. The *eccentricity*, $ec_{\mathcal{H}}(h)$, of a vertex $h \in \mathcal{V}_{\mathcal{H}}$ is described as $ec_{\mathcal{H}}(h) = \max\{d_{\mathcal{H}}(h, h_1) \mid h_1 \in \mathcal{V}_{\mathcal{H}}\}$. The *diameter* and the *radius* of $\mathcal{H}$, represented by $\mathrm{d}_{\mathcal{H}}$ and $\mathrm{r}_{\mathcal{H}}$, respectively, are described as:

$$\mathrm{d}_{\mathcal{H}} = \max_{h \in \mathcal{V}_{\mathcal{H}}} ec_{\mathcal{H}}(h), \qquad \mathrm{r}_{\mathcal{H}} = \min_{h \in \mathcal{V}_{\mathcal{H}}} ec_{\mathcal{H}}(h). \tag{1.1}$$

A *diametrical path* in $\mathcal{H}$ is a path of length equal to $\mathrm{d}_{\mathcal{H}}$. A vertex $h \in \mathcal{V}_{\mathcal{H}}$ is known as a *peripheral* vertex if $ec_{\mathcal{H}}(h) = \mathrm{d}_{\mathcal{H}}$. The induced subgraph of $\mathcal{H}$ constructed from the peripheral vertices is represented by $Per(\mathcal{H})$. If $ec_{\mathcal{H}}(h) = \mathrm{r}_{\mathcal{H}}$, then h is called a *central* vertex in $\mathcal{H}$. The *center* of $\mathcal{H}$ is induced subgraph of $\mathcal{H}$ created by the central vertices of $\mathcal{H}$ and is written by $C(\mathcal{H})$. A graph is recognized as a self-centered graph if its radius and diameter are equal. For $\mathcal{X} \subset \mathcal{V}_{\mathcal{H}}$, the graph $\mathcal{H} - \mathcal{X}$ is constructed from $\mathcal{H}$ by deleting all vertices and edges linked on the vertices of $\mathcal{X}$. For $\mathcal{E}_1 \subset \mathcal{E}_{\mathcal{H}}$, the graph $\mathcal{H} - \mathcal{E}_1$ is constructed from $\mathcal{H}$ by removing all edges of $\mathcal{E}_1$ from $\mathcal{H}$.

Example 1.1. Let $\mathcal{H}$ be a graph with $\mathcal{V}_{\mathcal{H}} = \{h_1, \ldots, h_9\}$ and its center as shown in Figure 1.3. Then the central vertices are h_4, h_5 and the peripheral vertices are h_1, h_7, h_9 of $\mathcal{H}$. The radius and diameter of $\mathcal{H}$ are 3 and 5, respectively.

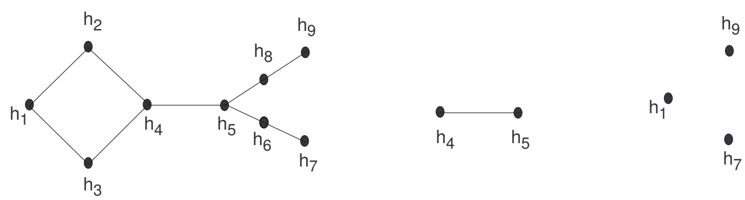

Figure 1.3: From left to right, a graph $\mathcal{H}$, $C(\mathcal{H})$ and $Per(\mathcal{H})$.

1.3 Matching, domination number, independence number and vertex cover

A *matching* M in $\mathcal{H}$ is a subset of $\mathcal{E}_{\mathcal{H}}$ such that any two elements of M do not incident to each other. A matching M in $\mathcal{H}$ is a largest matching if $|M| \geq |M'|$ for any other matching M' in $\mathcal{H}$. The cardinality of a largest matching in $\mathcal{H}$ is known as the matching number of $\mathcal{H}$ and is written by $m_{\mathcal{H}}$. A vertex $h \in \mathcal{V}_{\mathcal{H}}$ is represented as an M-saturated if it is an end-vertex of an edge in M. A matching M is a perfect matching in $\mathcal{H}$ if every vertex of $\mathcal{H}$ is M-saturated or $m_{\mathcal{H}} = \dfrac{n_{\mathcal{H}}}{2}$. A graph having a perfect matching is recognized as a *conjugated* graph.

A subset $\mathcal{A} \subset \mathcal{V}_{\mathcal{H}}$ is known as a *dominating set* of $\mathcal{H}$ if for every vertex $h_1 \in \mathcal{V}_{\mathcal{H}} \setminus \mathcal{A}$, there is a vertex $h_2 \in \mathcal{A}$ such that $h_1h_2 \in \mathcal{E}_{\mathcal{H}}$. For a dominating set $\mathcal{A}$ of $\mathcal{H}$ with $h_1, h_2 \in \mathcal{V}_{\mathcal{H}}$, if $h_1h_2 \in \mathcal{E}_{\mathcal{H}}$ then h_2 is dominated by h_1, where $h_1 \in \mathcal{A}$ and $h_2 \notin \mathcal{A}$. The domination number is the smallest cardinality between all the dominating sets of $\mathcal{H}$ and is represented by $\gamma_{\mathcal{H}}$.

A subset $\mathcal{I} \subset \mathcal{V}_{\mathcal{H}}$ is recognized as *independent set* of $\mathcal{H}$ if the elements in $\mathcal{I}$ are pairwise not linked in $\mathcal{H}$. The independence number of $\mathcal{H}$ is the largest cardinality among all independent sets of $\mathcal{H}$ and is represented by $\alpha_{\mathcal{H}}$.

A subset $\mathcal{C} \subset \mathcal{V}_{\mathcal{H}}$ is a *vertex cover* of $\mathcal{H}$ if and only if every edge $h_1h_2 \in \mathcal{E}_{\mathcal{H}}$, either $h_1 \in \mathcal{C}$ or $h_2 \in \mathcal{C}$ (or both). Clearly, $\mathcal{V}_{\mathcal{H}}$ is a vertex cover of $\mathcal{H}$. A vertex cover $\mathcal{C}$ of $\mathcal{H}$ is represented as a smallest vertex cover if $|\mathcal{C}| \leq |\mathcal{C}_1|$ for any other vertex cover $\mathcal{C}_1$ of $\mathcal{H}$ and $\mathcal{C}$ is a minimal vertex cover of $\mathcal{H}$ if there is no vertex cover $\mathcal{C}_1$, which is the proper subset of $\mathcal{C}$. The vertex covering number, $c_{\mathcal{H}}$, is the cardinality of a smallest vertex cover of $\mathcal{H}$.

A subset $\mathcal{F} \subset \mathcal{E}_{\mathcal{H}}$ is an *edge cover* of $\mathcal{H}$ if and only if every vertex in $\mathcal{H}$ is linked with an edge in $\mathcal{F}$. Clearly, $\mathcal{E}_{\mathcal{H}}$ is an edge cover of $\mathcal{H}$ when $\delta_{\mathcal{H}} > 0$. An edge cover $\mathcal{F}$ of $\mathcal{H}$ is called a smallest edge cover if $|\mathcal{F}| \leq |\mathcal{F}_1|$ for any other edge cover $\mathcal{F}_1$ of $\mathcal{H}$ and $\mathcal{F}$ is a minimal edge cover of $\mathcal{H}$ if there is no edge cover $\mathcal{F}_1$, which is the proper subset of $\mathcal{F}$. The edge covering number, $c'_{\mathcal{H}}$, is the cardinality of a smallest edge cover of $\mathcal{H}$.

Example 1.2. Let $\mathcal{H}$ be a graph with $\mathcal{V}_{\mathcal{H}} = \{h_1, h_2, \ldots, h_9, h_{10}\}$, shown in Figure 1.4. The minimum vertex cover and largest independent sets of $\mathcal{H}$ are $\{h_2, h_3, h_5, h_7\}$ and $\{h_1, h_4, h_6, h_8\}$, respectively. Therefore, the independence number and vertex covering number of $\mathcal{H}$ are $\alpha_{\mathcal{H}} = 4$ and $c_{\mathcal{H}} = 4$, respectively. Also the matching number of $\mathcal{H}$ is $m_{\mathcal{H}} = 4$.

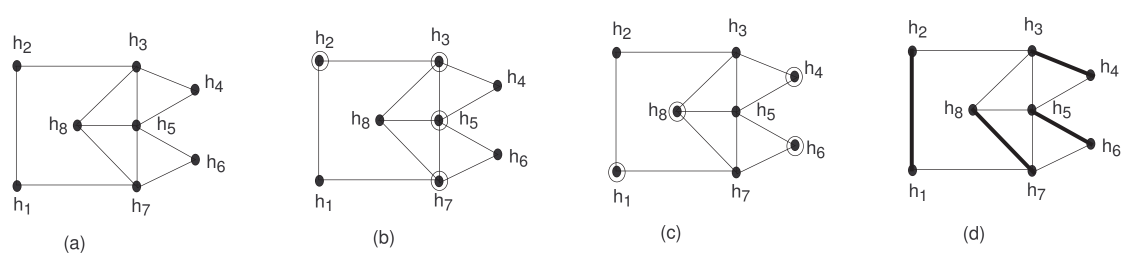

Figure 1.4: (a) A graph $\mathcal{H}$. (b) Circled vertices form a vertex cover. (c) Circled vertices form an independent set. (d) Bold edges form a maximum matching.

1.4 Trees and their related structures

In 1857, Sir Arthur Cayley [13] discussed the structure of trees, and he used the term "kenograms" for trees. Trees have many significant applications in various fields; particularly in road networks, data structure, the enumeration of saturated hydrocarbons, hierarchical data and communication networks. Furthermore, trees have a great utility in computer science, such as R-tree for spatial access methods, or in biology, such as evolutionary trees or cladograms. The spanning trees are used to look for minimum cost and in a road network problem to detect the shortest roots among the cities.

A connected graph $\mathcal{H}$ is known to be a *tree* if and only if it does not possess a cycle, and is expressed by T. In a tree T, a non-pendent vertex is said to be an internal vertex and each pair of distinct vertices of T are linked by a single path. The graph $\mathcal{H}$ is recognized as a forest if all connected components of it are trees.

A *star* S_n is an n-vertex tree that has a central vertex of $n-1$ degree and exactly $n-1$ pendent vertices. A tree is said to be a *double star* if it has exactly two non-pendent vertices. A tree T with $n \geq 3$ is known as *caterpillar* if extraction of pendent vertices of T constructs a path. A sub-tree T_1 of a connected graph $\mathcal{H}$ is known as a *spanning tree* of $\mathcal{H}$ if $\mathcal{V}_{T_1} = \mathcal{V}_{\mathcal{H}}$. If a vertex $h \in \mathcal{V}_T$ is labeled as the root of T, then T is represented as a rooted tree.

In the upcoming theorem, Gross and Yellen [40] manifested that every edge of a tree is a bridge. It signifies that by eliminating any edge from T transformed the tree into two components, each of which is a sub-tree of T.

Theorem 1.3 (Gross and Yellen [40]). *A graph T is a tree if and only if T is a connected graph, and every edge in it is a bridge.*

There are certain families of graphs, which are known as tree-like structures because they become a tree after deletion of a few edges. For example, n-vertex unicyclic and bicyclic graphs are connected graphs which contain n and $n+1$ edges, respectively. A connected graph $\mathcal{H}$ is said to be a cactus if its each block is either a cycle or an edge.

1.5 Extremal graph theory

Extremal graph theory is a significant field of graph theory, and it performs an essential role within the area of graph theory. In this theory, researchers analyze the influence of global properties (order, size, matching, independence number, etc.) of a graph on its local substructures.

In 1907, Mantel [70] gave the answer of an extremal problem "what is the largest size of a triangle-free graph $\mathcal{H}$" and he concluded the following outcome:

Theorem 1.4 (Mantel [70])**.** *Let $\mathcal{H}$ be a triangle-free graph. Then $\mathcal{H}$ contains at most $\frac{n_{\mathcal{H}}^2}{4}$ edges, equality if and only if $\mathcal{H} \cong K_{\lfloor n_{\mathcal{H}}/2 \rfloor, \lceil n_{\mathcal{H}}/2 \rceil}$.*

In 1941, Turán [90] started work on the advancement of extremal graph theory when he determined the generalization of Mantel's theorem.

Theorem 1.5 (Turán [90])**.** *Let $\mathcal{H}$ be a K_t-free graph with size $e_{\mathcal{H}}$, where $3 \leq t \leq n_{\mathcal{H}}$. Then we have $e_{\mathcal{H}} \leq \frac{n_{\mathcal{H}}^2((t-2)/(t-1))}{2}$.*

Erdős and Stone [30] generalized the Turán's theorem in 1946 and named it as *fundamental theorem* of extremal graph theory. They also extended the Turán's theorem for the graphs that do not contain the complete multi-partite graph as follows:

Theorem 1.6 (Erdős and Stone [30])**.** *For a given real number $a > 0$ and natural numbers r, s, $\exists$ an integer $b_0(r, s, a)$ such that if a graph $\mathcal{H}$ with $n_{\mathcal{H}} > b_0(r, s, a)$ and $e_{\mathcal{H}} \geq \frac{(r-1/r+a)n_{\mathcal{H}}^2}{2}$, then $\mathcal{H}$ contains a complete $r+1$-partite graph.*

In 1959, Erdős and Gallai [31] gave the answer of two problems proposed by Turán, that are, where the graph $\mathcal{H}$ attained the smallest size without containing a path and where it gained the largest size without containing a cycle of largest length.

Theorem 1.7 (Erdős and Gallai [31])**.** *Let $\mathcal{H}$ be a P_s-free, $(s \geq 2)$, graph with size $e_{\mathcal{H}}$. Then we have $e_{\mathcal{H}} \leq \frac{(s-2)n_{\mathcal{H}}}{2}$. Furthermore, equality holds if and only if $n_{\mathcal{H}}$ is divisible by $s-1$ and all connected components of $\mathcal{H}$ are K_{s-1}.*

Theorem 1.8 (Erdős and Gallai [31]). *Let $\mathcal{H}$ be a graph with $e_{\mathcal{H}} > \frac{1}{2}(s-1)(n_{\mathcal{H}}-1)$ edges, where $s \geq 3$. Then $\mathcal{H}$ have a cycle of length at least s. This bound is tight if $s-2$ is divided by $n_{\mathcal{H}}-1$.*

Up to now, identifying the extremal (smallest or largest) graphs in a given class of graphs with reference to topological invariants has turned out to be a significant direction in extremal graph theory. Along these lines, a number of excellent results have been obtained. We observe that the extremal graphs are the same for certain given classes of graphs. For further study on extremal graph theory, we refer [4, 5, 32, 35, 48, 51].

Chapter 2

Chemical graph theory and topological invariants

From the past two centuries, a lot of research work has been done in the implementations of Chemistry and graph theory in different fields by investigators. In later 18th century, chemical graphs were first used as the fundamental study of particles and matters. Cayley [12] used alkane trees to examine different categories of isomers. Sylvester [85] designed the structural formula for chemical graphs and then examined the similarity among them. William Cullen [88], who first termed them as affinity diagrams to symbolize the forces among pairs of molecules in chemical reactions. Chemical graph theory is the field of mathematical chemistry, which investigates the implementation of graph theory to figure out the molecular problems, and this theory performs a crucial part in the field of chemical science. A molecular graph $\mathcal{H}$ is a depiction of structural formula of chemical compound in the form of graph theory, and $\mathcal{H}$ is also generally known as a chemical graph, where edges and vertices of $\mathcal{H}$ correlate to chemical bonds and atoms, respectively.

In this dissertation, we will only concern with the topological properties or topological invariants of molecular graphs. The idea of topological invariants is implemented in molecular similarity analysis. Kopp [65] combined atoms of certain types in molecules to investigate volumes and densities of molecules. Topological indices are described as quantitative parameter of molecular graphs, and they perform a crucial part in the detection of the physical-chemical characterizations of molecules. For applications of topological indices, we refer the readers [50, 62].

This chapter is ordered as: In Section 2.1, we furnish a formal definition of a topological index with their implementations, and also we give details on some of most known topological indices. In Section 2.2, we present some known results related to topological descriptor.

2.1 Topological invariants

A *topological invariant* is figure out as the conversion of a molecular graph into a quantity which describes the graph-topology, and we also call it "graph invariant". A topological invariant of a graph $\mathcal{H}_1$, represented by $Top(\mathcal{H}_1)$, is equal to the topological index $Top(\mathcal{H}_2)$ of a graph $\mathcal{H}_2$ if $\mathcal{H}_1$ and $\mathcal{H}_2$ are isomorphic. A topological invariant is a mathematical quantity which brings together with the chemical structures of any finite simple graph. Topological indices generally reflect both the molecular shape and size of a molecular graph. A topological index of a molecular graph has numerous applications that are interconnection with its molecular properties [6]. These are also found effective for comparison and links between the biological and/or physico-chemical characterizations of molecules in non-empirical quantitative structure-property and quantitative structure-activity relationships [89]. These are also worthwhile in chemical documentation, isomer discrimination and pharmaceutical drug design [78, 79, 81].

Recently, topological invariants have earned a vital interest due to their significance in the field of computational chemistry. There are various varieties of topological invariants with respect to their specific topological features, including degrees of vertices, distances between vertices, eccentricities of vertices, connectivity, matching number, etc. Among these topological invariants, the degree based invariants are of extensive significant. Some degree and distance based topological invariants can also be computed by using matrices.

For a detailed study on this topic, we refer the reader [44, 77].

2.1.1 Some known topological invariants

Let $\mathcal{H}$ be a simple connected graph with $\mathcal{V}_{\mathcal{H}}$ vertex set and $\mathcal{E}_{\mathcal{H}}$ edge set. The first and the most noteworthy index, the *Wiener index*, was represented in 1947 by Harold Wiener [92]. At the beginning, this index was named as *path invariant* but after some time, it was retitled as Wiener index. In 1971, the notion of Wiener index was described by Hosoya [54] as:

$$\mathcal{W}(\mathcal{H}) = \sum_{\{h_1,h_2\}\subseteq \mathcal{V}_{\mathcal{H}}} d_{\mathcal{H}}(h_1, h_2).$$

The mathematical and chemical implementations of $\mathcal{W}(\mathcal{H})$ have been extensively investigated in [21]. Harold Wiener [92] also brought in another beneficial distance based topological invariant, known as *Wiener polarity index*. It can be described as cardinality of unordered pairs of $\{h_1, h_2\}$ vertices of $\mathcal{H}$ with $d_{\mathcal{H}}(h_1, h_2) = 3$ and mathematically defined as follows:

$$\mathcal{W}_p(\mathcal{H}) = |\{\{h_1, h_2\} \ | \ d_{\mathcal{H}}(h_1, h_2) = 3, \text{ for } h_1, h_2 \in \mathcal{V}_{\mathcal{H}}\}|.$$

Later on, the chemical and mathematical implementations of Wiener polarity index $\mathcal{W}_p(\mathcal{H})$ have been discussed by Lukovits and Linert, and Hosoya in [55, 69].

The *hyper Wiener index* of $\mathcal{H}$ is also an old index and is the extension of $\mathcal{W}(\mathcal{H})$. The hyper Wiener index $\mathcal{WW}(\mathcal{H})$ of $\mathcal{H}$, interpreted by Randić [76], is given by:

$$\mathcal{WW}(\mathcal{H}) = \frac{1}{2} \sum_{h_1\in \mathcal{V}_{\mathcal{H}}} \sum_{h_2\in \mathcal{V}_{\mathcal{H}}} (d_{\mathcal{H}}(h_1, h_2) + d_{\mathcal{H}}(h_1, h_2)^2).$$

Historically, the first degree based invariants that were described by Gutman and Trinajstić [45], and are named as *Zagreb group indices*. Now a days, these invariants are titled with the *Zagreb indices* and are specified as follows:

$$\mathcal{M}_1(\mathcal{H}) = \sum_{h_1\in \mathcal{V}_{\mathcal{H}}} (\deg_{\mathcal{H}}(h_1))^2 = \sum_{h_1h_2\in \mathcal{E}_{\mathcal{H}}} (\deg_{\mathcal{H}}(h_1) + \deg_{\mathcal{H}}(h_2)),$$

$$\mathcal{M}_2(\mathcal{H}) = \sum_{h_1h_2\in\mathcal{E}_\mathcal{H}} \deg_\mathcal{H}(h_1)\deg_\mathcal{H}(h_2).$$

These indices are approximate formulae of the structure-dependency of total π-electron energy and are also recommended to measure molecular complexity.

In 1975, Randić [75] investigated a novel topological invariant to judge the boundaries of branching of the carbon-atom skeleton of saturated hydrocarbons. He named it the *branching invariant*, but after some time it was retitled as *connectivity index*. Now a days, it is titled as *Randić index* and it is the most applied and known invariant among all invariants. It is the most-beneficial invariant in the study of structure property and activity relationships and is described as follows:

$$\mathcal{R}(H) = \sum_{h_1h_2\in\mathcal{E}_\mathcal{H}} (\deg_\mathcal{H}(h_1)\deg_\mathcal{H}(h_2))^{-1/2}.$$

Later, in 1998, Bollobás and Erdös [8] presented generalization of Randić invariant and called it *general Randić* invariant. It was specified as follows:

$$\mathcal{R}_\beta(\mathcal{H}) = \sum_{h_1h_2\in\mathcal{E}_\mathcal{H}} (\deg_\mathcal{H}(h_1)\deg_\mathcal{H}(h_2))^\beta,$$

where β is a real number. Therefore Randić invariant of $\mathcal{H}$ is $\mathcal{R}_{-1/2}$.

The *general sum-connectivity* invariant is a recent topological descriptor that was designed by Zhou and Trinajstić [100]. They replaced the product term $\deg_\mathcal{H}(h_1)\deg_\mathcal{H}(h_2)$ by $\deg_\mathcal{H}(h_1) + \deg_\mathcal{H}(h_2)$ in the general Randić invariant and written as follows:

$$\chi_\beta(\mathcal{H}) = \sum_{h_1h_2\in\mathcal{E}_\mathcal{H}} (\deg_\mathcal{H}(h_1) + \deg_\mathcal{H}(h_2))^\beta,$$

where β is a real number. Therefore $\chi_{-1/2}(\mathcal{H})$ is a classical sum-connectivity invariant, which was investigated by Zhou and Trinajstić [99]. For additional details on these degree based topological invariants, readers are referred to [6, 46, 62, 67, 68].

2.1.2 Some degree-distance based topological invariants

Recently, many eccentricity based invariants and their implementations in mathematics and chemistry have been introduced. Now we incorporated some distance-degree based topological invariants. The notion of the *average eccentricity index* was brought by Skorobogatov and Dobryninin [83] in 1988 and is interpreted as follows:

$$\overline{\varepsilon}(\mathcal{H}) = \frac{1}{n} \sum_{h \in \mathcal{V}_{\mathcal{H}}} ec_{\mathcal{H}}(h).$$

For more results on the average eccentricity index, we suggest the readers to [11, 23, 86].

One of the degree eccentricity invariant is *eccentric connectivity* invariant investigated by Sharma et al. [81] and is illustrated as:

$$\xi^{c}(\mathcal{H}) = \sum_{h \in \mathcal{V}_{\mathcal{H}}} ec_{\mathcal{H}}(h) \deg_{\mathcal{H}}(h).$$

In recent times, researchers have been attracted in analyzing the chemical and mathematical characteristics of $\xi^{c}(\mathcal{H})$. The eccentric connectivity invariant has been proved to provide extreme level of anticipatebility of pharmaceutical characteristics and allow directions for the advancement of beneficial and protected anti-HIV compounds [22]. Gupta et al. [44] examined the connection between the Wiener and the eccentric connectivity indices. It has been also applied in structure activity and structure property correspondences studies [66, 78], and its mathematical characteristics have been explored in [60, 79, 101].

The *connective eccentricity index* of $\mathcal{H}$ is the continuation of eccentric connectivity ξ^{c} index that was interpreted by Gupta et al. [42] and is defined as follows:

$$\xi^{ce}(\mathcal{H}) = \sum_{h \in \mathcal{V}_{\mathcal{H}}} \frac{\deg_{\mathcal{H}}(h)}{ec_{\mathcal{H}}(h)}.$$

Furthermore, the *eccentric adjacency index* (also renowned as Ediz eccentric connectivity invariant [27]) is the variation of the eccentric connectivity and the connective eccentricity invariants. Gupta et al. [43] suggested the eccentric adjacency index as follows:

$$\xi^{ad}(\mathcal{H}) = \sum_{h \in \mathcal{V}_{\mathcal{H}}} \frac{S_{\mathcal{H}}(h)}{ec_{\mathcal{H}}(h)}.$$

Additionally, they inquired the connection of anti-HIV activity of HEPT derivatives with the first-order molecular connectivity invariant and eccentric adjacency invariant. Moreover, the high discriminating power of ξ^{ad} extends a massive capability for structure-activity and structure-property studies.

Another topological index derived from the eccentric connectivity invariant, is the *total eccentricity* invariant and is given as:

$$\tau(\mathcal{H}) = \sum_{h\in\mathcal{V}_{\mathcal{H}}} ec_{\mathcal{H}}(h).$$

Vukičević and Graovac [91] defined the first and second *Zagreb eccentricity* invariants as follows:

$$\mathcal{E}_1(\mathcal{H}) = \sum_{h\in\mathcal{V}_{\mathcal{H}}} (ec_{\mathcal{H}}(h))^2, \qquad \mathcal{E}_2(\mathcal{H}) = \sum_{h_1h_2\in\mathcal{E}_{\mathcal{H}}} ec_{\mathcal{H}}(h_1)ec_{\mathcal{H}}(h_2).$$

Some computational and mathematical characteristics of the Zagreb eccentricity indices have been investigated in [16, 24, 39, 94].

2.2 Some known results of extremal graphs w.r.t. topological indices

In this section, we talk about some valuable results related to extremal graphs, with given parameters such as largest degree, matching number, diameter, etc., with respect to certain topological invariants. First we give some elementary results about Wiener index.

Theorem 2.1 (Entringer et al. [29], Gutman [47])**.** *Let T be a tree. Then $\mathcal{W}(S_{n_T}) \leq \mathcal{W}(T) \leq \mathcal{W}(P_{n_T})$, where first and second equalities satisfy if and only if $T \cong S_{n_T}$ and $T \cong P_{n_T}$, respectively.*

In the upcoming result, Entringer et al. [29] investigated the maximal graph with respect to Wiener index among all connected graphs.

Corollary 2.2 (Entringer et al. [29])**.** *For a connected graph $\mathcal{H}$, we have $\mathcal{W}(\mathcal{H}) \leq \mathcal{W}(P_{n_H})$, where equality if and only if $\mathcal{H} \cong P_{n_H}$.*

A tree T consisting of a path $P_{n_T-\triangle_T-1}$ and a star $S_{\triangle_T+1}$ whose one pendent vertex is attached with a pendent vertex of $P_{n_T-\triangle_T-1}$, is known as broom and is written by $B_{n_T,\triangle_T}$. The following theorem yields the maximal graph with respect to Wiener index between all connected graphs with a largest degree.

Theorem 2.3 (Stevanović [84]). *For any connected graph $\mathcal{H}$ with a largest degree $\triangle_{\mathcal{H}}$, we have $\mathcal{W}(\mathcal{H}) \leq \mathcal{W}(B_{n_{\mathcal{H}},\triangle_{\mathcal{H}}})$, equality if and only if $\mathcal{H} \cong B_{n_{\mathcal{H}},\triangle_{\mathcal{H}}}$.*

Let $S_{n,m}$ be a tree constructed from the star S_{n-m+1} by connecting a pendent edge to each $m-1$ pendent vertices in S_{n-m+1}. It is proved in [25] that among all trees with matching number m, $S_{n,m}$ has smallest Wiener index.

Theorem 2.4 (Du and Zhou [25]). *For any tree T with matching number m_T, where $2 \leq m_T \leq \left\lfloor \frac{n_T}{2} \right\rfloor$, we have $\mathcal{W}(T) \geq n_T^2 + (m_T-3)n_T - 3m_T + 4$, equality if and only if $T \cong S_{n_T,m_T}$.*

By $L_{n,g}$, we represent the unicyclic graph which is constructed from a cycle C_g and a path P_{n-g+1} by identifying a vertex of C_g with a pendent vertex of P_{n-g+1}. Let $U(n,g;n-g)$ be a unicyclic graph constructed from C_g by connecting $n-g$ pendent vertices to a vertex of C_g. The upcoming theorem gives the bounds on Wiener index of unicyclic graphs with a given girth.

Theorem 2.5 (Yu and Feng [96]). *Let U be a unicyclic graph with a given girth g. Then*

$$\mathcal{W}(U) \geq \begin{cases} \dfrac{g^3}{8} + (n_U - g)\left(\dfrac{g^2}{4} + n_U - 1\right) & \text{if } g \text{ is even,} \\ \dfrac{g^3 - g}{8} + (n_U - g)\left(\dfrac{g^2-1}{4} + n_U - 1\right) & \text{if } g \text{ is odd,} \end{cases}$$

equality if and only if $U \cong U(n_U, g; n_U - g)$. Moreover

$$\mathcal{W}(U) \leq \begin{cases} \dfrac{g^3}{8} + (n_U - g)\left(\dfrac{n_U^2 + n_U g + 3g - 1}{6} - \dfrac{g^2}{12}\right) & \text{if } g \text{ is even,} \\ \dfrac{g^3 - g}{8} + (n_U - g)\left(\dfrac{n_U^2 + n_U g + 3g - 1}{6} - \dfrac{g^2}{12} - \dfrac{1}{4}\right) & \text{if } g \text{ is odd,} \end{cases}$$

equality if and only if $U \cong L_{n_U,g}$.

Corollary 2.6 (Yu and Feng [96]). *For a unicyclic graph U with $n_U \geq 4$, we have* $n_U(n_U - 1) \leq \mathcal{W}(U) \leq \dfrac{n_U^3 - 7n_U + 12}{6}$, *with left inequality is equality if and only if* $U \cong U(n_U, 3; n_U - 3)$ *and right inequality is equality if and only if* $U \cong L_{n_U,3}$.

Now we provide some known results related to eccentricity based topological indices and their analogous extremal graphs. In the upcoming theorem, Zhou and Du [101] gives the lower and upper bounds on ξ^c of a graph.

Theorem 2.7 (Zhou and Du [101]). *Let $\mathcal{H}$ be a connected graph with size $e_{\mathcal{H}}$. Then*

$$2e_{\mathcal{H}} \cdot \mathrm{r}_{\mathcal{H}} \leq \xi^c(\mathcal{H}) \leq 2e_{\mathcal{H}} \cdot \mathrm{d}_{\mathcal{H}},$$

where both equalities hold if and only if $\mathcal{H}$ is a self-centered graph.

The next theorem shows that star S_n is the smallest graph with reference to eccentric connectivity index among all graphs.

Theorem 2.8 (Zhou and Du [101] and Morgan et al. [71]). *For a connected graph $\mathcal{H}$, we have $\xi^c(\mathcal{H}) \geq 3(n_{\mathcal{H}} - 1)$, where $n_{\mathcal{H}} \geq 4$ and equality if and only if $\mathcal{H} \cong S_{n_{\mathcal{H}}}$.*

Zhou and Du [101] give the smallest unicyclic graph with reference to the eccentric connectivity index in next result.

Theorem 2.9 (Zhou and Du [101]). *For a unicyclic graph U with $n_U \geq 4$, we have $\xi^c(U) \geq 3n_U + 1$, with equality holds if and only if $U \cong U(n_U, 3; n_U - 3)$.*

Let $\overline{B}$ be the bicyclic graph which is obtained from unicyclic graph $U(n, 3; n-3)$ by joining two pendent vertices with an edge of $U(n, 3; n-3)$.

Theorem 2.10 (Zhou and Du [101]). *For a bicyclic graph $\mathcal{H}$, where $n_{\mathcal{H}} \geq 5$, we have $\xi^c(\mathcal{H}) \geq 3n_{\mathcal{H}} + 5$, equality holds if and only if $\mathcal{H} \cong \overline{B}$.*

Hua and Das [58] discussed the connection among the Zagreb and the eccentric connectivity indices.

Theorem 2.11 (Hua and Das [58]). *For a connected graph $\mathcal{H}$ with $n_{\mathcal{H}} \geq 7$ and $\delta_{\mathcal{H}} \geq \frac{n_{\mathcal{H}}}{2} - 1$, we have $\xi^c(\mathcal{H}) \leq \mathcal{M}_i(\mathcal{H})$, for $i = 1, 2$.*

Theorem 2.12 (Hua and Das [58]). *Let $\mathcal{H}$ be a connected graph, where $n_{\mathcal{H}} \geq 6$, with the connected complement. Then*

- $\mathcal{M}_1(\mathcal{H}) + \mathcal{M}_1(\overline{\mathcal{H}}) \geq \xi^c(\mathcal{H}) + \xi^c(\overline{\mathcal{H}})$.
- $\mathcal{M}_2(\mathcal{H}) + \mathcal{M}_2(\overline{\mathcal{H}}) \geq \xi^c(\mathcal{H}) + \xi^c(\overline{\mathcal{H}})$.

Later on, Dankelmann et al. [15] determined the relation among the eccentric connectivity and the Wiener indices.

Theorem 2.13 (Dankelmann et al. [15]). *For a tree T, we have $\mathcal{W}(T) \leq \frac{n_T}{3}\xi^c(T) - n_T + 1$, equality holds if and only if $T \cong S_{n_T}$, where $n_T \geq 3$.*

Corollary 2.14 (Dankelmann et al. [15]). *Let $\mathcal{H}$ be a graph with $n_{\mathcal{H}} \geq 3$. Then $\mathcal{W}(\mathcal{H}) \leq \frac{2n_{\mathcal{H}}}{3}\xi^c(\mathcal{H}) - n_{\mathcal{H}} + 1$.*

Ilić and Gutman [60] derived the eccentric connectivity index of trees with a fixed largest vertex degree, fixed diameter, fixed radius, perfect matching, fixed number of pendent vertices and found their corresponding extremal graphs. Zhang et al. [102] gave lower bounds on the ξ^c in the form of size of graphs with a given diameter. Later on Zahng et al. [103] determined the largest eccentric connectivity invariant of connected n-vertex graphs with e edges ($n \leq e \leq n+4$), and gave a conjecture on the largest eccentric connectivity index of connected graphs for $e \geq n+5$. For further details on the eccentric connectivity index, see [72, 73, 93].

The relationship among the connective eccentricity and other topological indices is studied in the following result.

Theorem 2.15 (Yu and Feng [97]). *For a connected graph $\mathcal{H}$, we have*

- $\xi^{ce}(\mathcal{H}) \leq 2e_{\mathcal{H}} = n_{\mathcal{H}}(n_{\mathcal{H}} - 1)$, *equality if and only if $\mathcal{H} \cong K_{n_{\mathcal{H}}}$.*

- $\xi^{ce}(\mathcal{H}) \leq \xi^{c}(\mathcal{H})$, *equality if and only if* $\mathcal{H} \cong K_{n_{\mathcal{H}}}$.
- $\xi^{ce}(\mathcal{H}) \geq \dfrac{4e_{\mathcal{H}}^2}{\xi^{c}(\mathcal{H})}$, *equality if and only if* $ec_{\mathcal{H}}(h)$ *is a constant for all* h.
- $\xi^{ce}(\mathcal{H}) \geq \dfrac{M_1(\mathcal{H})}{\tau(\mathcal{H})}$.

Yu and Feng [97] present bounds for ξ^{ce} of graphs in the form of graph invariants such as the independence number, vertex connectivity, smallest degree and largest degree. Let K_n^s be the n-vertex graph constructed from a complete graph K_{n-s} by atthaching s pendent edges to a vertex of K_{n-s}.

Theorem 2.16 (Yu and Feng [97]). *Let* $\mathcal{H}$ *be a connected graph with* $s \geq 1$ *cut edges. Then* $\xi^{ce}(\mathcal{H}) \leq \frac{1}{2}(n_{\mathcal{H}}^2 - 2n_{\mathcal{H}}s + s^2 + 3s - 1)$, *equality if and only if* $\mathcal{H} \cong K_{n_{\mathcal{H}}}^s$.

Let C_n^s be a cactus obtained by adding s independent edges among the pendent vertices of S_n.

Theorem 2.17 (Yu and Feng [97]). *Let* $\mathcal{H}$ *be a cactus with* s *cycles, where* $n_{\mathcal{H}} \geq 5$. *Then* $\xi^{ce}(\mathcal{H}) \leq \frac{3}{2}n_{\mathcal{H}} + s - \frac{3}{2}$, *with equality holding if and only if* $\mathcal{H} \cong C_{n_{\mathcal{H}}}^s$.

Theorem 2.18 (Yu and Feng [97]). *For a given tree* T, *we have* $\xi^{ce}(T) \leq \dfrac{3(n_T - 1)}{2}$, *equality if and only if* $T = C_{n_T}^0 = S_{n_T}$.

Theorem 2.19 (Yu and Feng [97]). *For a given unicyclic graph* U, *we have* $\xi^{ce}(U) \leq \dfrac{3n_U - 1}{2}$, *equality if and only if* $T = C_{n_U}^1 = U(n_U, 3, n_U - 3)$.

De [17] derived some new bounds for ξ^{ce} in the form of some other graph parameters such as the largest degree ($\triangle$), smallest degree (δ), radius (r), diameter (d) and first Zagreb ($\mathcal{M}_1$) index. De et al. [18] presented ξ^{ce} index of certain graph operations. The following results give the smallest graphs with respect to the connective eccentricity index with the help of fixed matching number and a fixed order.

Theorem 2.20 (Xu et al. [95]). *For a given tree* T *with a fixed matching number* m_T, *where* $n_T \geq 2m_T$. *Then* $\xi^{ce}(T) \leq \frac{5}{6}n_T - \frac{1}{4}m_T - \frac{7}{12}$, *equality if and only if* $T \cong S_{n_T, m_T}$.

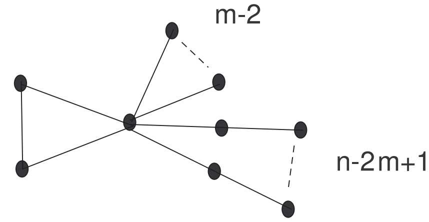

Figure 2.1: The graph U_{n_U,m_U}.

Theorem 2.21 (Xu et al. [95]). *Let U be a unicyclic graph with a fixed matching number m_U, where $n_U \geq 2m_U$. Then $\xi^{ce}(U) \leq \frac{5}{6}n_U - \frac{1}{4}m_U + \frac{1}{3}$, equality if and only if $U \cong U_{n_U,m_U}$, where U_{n_U,m_U} is given in Figure 2.1.*

Xu et al. [95] also discussed some relations between ξ^{ce} and ξ^{c} of graphs. For further details on the connective eccentricity index, see [87, 98]. Ediz [26] investigated some characteristics of the eccentric adjacency index of graphs. Furthermore, he determined some bounds on the eccentric adjacency invariant of graphs with parameters minimum degree and diameter, and radius and diameter in same paper.

Theorem 2.22 (Ediz [26]). *For a given connected graph $\mathcal{H}$, we have $\xi^{ad}(\mathcal{H}) \leq n_{\mathcal{H}}(n_{\mathcal{H}} - 1)^2$, with equality if and only if $\mathcal{H} \cong K_{n_H}$.*

Theorem 2.23 (Ediz [26]). *For a given tree T, we have $\xi^{ad}(T) \geq \xi^{c}(P_{n_T})$ and $\xi^{ad}(T) \leq \xi^{c}(S_{n_T})$, where $n_T \geq 2$.*

Theorem 2.24 (Ediz [26]). *For a given connected graph $\mathcal{H}$, we have $\xi^{ad}(\mathcal{H}) > \dfrac{n_{\mathcal{H}}\delta_{\mathcal{H}}}{\mathrm{d}_{\mathcal{H}}}$.*

Theorem 2.25 (Ediz [26]). *Let $\mathcal{H}$ be an s-regular graph with radius $\mathrm{r}_{\mathcal{H}}$ and diameter $\mathrm{d}_{\mathcal{H}}$. Then $\dfrac{n_{\mathcal{H}}s^2}{\mathrm{d}_{\mathcal{H}}} \leq \xi^{ad}(\mathcal{H}) \leq \dfrac{n_{\mathcal{H}}s^2}{\mathrm{r}_{\mathcal{H}}}$ with equality from the both sides if and only if $\mathcal{H} \cong K_{n_{\mathcal{H}}}$.*

Sharafdini and Safazadeh [80] calculated the eccentric adjacency index of several infinite classes of fullerene. For further details on the eccentric adjacency index, see [28, 34].

In following result, it is proved that the star S_{n_T} minimizes $\tau(T)$ among trees with a given order n_T.

Proposition 2.26 (Smith et al. [82]). *For any tree T with $n_T \geq 3$, we have $\tau(T) \geq 2n_T - 1$ with equality if and only if $T \cong S_{n_T}$.*

Smith et al. [82] also studied the extremal trees with the smallest and the largest total eccentricity invariant among trees with a given degree sequence. Farooq et al. [36, 37] found the extremal trees, unicyclic, bicyclic, conjugated unicyclic, and conjugated bicyclic graphs with reference to the total eccentricity invariant.

Theorem 2.27 (Farooq et al. [36]). *For a given tree T, we have $\tau(T) \leq \tau(P_{n_T}) = \frac{3}{4}n_T^2 - \frac{1}{2}n_T$.*

Theorem 2.28 (Farooq et al. [36]). *For a given unicyclic graph U with $n_U \geq 4$, we have $\tau(U) \geq 2n_U - 1$, equality satisfies if and only if $U \cong U_{n_U,3}$.*

Theorem 2.29 (Farooq et al. [36]). *For a given bicyclic graph B with $n_B \geq 4$, we have $\tau(B) \geq 2n_B - 1$, equality satisfies if and only if $B \cong \overline{B}$.*

Fathalikhani [38] and De et al. [19] determined the total eccentricity index of crucial graph operations. De et al. [20] find the total eccentricity index of subdivision graphs, double graph, extended double cover graph and certain generalized thorn graphs.

Chapter 3

Eccentric connectivity index and eccentric adjacency index of conjugated trees

One of the noteworthy problem in the chemical graph theory is to characterize the extremal graphs in a given family of graphs with reference to certain topological indices. Morgan et al. [71] computed sharp bounds of eccentric connectivity invariant of graphs in the form of order and also bounds for trees. Zhang et al. [102] gave lower bounds of eccentric connectivity invariant in the form of size of graphs with given diameter. Zhou et al. [101] found the bounds of eccentric connectivity invariant in the form of different graph invariants together with the order, size, degree distance and the first Zagreb index. Connection of eccentric adjacency and eccentric connectivity indices has been concluded by Gupta et al. [43].

Let $\mathcal{T}(2m, m)$, $m \geq 2$, be a class of conjugated trees of order $2m$, where m is a fixed matching number. In this chapter, we drive the conjugated trees with the extremal eccentric connectivity and eccentric adjacency indices among all n-vertex conjugated trees. This chapter is ordered as: Section 3.1, we derive trees in $\mathcal{T}(2m, m)$ with the smallest and the largest eccentric connectivity index. In Section 3.2, we find trees in $\mathcal{T}(2m, m)$

with the largest and the smallest eccentric adjacency index.

3.1 Smallest and largest eccentric connectivity index of conjugated trees

In this section, we determine the smallest and the largest eccentric connectivity index of trees in $\mathcal{T}(2m, m)$. Let $S^* \in \mathcal{T}(2m, m)$ be a tree obtained from S_{m+1} by subdividing $m-1$ edges of S_{m+1}. The tree S^* is depicted in Figure 3.1. We notice that all trees in $\mathcal{T}(2m, m)$ with radius 2 are isomorphic to S^*. If $m = 2$, then $S^* \cong P_4$ and $\xi^c(S^*) = 14$.

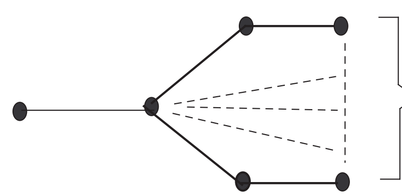

Figure 3.1: The tree S^*

Let $T \ncong S^*$ be a conjugated tree in $\mathcal{T}(2m, m)$ with a perfect matching M, $c \in \mathcal{V}_{C(T)}$ and $\mathrm{r}_T \geq 3$. Define

$$B_r(T) = \{uv \in \mathcal{E}_T \mid d_T(c, u) = d_T(c, v) - 1 = \mathrm{r}_T - 2 \text{ and } \deg_T(v) = 2\}. \qquad (3.1)$$

Observe that if uvw is a path in T with $d_T(c, w) = \mathrm{r}_T$ then w is a pendent vertex in T. Since T is a conjugated tree, we have $\deg_T(v) = 2$ and $vw \in M$.

In next lemma, we construct a new tree in $\mathcal{T}(2m, m)$ from a given tree in $\mathcal{T}(2m, m)$ with smaller eccentric connectivity index.

Lemma 3.1. *Let $T \ncong S^*$ be a conjugated tree in $\mathcal{T}(2m, m)$ with $m \geq 3$ and $c \in \mathcal{V}_{C(T)}$. Let w be a peripheral vertex of T and uvw be a path of length 2. Construct a new tree $T_1 = (T - \{uv\}) \cup \{cv\}$. Then $T_1 \in \mathcal{T}(2m, m)$ and $\xi^c(T) > \xi^c(T_1)$.*

Proof. Let M be a perfect matching in T. Take a diametrical w, w_1-path in T and $uv, vw \in \mathcal{E}_T$ such that $d_T(c, w) = \mathrm{r}_T$. Since T is a conjugated tree, we have $\deg_T(v) = 2$ and $vw \in M$. By the construction of T_1, it is obvious that M is also a perfect matching in T_1, that is, $T_1 \in \mathcal{T}(2m, m)$ and also

$$\deg_{T_1}(x) = \deg_T(x), \quad \forall\ x \in \mathcal{V}_T \setminus \{c, u\}. \tag{3.2}$$

Also, the degrees of vertices c and u in T_1 are given by

$$\deg_{T_1}(c) = \deg_T(c) + 1, \qquad \deg_{T_1}(u) = \deg_T(u) - 1. \tag{3.3}$$

Let $\mathcal{A} = \{y \in \mathcal{V}_T \mid ec_T(y) = d_T(y, w)\}$ and $x \in \mathcal{V}_T \setminus (\{v, w\} \cup \mathcal{A})$. Then

$$ec_{T_1}(x) = d_{T_1}(x, w_1) = d_T(x, w_1) = ec_T(x). \tag{3.4}$$

For each $y \in \mathcal{A} \backslash \{c\}$, either $ec_{T_1}(y) = d_{T_1}(y, u)$ or $ec_{T_1}(y) = d_{T_1}(y, w)$ or $ec_{T_1}(y) = d_{T_1}(y, z)$ for some peripheral vertex $z \in \mathcal{V}_{T_1} \setminus \{u, w\}$. If $ec_{T_1}(y) = d_{T_1}(y, z)$, then it is evident that $d_{T_1}(y, z) = d_T(y, z)$. Therefore

$$ec_{T_1}(y) = d_{T_1}(y, z) = d_T(y, z) \leq ec_T(y). \tag{3.5}$$

If $ec_{T_1}(y) = d_{T_1}(y, u)$, then

$$ec_{T_1}(y) = d_{T_1}(y, u) = d_T(y, u) < ec_T(y). \tag{3.6}$$

If $ec_{T_1}(y) = d_{T_1}(y, w)$ then it is obvious that $ec_T(y) = d_T(y, w) = d_T(y, c) + d_T(c, u) + 2$. Therefore

$$\begin{aligned} ec_{T_1}(y) &= d_{T_1}(y, w) = d_{T_1}(y, c) + d_{T_1}(c, w) \\ &= d_T(y, c) + 2 < ec_T(y). \end{aligned} \tag{3.7}$$

If w is the unique eccentric vertex of c in T then $ec_{T_1}(c) = d_{T_1}(c, w_1) = \mathrm{r}_T - 1 < ec_T(c)$. Also $d_T(v, c) \geq 2$ and $d_T(w, c) \geq 3$. It is evident that $ec_{T_1}(v) = ec_{T_1}(c) + 1$. Therefore

$$ec_{T_1}(v) = ec_{T_1}(c) + 1 < ec_T(c) + 1 < ec_T(c) + d_T(c, v) = ec_T(v). \tag{3.8}$$

Note that $vw \in \mathcal{E}_T \cap \mathcal{E}_{T_1}$. Therefore by using (3.8), we obtain

$$ec_{T_1}(w) = ec_{T_1}(v) + 1 < ec_T(v) + 1 = ec_T(w). \tag{3.9}$$

If w is not a unique eccentric vertex of c in T then by the construction of T_1, we have $ec_{T_1}(c) = ec_T(c)$. This gives

$$ec_{T_1}(v) = ec_{T_1}(c) + 1 = ec_T(c) + 1 < ec_T(c) + d_T(c, v) = ec_T(v). \tag{3.10}$$

Using (3.10), we obtain

$$ec_{T_1}(w) = ec_{T_1}(v) + 1 < ec_T(v) + 1 = ec_T(w). \tag{3.11}$$

Thus, from (3.2)$-$(3.11), we obtain

$$\begin{aligned}
\xi^c(T) - \xi^c(T_1) &= ec_T(c)\deg_T(c) - ec_{T_1}(c)\deg_{T_1}(c) + ec_T(u)\deg_T(u) - ec_{T_1}(u)\deg_{T_1}(u) \\
&\quad + ec_T(v)\deg_T(v) - ec_{T_1}(v)\deg_{T_1}(v) + ec_T(w)\deg_T(w) - ec_{T_1}(w)\deg_{T_1}(w) \\
\xi^c(T) - \xi^c(T_1) &> ec_T(c)\deg_T(c) - ec_T(c)(\deg_T(c) + 1) + ec_T(u)\deg_T(u) \\
&\quad - ec_T(u)(\deg_T(u) - 1) + 2ec_T(v) - 2ec_T(v) + ec_T(w) - ec_T(w) \\
&= ec_T(u) - ec_T(c) \geq 0.
\end{aligned}$$

This completes the proof. □

Next, we give an algorithm proposed by Farooq et al. [36] which reduces a given tree T in $\mathcal{T}(2m, m)$ into S^*.

Algorithm 1

Step 0: Take a conjugated tree $T \in \mathcal{T}(2m, m)$ and find r_T by (1.1), $c \in \mathcal{V}_{C(T)}$ and define $B_r(T)$ by (3.1).

Step 1: If $\mathrm{r}_T = 2$ then stop.

Step 2: For an edge $uv \in B_r(T)$, define $T := \{T - \{uv\}\} \cup \{cv\}$ and $B_r(T) := B_r(T) \setminus \{uv\}$.

Step 3: If $B_r(T) \neq \emptyset$ then go to Step 2; else find r_T by (1.1), $c \in \mathcal{V}_{C(T)}$ and $B_r(T)$ by (3.1); go to Step 1.

For termination and correctness of the Algorithm 1, we refer [36] to the reader.

In Theorem 3.2, we find the conjugated tree with the smallest eccentric connectivity index among all conjugated tress in $\mathcal{T}(2m, m)$ by using Lemma 3.1 and Algorithm 1.

Theorem 3.2. *Among all conjugated trees in $\mathcal{T}(2m, m)$, $m \geq 3$, the tree S^* shown in Figure 3.1 has the smallest eccentric connectivity index. Thus for any tree $T \in \mathcal{T}(2m, m)$, we have $\xi^c(T) \geq \xi^c(S^*)$.*

Proof. Let $T \ncong S^*$ be a conjugated tree in $\mathcal{T}(2m, m)$. By Lemma 3.1, the eccentric connectivity index of the modified tree decreases strictly at Step 2 in each iteration of the Algorithm 1. The Algorithm 1 terminates when $\mathrm{r}_T = 2$. Note that all n-vertex conjugated trees in $\mathcal{T}(2m, m)$ with radius 2 are isomorphic to S^*. This shows that S^* has the smallest eccentric connectivity index among trees in $\mathcal{T}(2m, m)$. □

Corollary 3.3. *If $T \in \mathcal{T}(2m, m)$, $m \geq 3$, then $\xi^c(T) \geq \xi^c(S^*) = 12m - 7$.*

Proof. Theorem 3.2 implies that $\xi^c(T) \geq \xi^c(S^*)$ for each $T \in \mathcal{T}(2m, m)$. The tree S^* (see Figure 3.1) has one vertex of eccentricity 2 and degree m, $m-1$ vertices of eccentricity 3 and degree 2, one vertex of eccentricity 3 and degree 1, and $m-1$ vertices of eccentricity 4 and degree 1. Therefore

$$\xi^c(S^*) = (1)(2)(m) + (m-1)(3)(2) + (1)(3)(1) + (m-1)(4)(1) = 12m - 7.$$

This completes the proof. □

Example 3.4. Consider a tree $T \in \mathcal{T}(16, 8)$ depicted in Figure 3.2. By using Algorithm 1 we obtain a sequence of trees $T,\ T_1,\ T_2,\ T_3,\ T_4,\ T_5,\ T_6$, where $T_6 \cong S^*$, satisfying the following:

$$\xi^c(T) > \xi^c(T_1) > \xi^c(T_2) > \xi^c(T_3) > \xi^c(T_4) > \xi^c(T_5) > \xi^c(T_6).$$

Note that the modification of trees at Step 2 in Algorithm 1 depends upon the choice of vertex u of T. Therefore this sequence of trees is not unique.

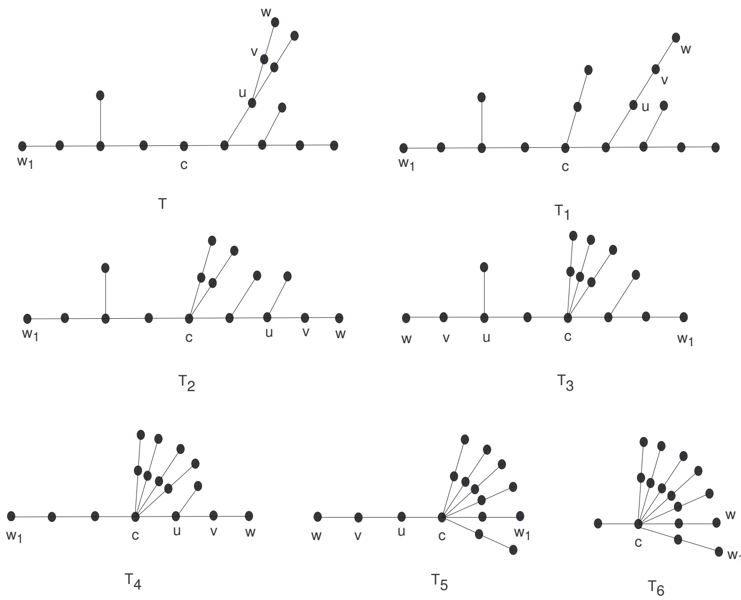

Figure 3.2: A sequence of trees generated by Algorithm 1.

Morgan et al. [71] showed that the path maximizes eccentric connectivity index among trees of fixed order n.

Theorem 3.5 (Morgan et al. [71]). *If T is an n-vertex tree, then*

$$\xi^c(T) \leq \xi^c(P_n) = \begin{cases} \frac{1}{2}(3n^2 - 6n + 4), & \text{for } n \text{ even,} \\ \frac{3}{2}(n-1)^2, & \text{for } n \text{ odd.} \end{cases} \tag{3.12}$$

Now we discuss the largest eccentric connectivity index of conjugated tree in $\mathcal{T}(2m, m)$.

Theorem 3.6. *If $T \in \mathcal{T}(2m, m)$, $m \geq 2$, then*

$$\xi^c(T) \leq \xi^c(P_{2m}) = 6m^2 - 6m + 2.$$

Proof. Theorem 3.5 implies that $\xi^c(T) \leq \xi^c(P_{2m})$. We notice that the order of a conjugated graph is even. Using $n = 2m$ in equation (3.12), we get the required result, that is,

$$\xi^c(P_{2m}) = 6m^2 - 6m + 2.$$

This completes the proof. □

3.2 Smallest and largest eccentric adjacency index of conjugated trees

In this section, we determine the smallest and the largest eccentric adjacency index of trees in $\mathcal{T}(2m, m)$. Note that all trees in $\mathcal{T}(2m, m)$ with radius 2 are isomorphic to S^*. If $m = 2$ then $S^* \cong P_4$ and $\xi^{ad}(P_4) = \frac{13}{3}$.

In next lemma, we construct a new tree in $\mathcal{T}(2m, m)$ from a given tree in $\mathcal{T}(2m, m)$ with larger eccentric adjacency index.

Lemma 3.7. *Let T be a conjugated tree in $\mathcal{T}(2m, m)$ with $\mathrm{r}_T \geq 3$ and $c \in \mathcal{V}_{C(T)}$. Take a vertex $u \in \mathcal{V}_T$ satisfying $d_T(c, u) = \mathrm{r}_T - 2$. Let $v_1, v_2, \ldots, v_k$ be those neighbors of u which satisfy $\deg_T(v_i) = 2$ and $d_T(c, v_i) = \mathrm{r}_T - 1$, for each $i = 1, 2, \ldots, k$. Construct a new tree $T_1 = (T - \{uv_1, uv_2, \ldots, uv_k\}) \cup \{cv_1, cv_2, \ldots, cv_k\}$. Then $T_1 \in \mathcal{T}(2m, m)$ and $\xi^{ad}(T) < \xi^{ad}(T_1)$.*

Proof. Let M be a perfect matching in T. Since T is a conjugated tree, there exists a unique pendent neighbor w_i of uv_i, $i = 1, 2, \ldots, k$. Note that $d_T(u, w_1) = d_T(u, w_2) = \cdots = d_T(u, w_k) = 2$. Let $w \in \{w_1, w_2, \ldots, w_k\}$ and take a diametrical w, w'-path in T. Since T is a conjugated tree, we have $\deg_T(v_i) = 2$ for each $i = 1, 2, \ldots, k$ and $v_1w_1, v_2w_2, \ldots, v_kw_k \in M$. By the construction of T_1, it is obvious to see that M is also a perfect matching in T_1, that is, $T_1 \in \mathcal{T}(2m, m)$.

Define $\mathcal{A}_1 = \{y \in \mathcal{V}_T \mid ec_T(y) = d_T(y, w)\}$. For each $y \in \mathcal{A}_1$, either $ec_{T_1}(y) = d_{T_1}(y, u)$ or $ec_{T_1}(y) = d_{T_1}(y, w)$ or $ec_{T_1}(y) = d_{T_1}(y, z)$ for some peripheral vertex $z \in \mathcal{V}_{T_1} \setminus \{u, w_1, w_2, \ldots, w_k\}$. If $ec_{T_1}(y) = d_{T_1}(y, z)$ then it is obvious that $d_{T_1}(y, z) = d_T(y, z)$. Therefore

$$ec_{T_1}(y) = d_{T_1}(y, z) = d_T(y, z) \leq ec_T(y). \tag{3.13}$$

If $ec_{T_1}(y) = d_{T_1}(y, u)$ then

$$ec_{T_1}(y) = d_{T_1}(y, u) = d_T(y, u) < ec_T(y). \tag{3.14}$$

Let $ec_{T_1}(y) = d_{T_1}(y, w)$. It is evident that $ec_T(y) = d_T(y, w) = d_T(y, c) + d_T(c, u) + 2$. Therefore

$$\begin{aligned} ec_{T_1}(y) &= d_{T_1}(y, w) = d_{T_1}(y, c) + d_{T_1}(c, w) \\ &= d_T(y, c) + 2 < ec_T(y). \end{aligned} \tag{3.15}$$

Now let $x \in \mathcal{V}_T \setminus (\{v_1, v_2, \ldots, v_k, w_1, w_2, \ldots, w_k\} \cup \mathcal{A}_1)$. Then we have

$$ec_{T_1}(x) = d_{T_1}(x, w') = d_T(x, w') = ec_T(x). \tag{3.16}$$

If c has no eccentric vertex other than $w_1, w_2, \ldots, w_k$ in T then $ec_{T_1}(c) = d_{T_1}(c, w') = \mathrm{r}_T - 1 < ec_T(c)$. Also $d_T(v_i, c) \geq 2$ and $d_T(w_i, c) \geq 3$, for $i = 1, 2, \ldots, k$. Moreover, $ec_{T_1}(v_i) = ec_{T_1}(c) + 1$ for each $i = 1, 2, \ldots, k$. Therefore

$$ec_{T_1}(v_i) = ec_{T_1}(c) + 1 < ec_T(c) + 1 < ec_T(c) + d_T(c, v_i) = ec_T(v_i), \tag{3.17}$$

for each $i = 1, 2, \ldots, k$. Note that $v_i w_i \in \mathcal{E}_T \cap \mathcal{E}_{T_1}$, for $i = 1, 2, \ldots, k$. Using (3.17), we obtain

$$ec_{T_1}(w_i) = ec_{T_1}(v_i) + 1 < ec_T(v_i) + 1 = ec_T(w_i), \tag{3.18}$$

for each $i = 1, 2, \ldots, k$.

If c has an eccentric vertex other than $w_1, w_2, \ldots, w_k$ in T then by the construction of T_1, we have $ec_{T_1}(c) = ec_T(c)$. Thus

$$ec_{T_1}(v_i) = ec_{T_1}(c) + 1 = ec_T(c) + 1 < ec_T(c) + d_T(c, v_i) = ec_T(v_i), \tag{3.19}$$

for each $i = 1, 2, \ldots, k$. By using (3.19), we have

$$ec_{T_1}(w_i) = ec_{T_1}(v_i) + 1 < ec_T(v_i) + 1 = ec_T(w_i), \tag{3.20}$$

for each $i = 1, 2, \ldots, k$. We note that $S_{T_1}(x) = S_T(x)$ for all $x \in \mathcal{V}_T \setminus (\Gamma_T(c) \cup \Gamma_T(u) \cup \{c, u\})$. Since T is a conjugated tree, it holds that $k + 1 \leq \deg_T(u) \leq k + 2$. That is, $S_T(v_i) = \deg_T(u) + 1 \leq k + 3$, for each $i = 1, 2, \ldots, k$. Thus

$$S_{T_1}(v_i) = (\deg_T(c) + k) + 1 \geq (2 + k) + 1 \geq S_T(v_i), \tag{3.21}$$

for each $i = 1, 2, \ldots, k$. Furthermore, either $u \in \Gamma_T(c)$ or $u \notin \Gamma_T(c)$. If $u \in \Gamma_T(c)$ then $\Gamma_T(c) \cap \Gamma_T(u) = \emptyset$. Thus

$$\begin{aligned} S_{T_1}(u) &= (S_T(u) - 2k) + k = S_T(u) - k, \\ S_{T_1}(c) &= (S_T(c) + 2k) - k = S_T(c) + k. \end{aligned} \tag{3.22}$$

Let $V_1 = \Gamma_T(u) \setminus \{c, v_1, v_2, \ldots, v_k\}$. Then

$$\begin{aligned} S_{T_1}(x) &= S_T(x) - k, \quad \forall\, x \in V_1, \\ S_{T_1}(y) &= S_T(y) + k, \quad \forall\, y \in \Gamma_T(c) \setminus \{u\}. \end{aligned} \tag{3.23}$$

Therefore, from (3.13)−(3.23), we obtain

$$\begin{aligned} \xi^{ad}(T_1) - \xi^{ad}(T) &= \frac{S_{T_1}(c)}{ec_{T_1}(c)} - \frac{S_T(c)}{ec_T(c)} + \frac{S_{T_1}(u)}{ec_{T_1}(u)} - \frac{S_T(u)}{ec_T(u)} + \sum_{i=1}^{k} \left(\frac{S_{T_1}(v_i)}{ec_{T_1}(v_i)} - \frac{S_T(v_i)}{ec_T(v_i)} \right) \\ &+ \sum_{i=1}^{k} \left(\frac{S_{T_1}(w_i)}{ec_{T_1}(w_i)} - \frac{S_T(w_i)}{ec_T(w_i)} \right) + \sum_{x \in V_1} \left(\frac{S_{T_1}(x)}{ec_{T_1}(x)} - \frac{S_T(x)}{ec_T(x)} \right) \\ &+ \sum_{y \in \Gamma_T(c) \setminus \{u\}} \left(\frac{S_{T_1}(y)}{ec_{T_1}(y)} - \frac{S_T(y)}{ec_T(y)} \right) \\ &> \frac{S_T(c) + k}{ec_T(c)} - \frac{S_T(c)}{ec_T(c)} + \frac{S_T(u) - k}{ec_T(u)} - \frac{S_T(u)}{ec_T(u)} + \sum_{i=1}^{k} \left(\frac{S_T(v_i)}{ec_T(v_i)} - \frac{S_T(v_i)}{ec_T(v_i)} \right) \\ &+ \sum_{i=1}^{k} \left(\frac{S_T(w_i)}{ec_T(w_i)} - \frac{S_T(w_i)}{ec_T(w_i)} \right) + \sum_{x \in V_1} \left(\frac{S_T(x) - k}{ec_T(x)} - \frac{S_T(x)}{ec_T(x)} \right) \\ &+ \sum_{y \in \Gamma_T(c) \setminus \{u\}} \left(\frac{S_T(y) + k}{ec_T(y)} - \frac{S_T(y)}{ec_T(y)} \right) \\ &= \frac{k}{ec_T(c)} - \frac{k}{ec_T(u)} - \sum_{x \in V_1} \frac{k}{ec_T(x)} + \sum_{y \in \Gamma_T(c) \setminus \{u\}} \frac{k}{ec_T(y)}. \end{aligned}$$

Observe that $ec_T(u) \geq \mathrm{r}_T = ec_T(c)$, equality if and only if $u \in \mathcal{V}_{C(T)} \setminus \{c\}$ and $w_1, w_2, \ldots, w_k$ are the peripheral vertices in T. Therefore $|\Gamma_T(u) \setminus (\{c, v_1, v_2 \ldots, v_k\})| \leq 1$. Note that c is a central vertex in T and $u \in \Gamma_T(c)$. Thus $|\Gamma_T(c) \setminus \{u\}| \geq 1$, $ec_T(y) \leq ec_T(x)$, for each $y \in \Gamma_T(c) \setminus \{u\}$ and $x \in V_1$. Therefore $\xi^{ad}(T_1) > \xi^{ad}(T)$.

Now, if $u \notin \Gamma_T(c)$ then $|\Gamma_T(u) \cap \Gamma_T(c)| \leq 1$ and

$$S_{T_1}(c) = S_T(c) + 2k, \quad S_{T_1}(u) = S_T(u) - 2k. \tag{3.24}$$

Let $V_2 = \Gamma_T(u) \setminus (\{v_1, v_2 \dots, v_k\} \cup (\Gamma_T(c) \cap \Gamma_T(u)))$ and $V_3 = \Gamma_T(c) \setminus (\Gamma_T(c) \cap \Gamma_T(u))$. Then

$$\begin{aligned} S_{T_1}(x) &= S_T(x) - k, && \forall\ x \in V_2, \\ S_{T_1}(y) &= S_T(y) + k, && \forall\ y \in V_3, \\ S_{T_1}(z) &= (S_T(z) - k) + k = S_T(z), && \forall\ z \in (\Gamma_T(c) \cap \Gamma_T(u)). \end{aligned} \tag{3.25}$$

Thus, from (3.13)−(3.21) and (3.24)−(3.25), we get

$$\begin{aligned} \xi^{ad}(T_1) - \xi^{ad}(T) &= \frac{S_{T_1}(c)}{ec_{T_1}(c)} - \frac{S_T(c)}{ec_T(c)} + \frac{S_{T_1}(u)}{ec_{T_1}(u)} - \frac{S_T(u)}{ec_T(u)} + \sum_{i=1}^{k} \left(\frac{S_{T_1}(v_i)}{ec_{T_1}(v_i)} - \frac{S_T(v_i)}{ec_T(v_i)} \right) \\ &+ \sum_{i=1}^{k} \left(\frac{S_{T_1}(w_i)}{ec_{T_1}(w_i)} - \frac{S_T(w_i)}{ec_T(w_i)} \right) + \sum_{y \in V_3} \left(\frac{S_{T_1}(y)}{ec_{T_1}(y)} - \frac{S_T(y)}{ec_T(y)} \right) \\ &+ \sum_{x \in V_2} \left(\frac{S_{T_1}(x)}{ec_{T_1}(x)} - \frac{S_T(x)}{ec_T(x)} \right) + \sum_{z \in (\Gamma_T(c) \cap \Gamma_T(u))} \left(\frac{S_{T_1}(z)}{ec_{T_1}(z)} - \frac{S_T(z)}{ec_T(z)} \right) \\ &> \frac{S_T(c) + 2k}{ec_T(c)} - \frac{S_T(c)}{ec_T(c)} + \frac{S_T(u) - 2k}{ec_T(u)} - \frac{S_T(u)}{ec_T(u)} \\ &+ \sum_{i=1}^{k} \left(\frac{S_T(v_i)}{ec_T(v_i)} - \frac{S_T(v_i)}{ec_T(v_i)} \right) + \sum_{i=1}^{k} \left(\frac{S_T(w_i)}{ec_T(w_i)} - \frac{S_T(w_i)}{ec_T(w_i)} \right) \\ &+ \sum_{y \in V_3} \left(\frac{S_T(y) + k}{ec_T(y)} - \frac{S_T(y)}{ec_T(y)} \right) + \sum_{x \in V_2} \left(\frac{S_T(x) - k}{ec_T(x)} - \frac{S_T(x)}{ec_T(x)} \right) \\ &+ \sum_{z \in (\Gamma_T(c) \cap \Gamma_T(u))} \left(\frac{S_T(z)}{ec_T(z)} - \frac{S_T(z)}{ec_T(z)} \right) \\ &= \frac{2k}{e_T(c)} - \frac{2k}{ec_T(u)} + \sum_{y \in V_3} \frac{k}{ec_T(y)} - \sum_{x \in V_2} \frac{k}{ec_T(x)}. \end{aligned}$$

We know that if $u \notin \Gamma_T(c)$ then $ec_T(u) > ec_T(c)$. Also as c is a central vertex in T, it holds that $|V_3| \geq |V_2|$ and $ec_T(y) \leq ec_T(x)$, for each $x \in V_2$ and $y \in V_3$. Thus $\xi^{ad}(T_1) > \xi^{ad}(T)$. This completes the proof. □

Next, we give a modified version of Algorithm 3 [36] which reduces a given tree $T \in \mathcal{T}(2m, m)$ into S^*.

Algorithm 2

Step 0: Take a conjugated tree $T \in \mathcal{T}(2m, m)$ and find r_T by (1.1), $c \in \mathcal{V}_{C(T)}$ and define $B_r(T)$ by (3.1).

Step 1: If $\mathrm{r}_T = 2$ then stop.

Step 2: Take a vertex $u \in \mathcal{V}_T$ satisfying $d_T(c, u) = \mathrm{r}_T - 2$ and let $v_1, v_2, \ldots, v_k$ be those neighbors of u for which $uv_i \in B_r(T)$, for each $i = 1, 2, \ldots, k$. Define $T := \{T - \{uv_1, uv_2, \ldots, uv_k\}\} \cup \{cv_1, cv_2, \ldots, cv_k\}$ and $B_r(T) := B_r(T) \setminus \{uv_1, uv_2, \ldots, uv_k\}$.

Step 3: If $B_r(T) \neq \emptyset$ then go to Step 2; else find r_T by (1.1), $c \in \mathcal{V}_{C(T)}$ and $B_r(T)$ by (3.1); go to Step 1.

For termination and correctness of the Algorithm 2, see [36].

Next, by using Lemma 3.7 and Algorithm 2, we find the conjugated tree with the largest eccentric adjacency index among all conjugated tress in $\mathcal{T}(2m, m)$.

Theorem 3.8. *Among all conjugated trees in $\mathcal{T}(2m, m)$, $m \geq 3$, the tree S^* shown in Figure 3.1 has the largest eccentric adjacency index. Thus for any tree $T \in \mathcal{T}(2m, m)$, we have $\xi^{ad}(T) \leq \xi^{ad}(S^*)$.*

Proof. Let $T \ncong S^*$ be a conjugated tree. By Lemma 3.7, the eccentric adjacency index of the modified tree increases strictly at Step 2 in each iteration of the Algorithm 2. The Algorithm 2 terminates when $\mathrm{r}_T = 2$ and note that all n-vertex conjugated trees with radius 2 are isomorphic to S^*. This shows that $\xi^{ad}(S^*) \geq \xi^{ad}(T)$. □

Corollary 3.9. *If $T \in \mathcal{T}(2m, m)$, $m \geq 3$, then $\xi^{ad}(T) \leq \xi^{ad}(S^*) = \frac{1}{6}(2m^2 + 11m - 8)$.*

Proof. Let $S^* \in \mathcal{T}(2m, m)$ and $c \in \mathcal{V}_{C(S^*)}$. The eccentricity of c in S^* is 2, $\deg_{S^*}(c) = m$ and $S_{S^*}(c) = 2(m-1) + 1 = 2m - 1$. If u is any neighbor of c in S^* then $ec_{S^*}(u) = 3$ and

$$\sum_{u \in \Gamma_{S^*}(c)} \frac{S_{S^*}(u)}{ec_{S^*}(u)} = \frac{(m-1)(m+1)}{3} + \frac{m}{3} = \frac{m^2 + m - 1}{3}.$$

Since there are $m-1$ peripheral vertices in S^* with eccentricity 4 and sum of degrees of neighbors of a peripheral vertex v is 2. Therefore

$$\begin{aligned}\xi^{ad}(S^*) &= \sum_{v\in\mathcal{V}_{S^*}\setminus(\{c\}\cup\Gamma_{S^*}(c))}\frac{S_{S^*}(v)}{ec_{S^*}(v)}+\sum_{u\in\Gamma_{S^*}(c)}\frac{S_{S^*}(u)}{ec_{S^*}(u)}+\frac{S_{S^*}(c)}{ec_{S^*}(c)}\\ &= \frac{2(m-1)}{4}+\frac{m^2+m-1}{3}+\frac{2m-1}{2}\\ &= \frac{2m^2+11m-8}{6}.\end{aligned}$$

The result $\xi^{ad}(T)\leq\xi^{ad}(S^*)$ follows from Theorem 3.8 for each $T\in\mathcal{T}(2m,m)$. □

Example 3.10. Consider a tree $T\in\mathcal{T}(20,10)$ with $c\in\mathcal{V}_{C(T))}$ shown in Figure 3.3. By the use of Algorithm 2, we obtain a sequence of trees $T,\ T_1,\ T_2,\ T_3,\ T_4,\ T_5$, where $T_5\cong S^*$. This sequence of trees is not unique because it depends upon the choice of vertex u. The relation of eccentric adjacency index of $T,\ T_1,\ T_2,\ T_3,\ T_4,\ T_5$ is as follows:

$$\xi^{ad}(T)<\xi^{ad}(T_1)<\xi^{ad}(T_2)<\xi^{ad}(T_3)<\xi^{ad}(T_4)<\xi^{ad}(T_5).$$

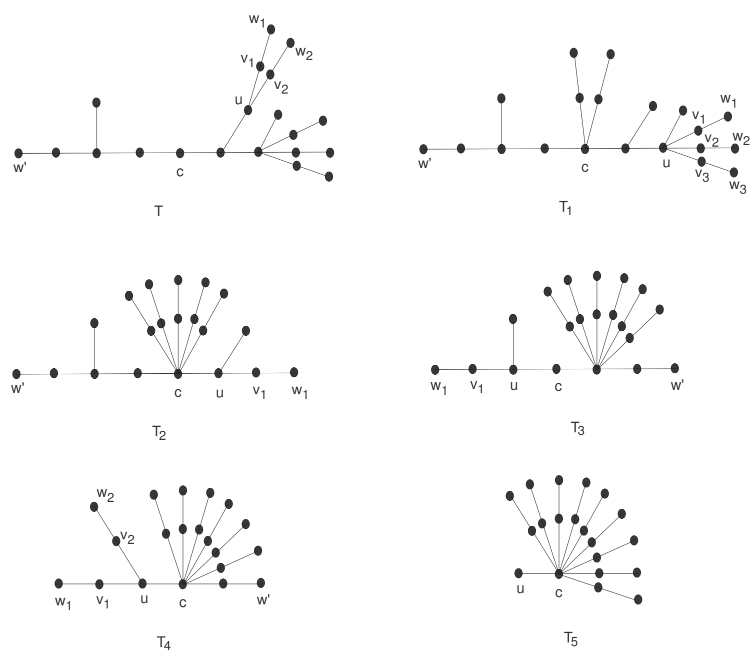

Figure 3.3: A sequence of trees generated by Algorithm 2

Ediz [26] proved that the path has the smallest eccentric adjacency index among trees of fixed order n.

Theorem 3.11 (Ediz [26]). *If T is an n-vertex tree, then*

$$\xi^{ad}(T) \geq \xi^{ad}(P_n) = \begin{cases} 2\left(\frac{2}{n-1} + \frac{3}{n-2} + \frac{4}{n-3} + \frac{4}{n-4} + \cdots + \frac{4}{\lfloor n/2 \rfloor + 1}\right) + \frac{4}{\lfloor n/2 \rfloor} & \text{if } n \text{ is odd,} \\ 2\left(\frac{2}{n-1} + \frac{3}{n-2} + \frac{4}{n-3} + \frac{4}{n-4} + \cdots + \frac{4}{n/2}\right) & \text{if } n \text{ is even.} \end{cases} \tag{3.26}$$

Now we find the smallest eccentric connectivity index of conjugated tree in $\mathcal{T}(2m, m)$.

Theorem 3.12. *If $T \in \mathcal{T}(2m, m)$, $m \geq 2$, then*

$$\xi^{ad}(T) \geq \xi^{ad}(P_{2m}) = 2\left(\frac{2}{2m-1} + \frac{3}{2m-2} + \frac{4}{2m-3} + \frac{4}{2m-4} + \cdots + \frac{4}{m}\right).$$

Proof. By Theorem 3.11, we have $\xi^{ad}(T) \geq \xi^{ad}(P_{2m})$ for each $T \in \mathcal{T}(2m, m)$. We notice that the order of a conjugated graph is even. Therefore by using $n = 2m$ in equation (3.26), we get

$$\begin{aligned} \xi^{ad}(P_{2m}) &= 2\left(\frac{2}{2m-1} + \frac{3}{2m-2} + \frac{4}{2m-3} + \frac{4}{2m-4} + \cdots + \frac{4}{2m/2}\right) \\ &= 2\left(\frac{2}{2m-1} + \frac{3}{2m-2} + \frac{4}{2m-3} + \frac{4}{2m-4} + \cdots + \frac{4}{m}\right). \end{aligned}$$

This completes the proof. □

3.3 Conclusion

In this chapter, we drive the conjugated trees with the smallest and the largest eccentric connectivity index among all conjugated trees. We also discuss the extremal conjugated trees with reference to eccentric adjacency index. It will be challenging to derive the extremal conjugated graphs with reference to eccentric connectivity invariant and eccentric adjacency index among all n-vertex conjugated graphs.

Chapter 4

Eccentric adjacency index of unicyclic graphs and trees

A lot of results have been obtained in the area of extremal graphs with reference to distance based topological invariants. Ediz [26,28] investigated certain properties of eccentric adjacency index and also calculated the eccentric adjacency index of one pentagonal carbon nanocones. Many research papers that study the extremal problems of topological indices focus on trees, unicyclic, bicyclic and sometimes to tricyclic graphs. In this regard, we find the results of extremal unicyclic graphs and trees with reference to eccentric adjacency index.

This chapter is ordered as: In Section 4.1, we find the graph with the largest eccentric adjacency index among all n-vertex unicyclic graphs with a fixed order and girth. Also, we find the graph with largest eccentric adjacency index among all n-vertex unicyclic graphs of fixed order in this section. In Section 4.2, we discuss the extremal n-vertex trees with the largest eccentric adjacency index in the family of all n-vertex trees with a given diameter and order.

4.1 The eccentric adjacency index of unicyclic graphs

Let $\mathcal{U}(n)$ be the family of all unicyclic graphs and $\mathcal{U}(n,g)$ be the family of all unicyclic graphs with girth g, where $n \geq 3$ and $3 \leq g \leq n$. Let $\widetilde{\mathcal{U}}(n,g) \subset \mathcal{U}(n,g)$ be the family of all n-vertex unicyclic graphs that are obtained from the cycle C_g by connecting $n-g$ pendent vertices to the vertices of C_g. Also let $U(n,g;n-g)$ be a unicyclic graph obtained from the cycle C_g by connecting $n-g$ pendent vertices with a unique vertex of C_g.

In this section, we find the extremal unicyclic graph in $\mathcal{U}(n,g)$ with respect to eccentric adjacency index. First, we prove some lemmas which will be used to prove our main results.

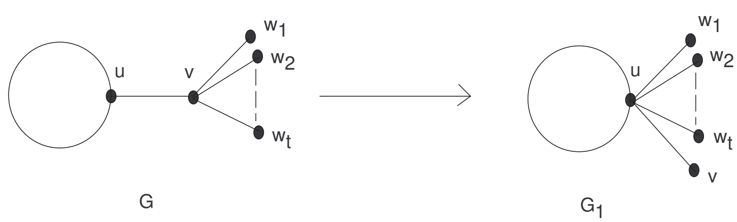

Figure 4.1: The graphs G and G_1 in Lemma 4.1.

Lemma 4.1. *Let G be an n-vertex simple and connected graph with $n_G \geq 4$. Assume there is an edge $uv \in \mathcal{E}_G$ with $\deg_G(u) \geq 2$ and $\Gamma_G(v) = \{u, w_1, w_2, \ldots, w_t\}$, where $w_1, w_2, \ldots, w_t \in P_G(v)$. Construct a new graph G_1 from G as $G_1 = (G - \{vw_1, \ldots, vw_t\}) \cup \{uw_1, \ldots, uw_t\}$ (see Figure 4.1). Then we have $\xi^{ad}(G_1) > \xi^{ad}(G)$.*

Proof. Take $w \in P_G(v)$ and define $A = \{y \in \mathcal{V}_G \mid ec_G(y) = d_G(y,w)\}$. Let $y \in A$ and $z \in \mathcal{V}_G$ such that $d_{G_1}(y,z) = ec_{G_1}(y)$. There are two possibilities: either $z \in P_G(v)$ or $z \notin P_G(v)$. If $z \in P_G(v)$ then we have

$$ec_{G_1}(y) = d_{G_1}(y,z) = d_{G_1}(y,u) + d_{G_1}(u,z) = d_G(y,u) + 1 < ec_G(y). \tag{4.1}$$

If $z \notin P_G(v)$ then we obtain

$$ec_{G_1}(y) = d_{G_1}(y,z) = d_G(y,z) \leq ec_G(y). \tag{4.2}$$

Let $a \in \mathcal{V}_G$ with $ec_G(w) = d_G(w,a)$. Then $ec_G(w) = d_G(u,a)+2$ and $d_{G_1}(u,a) = d_G(u,a)$. Therefore we have

$$ec_{G_1}(w) = d_{G_1}(w,a) = d_{G_1}(w,u) + d_{G_1}(u,a) = 1 + d_G(u,a) < ec_G(w).$$

Note that $ec_{G_1}(x) = ec_G(x)$ for any $x \in \mathcal{V}_G \setminus (A \cup P_G(v))$. By the construction of G_1, it is obvious that $S_{G_1}(x) = S_G(x)$, for all $x \in \mathcal{V}_G \setminus (\Gamma_G(u) \cup \Gamma_G(v))$. We know that $\deg_G(v) = t+1$. Therefore

$$\begin{aligned} S_{G_1}(u) &= \sum_{x \in \Gamma_G(u)\setminus\{v\}} \deg_G(x) + \sum_{x \in \Gamma_G(v)\setminus\{u\}} \deg_G(x) + 1 \\ &= \sum_{x \in \Gamma_G(u)\setminus\{v\}} \deg_G(x) + \deg_G(v) = S_G(u). \end{aligned} \tag{4.3}$$

Note that $S_G(v) = \deg_G(u) + t$ and $S_G(w) = \deg_G(v) = t+1$. Therefore

$$\begin{aligned} S_{G_1}(v) &= \deg_{G_1}(u) = \deg_G(u) + t = S_G(v), \\ S_{G_1}(w) &= \deg_{G_1}(u) = \deg_G(u) + t \geq 2 + t = S_G(w) + 1. \end{aligned} \tag{4.4}$$

If $x \in \Gamma_G(u) \setminus \{v\}$ then $|\Gamma_G(u) \setminus \{v\}| \geq 1$. Thus

$$\begin{aligned} S_{G_1}(x) &= \sum_{y \in \Gamma_G(x)\setminus\{u\}} \deg_{G_1}(y) + \deg_{G_1}(u) \\ &= \sum_{y \in \Gamma_G(x)\setminus\{u\}} \deg_G(y) + \deg_G(u) + t \\ &= S_G(x) + t. \end{aligned} \tag{4.5}$$

From (4.1)-(4.5), we obtain

$$\begin{aligned} \xi^{ad}(G_1) = {} & \frac{S_{G_1}(u)}{ec_{G_1}(u)} + \frac{S_{G_1}(v)}{ec_{G_1}(v)} + \sum_{w \in P_G(v)} \frac{S_{G_1}(w)}{ec_{G_1}(w)} + \sum_{x \in \Gamma_G(u)\setminus\{v\}} \frac{S_{G_1}(x)}{ec_{G_1}(x)} \\ & + \sum_{z \in \mathcal{V}_G \setminus (\Gamma_G(u) \cup \Gamma_G(v))} \frac{S_{G_1}(z)}{ec_{G_1}(z)} \\ & > \frac{S_G(u)}{ec_G(u)} + \frac{S_G(v)}{ec_G(v)} + \sum_{w \in P_G(v)} \frac{S_G(w)+1}{ec_G(w)} + \sum_{x \in \Gamma_G(u)\setminus\{v\}} \frac{S_G(x)+t}{ec_G(x)} \\ & + \sum_{z \in \mathcal{V}_G \setminus (\Gamma_G(u) \cup \Gamma_G(v))} \frac{S_G(z)}{ec_G(z)} \\ & = \xi^{ad}(G) + \sum_{w \in P_G(v)} \frac{1}{ec_G(w)} + \sum_{x \in \Gamma_G(u)\setminus\{v\}} \frac{t}{ec_G(x)}. \end{aligned}$$

Thus $\xi^{ad}(G_1) > \xi^{ad}(G)$. □

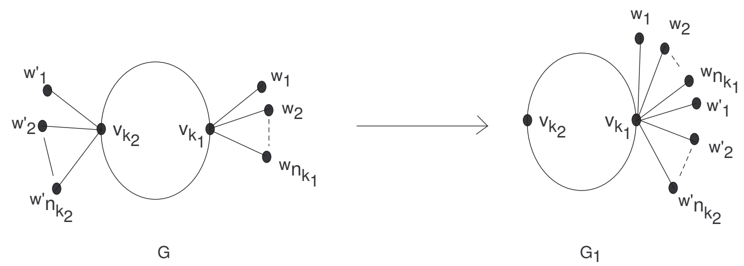

Figure 4.2: The graphs G and G_1 in Lemma 4.2.

In the following lemma, we construct a unicyclic graph in $\widetilde{\mathcal{U}}(n,g)$ from a given unicyclic graph in $\widetilde{\mathcal{U}}(n,g)$ such that the new unicyclic graph has larger eccentric adjacency index.

Lemma 4.2. *Let $G \in \widetilde{\mathcal{U}}(n,g)$ be an n-vertex unicyclic graph with $n_G \geq 4$. Assume there are two vertices $v_{k_1}, v_{k_2} \in \mathcal{V}_{C_g}$, where $1 \leq k_1, k_2 \leq g$ and $k_1 \neq k_2$, with $ec_G(v_{k_1}) \leq ec_G(v_{k_2})$. Let $P_G(v_{k_1}) = \{w_1, w_2, \ldots, w_{n_{k_1}}\}$ and $P_G(v_{k_2}) = \{w'_1, w'_2, \ldots, w'_{n_{k_2}}\}$, where $n_{k_1}, n_{k_2} \geq 1$. Construct a new graph G_1 from G as $G_1 = (G - \{v_{k_2}w'_1, \ldots, v_{k_2}w'_{n_{k_2}}\}) \cup \{v_{k_1}w'_1, \ldots, v_{k_1}w'_{n_{k_2}}\}$ (see Figure 4.2). Then we have $\xi^{ad}(G_1) > \xi^{ad}(G)$.*

Proof. Take $w' \in P_G(v_{k_2})$ and define $B = \{x \in \mathcal{V}_G \mid ec_G(x) = d_G(x, w')\}$. Let $x \in B$ and $z \in \mathcal{V}_G$ such that $d_{G_1}(x,z) = ec_{G_1}(x)$. Then either $z = v_{k_2}$ or $z \in \mathcal{V}_G \setminus \{v_{k_2}\}$ in G_1. If $z = v_{k_2}$ then we have

$$ec_{G_1}(x) = d_{G_1}(x, v_{k_2}) = d_G(x, v_{k_2}) < d_G(x, w') = ec_G(x). \tag{4.6}$$

Now if $z \in \mathcal{V}_G \setminus \{v_{k_2}\}$ then we have

$$ec_{G_1}(x) = d_{G_1}(x, z) = d_G(x, z) \leq d_G(x, w') = ec_G(x). \tag{4.7}$$

Note that $ec_G(v_{k_1}) \leq ec_G(v_{k_2})$. Then

$$ec_{G_1}(w') = ec_{G_1}(v_{k_1}) + 1 = ec_G(v_{k_1}) + 1 \leq ec_G(v_{k_2}) + 1 = ec_G(w'). \tag{4.8}$$

It is easily seen that $ec_{G_1}(y) = ec_G(y)$ for all $y \in \mathcal{V}_G \setminus (B \cup P_G(v_{k_2}))$. By the construction of G_1, we have $S_{G_1}(x) = S_G(x)$, for all $x \in \mathcal{V}_G \setminus (\Gamma_G(v_{k_1}) \cup \Gamma_G(v_{k_2}) \cup \{v_{k_1}, v_{k_2}\})$. For each $x \in \Gamma_G(v_{k_1}) \cap \Gamma_G(v_{k_2})$, we have

$$S_{G_1}(x) = S_G(x). \tag{4.9}$$

Let $H_1 = \Gamma_G(v_{k_1}) \setminus (\{v_{k_2}\} \cup (\Gamma_G(v_{k_1}) \cap \Gamma_G(v_{k_2})))$ and for each $x \in H_1$ we have

$$\begin{aligned} S_{G_1}(x) &= \sum_{y \in \Gamma_G(x) \setminus \{v_{k_1}\}} \deg_{G_1}(y) + \deg_{G_1}(v_{k_1}) \\ &= \sum_{y \in \Gamma_G(x) \setminus \{v_{k_1}\}} \deg_G(y) + \deg_G(v_{k_1}) + n_{k_2} \\ &= S_G(x) + n_{k_2}. \end{aligned} \tag{4.10}$$

Also, let $H_2 = \Gamma_G(v_{k_2}) \setminus (P_G(v_{k_2}) \cup \{v_{k_1}\} \cup (\Gamma_G(v_{k_1}) \cap \Gamma_G(v_{k_2})))$ and for each $x \in H_2$ we have

$$\begin{aligned} S_{G_1}(x) &= \sum_{y \in \Gamma_G(x) \setminus \{v_{k_2}\}} \deg_{G_1}(y) + \deg_{G_1}(v_{k_2}) \\ &= \sum_{y \in \Gamma_G(x) \setminus \{v_{k_1}\}} \deg_G(y) + \deg_G(v_{k_2}) - n_{k_2} \\ &= S_G(x) - n_{k_2}. \end{aligned} \tag{4.11}$$

If $w' \in P_G(v_{k_2})$ then we obtain

$$\begin{aligned} S_{G_1}(w') = \deg_{G_1}(v_{k_1}) &= \deg_G(v_{k_1}) + n_{k_2} \\ &= n_{k_1} + 2 + n_{k_2} \\ &= n_{k_1} + \deg_G(v_{k_2}) = S_G(w') + n_{k_1}. \end{aligned} \tag{4.12}$$

Case I: If $v_{k_1}v_{k_2} \in \mathcal{E}_G$, then we have

$$\begin{aligned} S_{G_1}(v_{k_1}) &= \sum_{x \in \Gamma_G(v_{k_1}) \setminus \{v_{k_2}\}} \deg_{G_1}(x) + \deg_{G_1}(v_{k_2}) \\ &= \sum_{x \in \Gamma_G(v_{k_1}) \setminus \{v_{k_2}\}} \deg_G(x) + n_{k_2} + (\deg_G(v_{k_2}) - n_{k_2}) \\ &= S_G(v_{k_1}). \end{aligned} \tag{4.13}$$

$$
\begin{aligned}
S_{G_1}(v_{k_2}) &= \sum_{x\in\Gamma_G(v_{k_2})\setminus\{v_{k_1}\}} \deg_{G_1}(x) + \deg_{G_1}(v_{k_1}) \\
&= \sum_{x\in\Gamma_G(v_{k_2})\setminus\{v_{k_1}\}} \deg_G(x) - n_{k_2} + (\deg_G(v_{k_1}) + n_{k_2}) \qquad (4.14)\\
&= (S_G(v_{k_2}) - n_{k_2}) + n_{k_2} = S_G(v_{k_2}).
\end{aligned}
$$

By the definition of eccentric adjacency index and (4.6)−(4.14), it follows that

$$
\begin{aligned}
\xi^{ad}(G_1) &= \frac{S_{G_1}(v_{k_1})}{ec_{G_1}(v_{k_1})} + \frac{S_{G_1}(v_{k_2})}{ec_{G_1}(v_{k_2})} + \sum_{x\in H_1} \frac{S_{G_1}(x)}{ec_{G_1}(x)} + \sum_{w'\in P_G(v_{k_2})} \frac{S_{G_1}(w')}{ec_{G_1}(w')} \\
&+ \sum_{x\in H_2} \frac{S_{G_1}(x)}{ec_{G_1}(x)} + \sum_{x\in\Gamma_G(v_{k_1})\cap\Gamma_G(v_{k_2})} \frac{S_{G_1}(x)}{ec_{G_1}(x)} + \sum_{x\in\mathcal{V}_G\setminus(\Gamma_G(v_{k_1})\cup\Gamma_G(v_{k_2})\cup\{v_{k_1},v_{k_2}\})} \frac{S_{G_1}(x)}{ec_{G_1}(x)} \\
&> \frac{S_G(v_{k_1})}{ec_G(v_{k_1})} + \frac{S_G(v_{k_2})}{ec_G(v_{k_2})} + \sum_{x\in H_1} \frac{S_G(x)+n_{k_2}}{ec_G(x)} + \sum_{w'\in P_G(v_{k_2})} \frac{S_G(w')+n_{k_1}}{ec_G(w')} \\
&+ \sum_{x\in H_2} \frac{S_G(x)-n_{k_2}}{ec_G(x)} + \sum_{x\in\Gamma_G(v_{k_1})\cap\Gamma_G(v_{k_2})} \frac{S_G(x)}{ec_G(x)} + \sum_{x\in\mathcal{V}_G\setminus(\Gamma_G(v_{k_1})\cup\Gamma_G(v_{k_2})\cup\{v_{k_1},v_{k_2}\})} \frac{S_G(x)}{ec_G(x)} \\
&= \xi^{ad}(G) + \sum_{w'\in P_G(v_{k_2})} \frac{n_{k_1}}{ec_G(w')} + \sum_{x\in H_1} \frac{n_{k_2}}{ec_G(x)} - \sum_{x\in H_2} \frac{n_{k_2}}{ec_G(x)} \\
&= \xi^{ad}(G) + \sum_{w'\in P_G(v_{k_2})} \frac{n_{k_1}}{ec_G(w')} + \sum_{w\in P_G(v_{k_1})} \frac{n_{k_2}}{ec_G(w)} + \sum_{x\in H_1\setminus P_G(v_{k_1})} \frac{n_{k_2}}{ec_G(x)} \\
&- \sum_{x\in H_2} \frac{n_{k_2}}{ec_G(x)} \\
&\geq \xi^{ad}(G) + \sum_{w'\in P_G(v_{k_2})} \frac{n_{k_1}}{\mathrm{d}_G} + \sum_{w\in P_G(v_{k_1})} \frac{n_{k_2}}{\mathrm{d}_G} + \sum_{x\in H_1\setminus P_G(v_{k_1})} \frac{n_{k_2}}{ec_G(x)} - \sum_{x\in H_2} \frac{n_{k_2}}{ec_G(x)}.
\end{aligned}
$$

Note that $\lfloor \frac{g}{2} \rfloor \leq ec_G(v_i) \leq \lfloor \frac{g}{2} \rfloor + 1$ for each vertex $v_i \in \mathcal{V}_{C_g}$, $1 \leq i \leq g$. Therefore

$$
\begin{aligned}
\xi^{ad}(G_1) &\geq \xi^{ad}(G) + \frac{n_{k_1}n_{k_2}}{\mathrm{d}_G} + \frac{n_{k_2}n_{k_1}}{\mathrm{d}_G} + \sum_{x\in H_1\setminus P_G(v_{k_1})} \frac{n_{k_2}}{\lfloor \frac{g}{2} \rfloor + 1} - \sum_{x\in H_2} \frac{n_{k_2}}{\lfloor \frac{g}{2} \rfloor} \\
&= \xi^{ad}(G) + \frac{2n_{k_1}n_{k_2}}{\mathrm{d}_G} + \frac{n_{k_2}|H_1 \setminus P_G(v_{k_1})|}{\lfloor \frac{g}{2} \rfloor + 1} - \frac{n_{k_2}|H_2|}{\lfloor \frac{g}{2} \rfloor}.
\end{aligned}
$$

Now we have following three cases:

(1). If $v_{k_1}v_{k_2} \in \mathcal{E}_{C_g}$ then $|H_1 \setminus P_G(v_{k_1})| = 1$ and $|H_2| = 1$. Therefore

$$
\xi^{ad}(G_1) \geq \xi^{ad}(G) + \frac{2n_{k_1}n_{k_2}}{\mathrm{d}_G} - \frac{n_{k_2}}{\lfloor \frac{g}{2} \rfloor(\lfloor \frac{g}{2} \rfloor + 1)}.
$$

(2). If $v_{k_1}v_{k_2} \notin \mathcal{E}_{C_g}$ and $\Gamma_G(v_{k_1}) \cap \Gamma_G(v_{k_2}) = \emptyset$ then $|H_1 \setminus P_G(v_{k_1})| = 2$ and $|H_2| = 2$. Therefore

$$\xi^{ad}(G_1) \geq \xi^{ad}(G) + \frac{2n_{k_1}n_{k_2}}{\mathrm{d}_G} - \frac{2n_{k_2}}{\lfloor\frac{g}{2}\rfloor(\lfloor\frac{g}{2}\rfloor+1)}.$$

(3). If $v_{k_1}v_{k_2} \notin \mathcal{E}_{C_g}$ and $\Gamma_G(v_{k_1}) \cap \Gamma_G(v_{k_2}) \neq \emptyset$ then $|H_1 \setminus P_G(v_{k_1})| = 1$ and $|H_2| = 1$. Therefore

$$\xi^{ad}(G_1) \geq \xi^{ad}(G) + \sum_{x\in\Gamma_G(v_{k_1})\cap\Gamma_G(V_{k_2})} \frac{S_G(x)}{ec_G(x)} + \frac{2n_{k_1}n_{k_2}}{\mathrm{d}_G} - \frac{n_{k_2}}{\lfloor\frac{g}{2}\rfloor(\lfloor\frac{g}{2}\rfloor+1)}.$$

Since $\lfloor\frac{g}{2}\rfloor(\lfloor\frac{g}{2}\rfloor+1) > \mathrm{d}_G$, it holds that $\xi^{ad}(G_1) > \xi^{ad}(G)$ in either case.

Case II: If $v_{k_1}v_{k_2} \notin \mathcal{E}_G$, then we have

$$\begin{aligned} S_{G_1}(v_{k_1}) &= \sum_{x\in\Gamma_G(v_{k_1})\}} \deg_G(x) + n_{k_2} = S_G(v_{k_1}) + n_{k_2}. \\ S_{G_1}(v_{k_2}) &= \sum_{x\in\Gamma_G(v_{k_2})\}} \deg_G(x) - n_{k_2} + (\deg_G(v_{k_1}) + n_{k_2}) = S_G(v_{k_2}) - n_{k_2}. \end{aligned} \tag{4.15}$$

By the definition of eccentric adjacency index, (4.6)−(4.12) and (4.15), it follows that

$$\begin{aligned} \xi^{ad}(G_1) &= \frac{S_{G_1}(v_{k_1})}{ec_{G_1}(v_{k_1})} + \frac{S_{G_1}(v_{k_2})}{ec_{G_1}(v_{k_2})} + \sum_{x\in H_1} \frac{S_{G_1}(x)}{ec_{G_1}(x)} + \sum_{w'\in P_G(v_{k_2})} \frac{S_{G_1}(w')}{ec_{G_1}(w')} \\ &+ \sum_{x\in H_2} \frac{S_{G_1}(x)}{ec_{G_1}(x)} + \sum_{x\in\Gamma_G(v_{k_1})\cap\Gamma_G(v_{k_2})} \frac{S_{G_1}(x)}{ec_{G_1}(x)} + \sum_{x\in\mathcal{V}_G\setminus(\Gamma_G(v_{k_1})\cup\Gamma_G(v_{k_2})\cup\{v_{k_1},v_{k_2}\})} \frac{S_{G_1}(x)}{ec_{G_1}(x)} \\ &> \frac{S_G(v_{k_1}) + n_{k_2}}{ec_G(v_{k_1})} + \frac{S_G(v_{k_2}) - n_{k_2}}{ec_G(v_{k_2})} + \sum_{x\in H_1} \frac{S_G(x) + n_{k_2}}{ec_G(x)} + \sum_{w'\in P_G(v_{k_2})} \frac{S_G(w') + n_{k_1}}{ec_G(w')} \\ &+ \sum_{x\in H_2} \frac{S_G(x) - n_{k_2}}{ec_G(x)} + \sum_{x\in\Gamma_G(v_{k_1})\cap\Gamma_G(v_{k_2})} \frac{S_G(x)}{ec_G(x)} + \sum_{x\in\mathcal{V}_G\setminus(\Gamma_G(v_{k_1})\cup\Gamma_G(v_{k_2})\cup\{v_{k_1},v_{k_2}\})} \frac{S_G(x)}{ec_G(x)} \end{aligned}$$

Given that $ec_G(v_{k_1}) \leq ec_G(v_{k_2})$, therefore we get

$$\xi^{ad}(G_1) \geq \xi^{ad}(G) + \sum_{w'\in P_G(v_{k_2})} \frac{n_{k_1}}{ec_G(w')} + \sum_{x\in H_1\cup\{v_{k_1}\}} \frac{n_{k_2}}{ec_G(x)} - \sum_{x\in H_2\cup\{v_{k_2}\}} \frac{n_{k_2}}{ec_G(x)}.$$

Thus by similar arguments as given in Case I, we obtain $\xi^{ad}(G_1) > \xi^{ad}(G)$. This completes the proof. □

Example 4.3. Consider a unicyclic graph $U \in \mathcal{U}(17, 6)$ given in Figure 4.3. From Lemma 4.1, we construct a sequence of unicyclic graphs $U, U_1, U_2, U_3, U_4,$ where $U_4 \in \widetilde{\mathcal{U}}(17, 6)$, satisfying $\xi^{ad}(U) < \xi^{ad}(U_1) < \xi^{ad}(U_2) < \xi^{ad}(U_3) < \xi^{ad}(U_4)$. This sequence of unicyclic graphs is not unique because it depends upon the choice of edge uv.

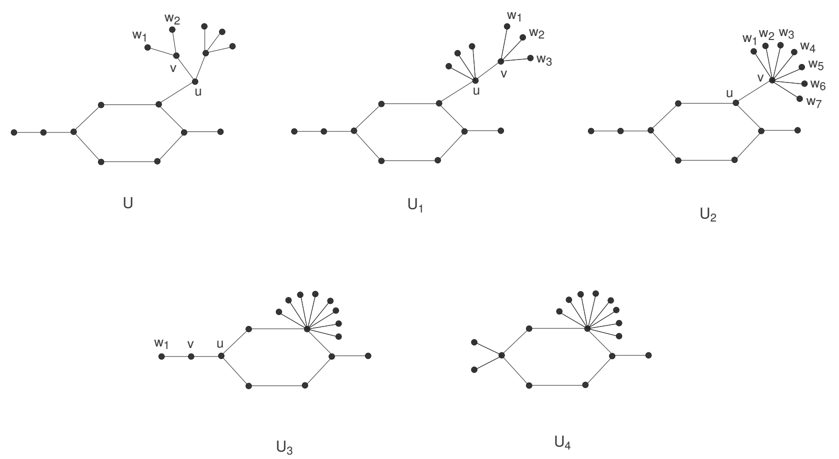

Figure 4.3: A sequence of unicyclic graphs obtained after applying Lemma 4.1.

Now we apply the Lemma 4.2 on the unicyclic graph U_4 to get $U(17, 6; 11)$. We generate a sequence of unicyclic graphs $U_4, U_5, U_6,$ where $U_6 \cong U(17, 6; 11)$ satisfying $\xi^{ad}(U_4) < \xi^{ad}(U_5) < \xi^{ad}(U_6)$. The sequence of trees is shown in Figure 4.4. This sequence of unicyclic graphs is not unique because it depends upon the choice of vertices v_{k_1} and v_{k_2}.

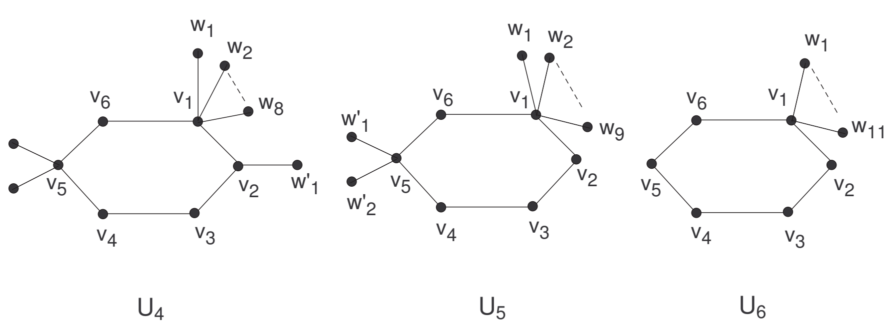

Figure 4.4: A sequence of unicyclic graphs obtained after applying Lemma 4.2.

In upcoming theorem, we derive the unicyclic graph in $\mathcal{U}(n,g)$ with the largest eccentric adjacency index, by using Lemmas 4.1 and 4.2.

Theorem 4.4. *Let $U \in \mathcal{U}(n,g)$ be an n-vertex unicyclic graph, where $3 \leq g \leq n$ and $n \geq 4$. Then $\xi^{ad}(U) \leq \xi^{ad}(U(n,g;n-g))$ with equality if and only if $U \cong U(n,g;n-g)$.*

Proof. Let $U \in \mathcal{U}(n,g)$ and C_g be its unique cycle of length g. If $U \notin \widetilde{\mathcal{U}}(n,g)$ then there is an edge $uv \in \mathcal{E}_U \setminus \mathcal{E}_{C_g}$ with $\deg_U(u) \geq 2$ and $\Gamma_U(v) = \{u, w_1, \dots, w_t\}$, where $w_i \in P_U(v)$, $i = 1, 2, \dots, t$. By applying Lemma 4.1, we get a unicyclic graph $U_1 = (U - \{vw_1, \dots, vw_t\}) \cup \{uw_1, \dots, uw_t\}$ such that $\xi^{ad}(U) < \xi^{ad}(U_1)$. Again, if $U_1 \notin \widetilde{\mathcal{U}}(n,g)$ then there is an edge $u_1v_1 \in \mathcal{E}_{U_1} \setminus \mathcal{E}_{C_g}$ with $\deg_{U_1}(u_1) \geq 2$ and $\Gamma_{U_1}(v_1) = \{u_1, w'_1, \dots, w'_t\}$ where $w'_i \in P_{U_1}(v_1)$, $i = 1, 2, \dots, t$. By applying Lemma 4.1, we get a unicyclic graph $U_2 = (U_1 - \{v_1w'_1, \dots, v_1w'_t\}) \cup \{u_1w'_1, \dots, u_1w'_t\}$ such that $\xi^{ad}(U_1) < \xi^{ad}(U_2)$. Repeatedly applying Lemma 4.1, we get a sequence of unicyclic graphs $U, U_1, U_2, \dots, U_l$ satisfying $\xi^{ad}(U) < \xi^{ad}(U_1) < \xi^{ad}(U_2) < \dots < \xi^{ad}(U_l)$ such that $U_l \in \widetilde{\mathcal{U}}(n,g)$.

Now if $U_l \ncong U(n,g;n-g)$ then there are two vertices $v_r, v_s \in \mathcal{V}_{C_g}$, $r, s = 1, 2, \dots, g$ and $r \neq s$, with $ec_{U_l}(v_r) \leq ec_{U_l}(v_s)$. Assume that $P_{U_l}(v_r) = \{x_1, x_2, \dots, x_{n_r}\}$ and $P_{U_l}(v_s) = \{y_1, y_2, \dots, y_{n_s}\}$, where $n_r \geq 1, n_s \geq 1$. By applying Lemma 4.2, we obtain a unicyclic graph $U_{l_1} = (U_l - \{v_sy_1, \dots, v_sy_{n_s}\}) \cup \{v_ry_1, \dots, v_ry_{n_s}\}$ that satisfies $\xi^{ad}(U_l) < \xi^{ad}(U_{l_1})$. Again, if $U_{l_1} \ncong U(n,g,n-g)$ then there are two vertices $v_{r'}, v_{s'} \in \mathcal{V}_{C_g}$, $r', s' = 1, 2, \dots, g$ and $r' \neq s'$, with $ec_{U_{l_1}}(v_{r'}) \leq ec_{U_{l_1}}(v_{s'})$. Assume that $P_{U_{l_1}}(v_{k'_1}) = \{x'_1, x'_2, \dots, x'_{n_{k'_1}}\}$ and $P_{U_{l_1}}(v_{k'_2}) = \{y'_1, y'_2, \dots, y'_{n_{k'_2}}\}$, where $n_{r'}, n_{s'} \geq 1$. By applying Lemma 4.2, we obtain a unicyclic graph $U_{l_2} = (U_{l_1} - \{v_{s'}y'_1, \dots, v_{s'}y'_{n_{s'}}\}) \cup \{v_{r'}y'_1, \dots, v_{r'}y'_{n_{s'}}\}$ such that $\xi^{ad}(U_{l_1}) < \xi^{ad}(U_{l_2})$. Applying repeatedly Lemma 4.2, we obtain a sequence of unicyclic graphs $U_l, U_{l_1}, U_{l_2}, \dots, U_{l_m}$ satisfying $\xi^{ad}(U_l) < \xi^{ad}(U_{l_1}) < \xi^{ad}(U_{l_2}) < \dots < \xi^{ad}(U_{l_m})$ such that $U_{l_m} \cong U(n,g;n-g)$. This completes the proof. □

By Theorem 4.4 and simple calculations we have the next result.

Corollary 4.5. *Let $U \in \mathcal{U}(n,g)$ be an n-vertex unicyclic graph where $n \geq 4$. Then*

$$\xi^{ad}(U) \leq \begin{cases} \frac{n^2+7}{2} & \text{if } g = 3, \\ \frac{2(3n+g-8)}{g-1} + \frac{2(n^2+g^2-2ng+2n-2g+8)}{g+1} & \text{if } 3 < g < n \text{ and } g \text{ is odd}, \\ \frac{2(3n+g-4)}{g} + \frac{2(n^2+g^2-2ng+2n-2g+4)}{g+2} & \text{if } 3 < g < n \text{ and } g \text{ is even}, \\ \frac{4n}{\lfloor \frac{n}{2} \rfloor} & \text{if } g = n, \end{cases} \tag{4.16}$$

equality if and only if $U \cong U(n,g;n-g)$.

In the upcoming theorem, we find the unicyclic graph in $\mathcal{U}(n)$ with the largest eccentric adjacency index, by using Theorem 4.4 and Corollary 4.5.

Theorem 4.6. *Let $U \in \mathcal{U}(n)$ be an n-vertex unicyclic graph with $n \geq 4$. Then*

$$\xi^{ad}(U) \leq \frac{n^2+7}{2},$$

with equality if and only if $U \cong U(n,3;n-3)$.

Proof. Let $U \in \mathcal{U}(n,g)$ be an n-vertex unicyclic graph. Then (4.16) holds true. We prove that $\xi^{ad}(U(n,g;n-g)) \leq \xi^{ad}(U(n,3;n-3))$. Let

$$h(g) = \begin{cases} \frac{n^2+7}{2} & \text{if } g = 3, \\ \frac{2(3n+g-8)}{g-1} + \frac{2(n^2+g^2-2ng+2n-2g+8)}{g+1} & \text{if } 3 < g < n \text{ and } g \text{ is odd}, \\ \frac{2(3n+g-4)}{g} + \frac{2(n^2+g^2-2ng+2n-2g+4)}{g+2} & \text{if } 3 < g < n \text{ and } g \text{ is even}, \\ \frac{4n}{\lfloor \frac{n}{2} \rfloor} & \text{if } g = n. \end{cases}$$

Let g be odd, $3 < g < n$. Then we have

$$h(g) = \frac{2(3n+g-8)}{g-1} + \frac{2(n^2+g^2-2ng+2n-2g+8)}{g+1}.$$

This gives

$$h'(g) = \frac{-2(3n-7)}{(g-1)^2} - \frac{2(n^2-g^2+4n-2g+10)}{(g+1)^2}.$$

Note that $n^2 - g^2 + 4n - 2g + 10 > 0$ for $n > g > 3$. This implies that $h'(g) < 0$. Thus $h(g)$ is a decreasing function for $3 < g < n$ and g is odd. Also

$$h(5) = \frac{2n^2 - 7n + 37}{6}. \tag{4.17}$$

Now let g be even, $3 < g < n$. Then we have

$$h(g) = \frac{2(3n + g - 4)}{g} + \frac{2(n^2 + g^2 - 2ng + 2n - 2g + 4)}{g + 2}.$$

This gives

$$h'(g) = \frac{-2(3n - 4)}{g^2} - \frac{2(n^2 - g^2 + 6n - 4g + 8)}{(g + 2)^2}.$$

Note that $n^2 - g^2 + 6n - 4g + 8 > 0$ for $n > g > 3$. This implies that $h'(g) < 0$. Thus $h(g)$ is a decreasing function for $3 < g < n$ and g is even. Also

$$h(4) = \frac{2n^2 - 3n + 24}{6}. \tag{4.18}$$

From (4.17) and (4.18), we have

$$h(5) - h(4) = \frac{-(4n - 13)}{6} < 0.$$

Also

$$h(4) - h(3) = \frac{-n^2 - 3n + 3}{6} < 0.$$

Finally, it is easily seen that $h(3) = \frac{n^2+7}{2} > \frac{4n}{\lfloor \frac{n}{2} \rfloor} = h(n)$, where $n \geq 4$. Thus $\xi^{ad}(U) \leq \frac{n^2+7}{2}$, with equality if and only if $U \cong U(n, 3; n - 3)$. This completes the proof. □

4.2 The eccentric adjacency index of trees with fixed diameter

Let $\mathcal{T}(n, \mathrm{d})$ be the family of all trees of order $n \geq 2$ with a fixed diameter d, where $2 \leq \mathrm{d} \leq n - 1$. Let $\widetilde{\mathcal{T}}(n, \mathrm{d})$ be the family of caterpillars with diameter d that are obtained from a diametrical path $P_{\mathrm{d}+1} = v_0 v_1 \ldots v_{\mathrm{d}}$ such that $n - \mathrm{d} - 1$ pendent vertices and attached to the vertices $v_1, v_2, \ldots, v_{\mathrm{d}-1}$. Also $T(n, \mathrm{d}; n - \mathrm{d} - 1)$ denotes a caterpillar obtained by connecting $n - \mathrm{d} - 1$ pendent vertices to a central vertex $v_{\lfloor \mathrm{d}/2 \rfloor}$ of path $P_{\mathrm{d}+1}$.

In the following theorem, we find the tree in $T \in \mathcal{T}(n, \mathrm{d})$ with the largest eccentric adjacency index, by using Lemma 4.1.

Theorem 4.7. *Let $T \in \mathcal{T}(n, \mathrm{d})$ be an n-vertex tree, where $n \geq 2$. Then $\xi^{ad}(T) \leq \xi^{ad}(T(n, \mathrm{d}; n - \mathrm{d} - 1))$ with equality if and only if $T \cong T(n, \mathrm{d}; n - \mathrm{d} - 1)$.*

Proof. Let $T \in \mathcal{T}(n, \mathrm{d})$ and $P_{\mathrm{d}+1} = v_0 v_1 \ldots v_{\mathrm{d}}$ be its diametrical path. If $T \notin \widetilde{\mathcal{T}}(n, \mathrm{d})$ then there is an edge $uv \in \mathcal{E}_T \setminus \mathcal{E}_{P_{\mathrm{d}+1}}$ with $\deg_T(u) \geq 2$ and $\Gamma_T(v) = \{u, w_1, \ldots, w_t\}$ where $w_i \in P_T(v)$, $i = 1, 2, \ldots, t$. By applying Lemma 4.1, we get a tree $T_1 = (T - \{vw_1, \ldots, vw_t\}) \cup \{uw_1, \ldots, uw_t\}$ such that $\xi^{ad}(T) < \xi^{ad}(T_1)$. Again, if $T_1 \notin \widetilde{\mathcal{T}}(n, \mathrm{d})$ then there is an edge $u'v' \in \mathcal{E}_{T_1} \setminus \mathcal{E}_{P_{\mathrm{d}+1}}$ with $\deg_{T_1}(u') \geq 2$ and $\Gamma_{T_1}(v') = \{u_1, w_1, \ldots, w_t\}$ where $w_i \in P_{T_1}(v')$, $i = 1, 2, \ldots, t$. By applying Lemma 4.1, we get a new tree $T_2 = (T_1 - \{v'w_1, \ldots, v'w_t\}) \cup \{u'w_1, \ldots, u'w_t\}$ such that $\xi^{ad}(T_1) < \xi^{ad}(T_2)$. Thus by repeatedly applying Lemma 4.1, we generate a sequence of tress $T, T_1, T_2, \ldots, T_l$ such that $\xi^{ad}(T) < \xi^{ad}(T_1) < \xi^{ad}(T_2) < \cdots < \xi^{ad}(T_l)$, where $T_l \in \widetilde{\mathcal{T}}(n, \mathrm{d})$.

Now if $T_l \in \widetilde{\mathcal{T}}(n, \mathrm{d})$ then there exists some vertices v_k of $P_{\mathrm{d}+1}$ with $k \neq \lfloor \frac{\mathrm{d}}{2} \rfloor$ and $\deg_{T_l}(v_k) \geq 3$. Without loss of generality, suppose that $\lfloor \frac{\mathrm{d}}{2} \rfloor < k \leq \mathrm{d} - 1$, that is, $ec_{T_l}(v_k) = k$. Let $w_1, \ldots, w_t$ be the pendent vertices adjacent at v_k, where $1 \leq k \leq \mathrm{d} - 1$. Construct a new tree T_{l_1} from T_l as $T_{l_1} = (T_l - \{v_k w_1, \ldots, v_k w_t\}) \cup \{v_{\lfloor \frac{\mathrm{d}}{2} \rfloor} w_1, \ldots, v_{\lfloor \frac{\mathrm{d}}{2} \rfloor} w_t\}$ and $T_{l_1} \in \widetilde{\mathcal{T}}(n, \mathrm{d})$. Note that $ec_{T_{l_1}}(v) \leq ec_{T_l}(v)$ for any $v \in \mathcal{V}_{T_l}$. Take $w \in P_{T_l}(v_k)$ and we know that $S_{T_l}(w) = \deg_{T_l}(v_k) = t + 2$. Therefore

$$S_{T_{l_1}}(w) = \deg_{T_{l_1}}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) + t \geq 2 + t = S_{T_l}(w). \tag{4.19}$$

There are two cases, either $v_k v_{\lfloor \frac{\mathrm{d}}{2} \rfloor} \in \mathcal{E}_{P_{\mathrm{d}+1}}$ or $v_k v_{\lfloor \frac{\mathrm{d}}{2} \rfloor} \notin \mathcal{E}_{P_{\mathrm{d}+1}}$.

Case I: If $v_k v_{\lfloor \frac{\mathrm{d}}{2} \rfloor} \notin \mathcal{E}_{P_{\mathrm{d}+1}}$ then by the construction of T_{l_1}, we have

$$S_{T_{l_1}}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) = S_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) + t, \quad S_{T_{l_1}}(v_k) = S_{T_l}(v_k) - t. \tag{4.20}$$

Let $B_1 = \Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \setminus (\Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \cap \Gamma_{T_l}(v_k))$ and $B_2 = \Gamma_{T_l}(v_k) \setminus (P_{T_l}(v_k) \cup (\Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \cap \Gamma_{T_l}(v_k)))$. Then

$$\begin{aligned} S_{T_{l_1}}(x) &= S_{T_l}(x), && \forall\ x \in \Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \cap \Gamma_{T_l}(v_k), \\ S_{T_{l_1}}(x) &= S_{T_l}(x) + t, && \forall\ x \in B_1, \\ S_{T_{l_1}}(x) &= S_{T_l}(x) - t, && \forall\ x \in B_2. \end{aligned} \tag{4.21}$$

By the construction of T_{l_1}, we have

$$S_{T_{l_1}}(z)=S_{T_l}(z),\quad \forall\ z\in \mathcal{V}_{T_l}\setminus(\{v_{\lfloor\frac{d}{2}\rfloor},v_k\}\cup\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cup\Gamma_{T_l}(v_k)). \tag{4.22}$$

From the definition of eccentric adjacency index and (4.19)−(4.22), we obtain

$$\begin{aligned}
\xi^{ad}(T_{l_1}) &= \frac{S_{T_{l_1}}(v_{\lfloor\frac{d}{2}\rfloor})}{ec_{T_{l_1}}(v_{\lfloor\frac{d}{2}\rfloor})}+\frac{S_{T_{l_1}}(v_k)}{ec_{T_{l_1}}(v_k)}+\sum_{w\in P_{T_l}(v_k)}\frac{S_{T_{l_1}}(w)}{ec_{T_{l_1}}(w)}+\sum_{z\in B_1}\frac{S_{T_{l_1}}(z)}{ec_{T_{l_1}}(z)}+\sum_{x\in B_2}\frac{S_{T_{l_1}}(x)}{ec_{T_{l_1}}(x)}\\
&+\sum_{x\in\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cap\Gamma_{T_l}(v_k)}\frac{S_{T_{l_1}}(x)}{ec_{T_{l_1}}(x)}+\sum_{z\in\mathcal{V}_{T_l}\setminus(\{v_{\lfloor\frac{d}{2}\rfloor},v_k\}\cup\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cup\Gamma_{T_l}(v_k))}\frac{S_{T_{l_1}}(z)}{ec_{T_{l_1}}(z)}\\
&>\frac{S_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})+t}{ec_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})}+\frac{S_{T_l}(v_k)-t}{ec_{T_l}(v_k)}+\sum_{w\in P_{T_l}(v_k)}\frac{S_{T_l}(w)}{ec_{T_l}(w)}+\sum_{z\in B_1}\frac{S_{T_l}(z)+t}{ec_{T_l}(z)}\\
&+\sum_{x\in B_2}\frac{S_{T_l}(x)-t}{ec_{T_l}(x)}+\sum_{x\in\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cap\Gamma_{T_l}(v_k)}\frac{S_{T_l}(x)}{ec_{T_l}(x)}+\sum_{z\in\mathcal{V}_{T_l}\setminus(\{v_{\lfloor\frac{d}{2}\rfloor},v_k\}\cup\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cup\Gamma_{T_l}(v_k))}\frac{S_{T_l}(z)}{ec_{T_l}(z)}\\
&=\xi^{ad}(T_l)+\frac{t}{ec_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})}-\frac{t}{ec_{T_l}(v_k)}+\sum_{z\in B_1}\frac{t}{ec_{T_l}(z)}-\sum_{x\in B_2}\frac{t}{ec_{T_l}(x)}\\
&=\xi^{ad}(T_l)+\frac{t}{\lceil\frac{d}{2}\rceil}-\frac{t}{k}+\sum_{z\in B_1}\frac{t}{ec_{T_l}(z)}-\sum_{x\in B_2}\frac{t}{ec_{T_l}(x)}.
\end{aligned}$$

Given that $\lceil\frac{d}{2}\rceil<k$ and for each $x\in B_1$, we have $ec_{T_l}(x)=\lceil\frac{d}{2}\rceil+1$. Note that if $x\in B_2$ then we have $\lceil\frac{d}{2}\rceil+1<ec_{T_l}(x)<d$. Therefore

$$\xi^{ad}(T_{l_1})>\xi^{ad}(T_l)+\sum_{z\in B_1}\frac{t}{\lceil\frac{d}{2}\rceil+1}-\sum_{x\in B_2}\frac{t}{\lceil\frac{d}{2}\rceil+1}.$$

Now we have two subcases; either $\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cap\Gamma_{T_l}(v_k)=\emptyset$ or $\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cap\Gamma_{T_l}(v_k)\neq\emptyset$.

(1). If $\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cap\Gamma_{T_l}(v_k)=\emptyset$ then we have $|B_1|=2$ and $|B_2|=2$.

(2). If $\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cap\Gamma_{T_l}(v_k)\neq\emptyset$ then we have $|B_1|\geq 1$ and $|B_2|=1$.

Thus from above two subcases, it holds that $\xi^{ad}(T_{l_l})>\xi^{ad}(T_l)$.

Case II: If $v_kv_{\lfloor\frac{d}{2}\rfloor}\in\mathcal{E}_{P_{d+1}}$ then by the construction of T_{l_1}, we get

$$\begin{aligned}
&S_{T_{l_1}}(v_{\lfloor\frac{d}{2}\rfloor})=S_{T_l}(v_{\lfloor\frac{d}{2}\rfloor}),\quad S_{T_{l_1}}(v_k)=S_{T_l}(v_k),\\
&S_{T_{l_1}}(x)=S_{T_l}(x)+t,\qquad \forall\ x\in\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\setminus\{v_k\},\\
&S_{T_{l_1}}(x)=S_{T_l}(x)-t,\qquad \forall\ x\in\Gamma_{T_l}(v_k)\setminus(P_{T_l}(v_k)\cup\{v_{\lfloor\frac{d}{2}\rfloor}\}),\\
&S_{T_{l_1}}(z)=S_{T_l}(z),\qquad\quad \forall\ z\in\mathcal{V}_{T_l}\setminus(\Gamma_{T_l}(v_{\lfloor\frac{d}{2}\rfloor})\cup\Gamma_{T_l}(v_k)).
\end{aligned}\tag{4.23}$$

Therefore from the definition of eccentric adjacency index, (4.19) and (4.23), we obtain

$$
\begin{aligned}
\xi^{ad}(T_{l_1}) &= \frac{S_{T_{l_1}}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor})}{ec_{T_{l_1}}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor})} + \frac{S_{T_{l_1}}(v_k)}{ec_{T_{l_1}}(v_k)} + \sum_{w \in P_{T_l}(v_k)} \frac{S_{T_{l_1}}(w)}{ec_{T_{l_1}}(w)} + \sum_{z \in \Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \setminus \{v_k\}} \frac{S_{T_{l_1}}(z)}{ec_{T_{l_1}}(z)} \\
&+ \sum_{z \in \Gamma_{T_l}(v_k) \setminus (P_{T_l}(v_k) \cup \{v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}\})} \frac{S_{T_{l_1}}(z)}{ec_{T_{l_1}}(z)} + \sum_{z \in \mathcal{V}_{T_l} \setminus (\Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \cup \Gamma_{T_l}(v_k))} \frac{S_{T_{l_1}}(z)}{ec_{T_{l_1}}(z)} \\
&> \frac{S_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor})}{ec_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor})} + \frac{S_{T_l}(v_k)}{ec_{T_l}(v_k)} + \sum_{w \in P_{T_l}(v_k)} \frac{S_{T_l}(w)}{ec_{T_l}(w)} + \sum_{z \in \Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \setminus \{v_k\}} \frac{S_{T_l}(z) + t}{ec_{T_l}(z)} \\
&+ \sum_{z \in \Gamma_{T_l}(v_k) \setminus (P_{T_l}(v_k) \cup \{v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}\})} \frac{S_{T_l}(z) - t}{ec_{T_l}(z)} + \sum_{z \in \mathcal{V}_{T_l} \setminus (\Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \cup \Gamma_{T_l}(v_k))} \frac{S_{T_l}(z)}{ec_{T_l}(z)} \\
&= \xi^{ad}(T_l) + \sum_{z \in \Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \setminus \{v_k\}} \frac{t}{ec_{T_l}(z)} - \sum_{z \in \Gamma_{T_l}(v_k) \setminus (P_{T_l}(v_k) \cup \{v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}\})} \frac{t}{ec_{T_l}(z)}.
\end{aligned}
$$

Since v_k has a unique neighbor in $V_{P_{\mathrm{d}+1}}$ other than $v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}$, such that $ec_{T_l}(x) = k+1$, where $x \in \Gamma_{T_l}(v_k) \setminus (P_{T_l}(v_k) \cup \{v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}\})$. Also for each $x \in \Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \setminus \{v_k\}$, we have $ec_{T_l}(x) = \lceil \frac{\mathrm{d}}{2} \rceil + 1$. Therefore

$$
\xi^{ad}(T_{l_1}) > \xi^{ad}(T_l) + \sum_{z \in \Gamma_{T_l}(v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}) \setminus \{v_k\}} \frac{t}{\lceil \frac{\mathrm{d}}{2} \rceil + 1} - \sum_{z \in \Gamma_{T_l}(v_k) \setminus (P_{T_l}(v_k) \cup \{v_{\lfloor \frac{\mathrm{d}}{2} \rfloor}\})} \frac{t}{k+1}.
$$

As we know that $\lfloor \frac{\mathrm{d}}{2} \rfloor < k \leq \mathrm{d} - 1$. Thus $\xi^{ad}(T_{l_1}) > \xi^{ad}(T_l)$.

Again, if $T_{l_1} \notin \widetilde{\mathcal{T}}(n, \mathrm{d})$ then there exists some vertices $v_k \in V_{P_{\mathrm{d}+1}}$ with $k \neq \lfloor \frac{\mathrm{d}}{2} \rfloor$ and $\deg_{T_{l_1}}(v_k) \geq 3$. Without loss of generality, suppose that $\lfloor \frac{\mathrm{d}}{2} \rfloor < k \leq \mathrm{d} - 1$, that is, $ec_{T_{l_1}}(v_k) = k$. Let $w_1, \ldots, w_t$ be the pendent vertices adjacent at v_k, where $1 \leq k \leq \mathrm{d} - 1$. Construct a new tree T_{l_2} from T_{l_1} as $T_{l_2} = (T_{l_1} - \{v_k w_1, \ldots, v_k w_t\}) \cup \{v_{\lfloor \frac{\mathrm{d}}{2} \rfloor} w_1, \ldots, v_{\lfloor \frac{\mathrm{d}}{2} \rfloor} w_t\}$ and $T_{l_2} \in \widetilde{\mathcal{T}}(n, \mathrm{d})$. We can apply repeatedly above transformation on T_l and construct a sequence of trees $T_l, T_{l_1}, \ldots, T_{l_m}$ such that $\xi^{ad}(T_l) < \xi^{ad}(T_{l_1}) < \cdots < \xi^{ad}(T_{l_m})$, where $T_{l_m} \cong T(n, \mathrm{d}; n - \mathrm{d} - 1)$. Therefore $\xi^{ad}(T) \leq \xi^{ad}(T(n, \mathrm{d}; n - \mathrm{d} - 1))$ with equality if and only if $T \cong T(n, \mathrm{d}; n - \mathrm{d} - 1)$. This completes the proof. □

By simple calculations and using Theorem 4.7, we have following result.

Corollary 4.8. *Let $T \in \mathcal{T}(n, \mathrm{d})$ be an n-vertex tree with $n \geq 3$. Then*

$$\xi^{ad}(T) \leq \begin{cases} \frac{n^2-1}{2} & \text{if } \mathrm{d} = 2, \\ \frac{2n^2-9n-17}{6} & \text{if } \mathrm{d} = 4, \\ 2\left(\frac{2}{\mathrm{d}} + \frac{3}{\mathrm{d}-1} + \frac{4}{\mathrm{d}-2} + \frac{4}{\mathrm{d}-3} + \cdots + \frac{4}{\mathrm{d}/2+2}\right) & \\ +\frac{2(n^2+\mathrm{d}^2-2nd+2n-2\mathrm{d}+5)}{d+2} + \frac{2(n-\mathrm{d}+3)}{\mathrm{d}} & \text{if } \mathrm{d} \geq 6 \text{ and is even,} \\ 2\left(\frac{2}{n-1} + \frac{3}{n-2} + \frac{4}{n-3} + \frac{4}{n-4} + \cdots + \frac{4}{n/2}\right) & \text{if } \mathrm{d} \geq 3 \text{ and is odd,} \end{cases}$$

with equality if and only if $T \cong T(n, \mathrm{d}; n - \mathrm{d} - 1)$.

4.3 Conclusion

The center of interest of this chapter is to study the unicyclic graphs with the largest eccentric adjacency index between all n-vertex unicyclic graphs with a given girth. Also we find the largest unicyclic graph with respect to eccentric adjacency index. Furthermore, we determined the tree with the largest eccentric adjacency index among all the n-vertex trees with a fixed diameter. It is interesting to investigate eccentric adjacency index for unicyclic graphs and trees with fixed parameters like maximum vertex degree, independence number, degree sequence, domination number, bipartition and fixed pendent vertices.

Chapter 5

Two degree distance based topological indices of chemical trees

The present-day trend is to study the extremal determinations in graph theory with some graph parameters, for example, vertex degree, bipartition, matching number, independence number, vertex cover, etc., and it has established its significance quite successful. In [1], the authors found the extremal conjugated trees with respect to eccentric connectivity and eccentric adjacency indices. Hua et al. [59] determined the graphs having smallest eccentric distance sum within all n-vertex graphs with k cut edges. Qi et al. [74] gave the trees with extremal Zagreb eccentricity invariants among the trees with fixed domination number, largest degree and bipartition.

Motivated by the above statements, it is quite natural for us to carry on the investigation on the eccentric connectivity and the eccentric adjacency indices with some given parameters. The rest of the chapter is structured as follows. In Section 5.1, we determine trees with the smallest eccentric connectivity and largest eccentric adjacency indices among the n-vertex trees with a given bipartition. Section 5.2 contains results of trees with the smallest eccentric connectivity and the largest eccentric adjacency indices in the class of trees with fixed matching number and independence number. Section 5.3 incorporated a bit discussion about eccentric connectivity index of the smallest trees with fixed domination number.

5.1 Eccentric connectivity index and the eccentric adjacency index of trees with a (r, s)-bipartition

Let $\mathcal{T}(n; r, s)$ be the family of n-vertex trees, every one of which has a (r, s)-bipartition, where $r \leq s$ and $r + s = n$. Note that $\mathcal{T}(n; 1, n-1) = \{S_n\}$. Let $T(n, r, s)$ be the n-vertex tree acquired by connecting $r-1$ and $s-1$ pendent vertices to the two vertices of P_2, respectively, where $2 \leq r \leq s$ and $r + s = n$. The graph $T(n, r, s)$ is depicted in Figure 5.1. In this section, we find the tree with smallest eccentric connectivity index in $\mathcal{T}(n; r, s)$ and also determine the tree with largest eccentric adjacency index in $\mathcal{T}(n; r, s)$.

Figure 5.1: The graph $T(n, r, s)$.

In Lemma 5.1, we establish a new tree in $\mathcal{T}(n; r, s)$ from a given tree in $\mathcal{T}(n; r, s)$ such that the new tree has smaller eccentric connectivity index and has larger eccentric adjacency index.

Lemma 5.1. *Let $T \in \mathcal{T}(n; r, s)$ with $uv, vw \in \mathcal{E}_T$, $\deg_T(u) \geq 2$ and $\Gamma_T(w) = \{v, w_1, w_2, \ldots, w_t\}$, where $w_1, w_2, \ldots, w_t \in P_T(w)$, $t \geq 1$ and also $w_1, w_2, \ldots, w_t$ be the end vertices of a diametrical path in T. Construct a new tree T_1 from T as $T_1 = (T - \{ww_1, \ldots, ww_t\}) \cup \{uw_1, \ldots, uw_t\}$. Then $\xi^c(T_1) \leq \xi^c(T)$ and $\xi^{ad}(T_1) \geq \xi^{ad}(T)$.*

Proof. By the construction of T_1, it is obvious that $T_1 \in \mathcal{T}(n; r, s)$. Let T_v be the component of $T - \{u, w\}$ which includes the vertex v and take $x \in P_T(w)$, define

$\mathcal{A} = \{y \in \mathcal{V}_T \mid d_T(x, y) = ec_T(y)\}$. It is natural to see that for any $x_1 \in \mathcal{V}_T \setminus (\mathcal{A} \cup P_T(w))$, we have

$$ec_{T_1}(x_1) = ec_T(x_1). \tag{5.1}$$

- If $ec_{T_v}(v) = 2$ then for any $y \in \mathcal{A}$, we have $ec_{T_1}(y) = ec_T(y)$.

- If $ec_{T_v}(v) \in \{0, 1\}$ then there are some vertex $z \in \mathcal{V}_T$ such that $d_{T_1}(y, z) = ec_{T_1}(y)$, for any $y \in \mathcal{A}$. There are two possibilities: either $z = w$ or $z \in \mathcal{V}_T \setminus \{w\}$. If $z = w$ then we have

$$ec_{T_1}(y) = d_{T_1}(y, w) = d_T(y, w) = ec_T(y) - 1. \tag{5.2}$$

  Now if $z \in \mathcal{V}_T \setminus \{w\}$ then we have

$$ec_{T_1}(y) = d_{T_1}(y, z) = d_T(y, z) \leq ec_T(y). \tag{5.3}$$

Note that $ec_T(x) = ec_T(w) + 1$ for any $x \in P_T(w)$. Therefore from (5.1)-(5.3), we get

$$ec_{T_1}(x) = ec_{T_1}(u) + 1 \leq ec_T(u) + 1. \tag{5.4}$$

Case I: By the construction of T_1, it is easily seen that

$$\deg_{T_1}(y) = \deg_T(y), \ \forall \ y \in \mathcal{V}_T \setminus \{u, w\}. \tag{5.5}$$

Also, the degrees of vertices u and w are given by

$$\deg_{T_1}(w) = \deg_T(w) - t = 1, \quad \deg_{T_1}(u) = \deg_T(u) + t. \tag{5.6}$$

Thus from (5.1)-(5.6), we obtain

$$
\begin{aligned}
\xi^c(T_1) - \xi^c(T) &= ec_{T_1}(u)\deg_{T_1}(u) - ec_T(u)\deg_T(u) + ec_{T_1}(w)\deg_{T_1}(w) - ec_T(w)\deg_T(w) \\
&+ \sum_{x\in P_T(w)} ec_{T_1}(x)\deg_{T_1}(x) - \sum_{x\in P_T(w)} ec_T(x)\deg_T(x) \\
&\leq ec_T(u)(\deg_T(u)+t) - ec_T(u)\deg_T(u) + ec_T(w)(\deg_T(w)-t) \\
&- ec_T(w)\deg_T(w) + \sum_{x\in P_T(w)} (ec_T(u)+1)\deg_T(x) \\
&- \sum_{x\in P_T(w)} (ec_T(w)+1)\deg_T(x) \\
&= t\ ec_T(u) - t\ ec_T(w) + t\ ec_T(u) - t\ ec_T(w) \\
&= 2t(ec_T(u) - ec_T(w)).
\end{aligned}
$$

Note that $ec_T(u) \leq ec_T(w)$, equality holds if $\mathrm{d}_T = 4$. Therefore $\xi^c(T_1) \leq \xi^c(T)$.

Case II: By the construction of T_1, we have

$$S_{T_1}(y) = S_T(y),\ \forall\ y \in \mathcal{V}_T \setminus (\Gamma_T(v) \cup \Gamma_T(w) \cup \{u,w\}). \tag{5.7}$$

Also, the sum of the degrees of neighbor vertices of v in T_1 is given by

$$
\begin{aligned}
S_{T_1}(v) &= \sum_{x\in\Gamma_T(v)\setminus\{u,w\}} \deg_{T_1}(x) + \deg_{T_1}(w) + \deg_{T_1}(u) \\
&= \sum_{x\in\Gamma_T(v)\setminus\{u,w\}} \deg_T(x) + (\deg_T(w)-t) + (\deg_T(u)+t) \\
&= S_T(v).
\end{aligned} \tag{5.8}
$$

Also

$$
\begin{aligned}
&S_{T_1}(u) = S_T(u)+t, \quad S_{T_1}(w) = S_T(w)-t \\
&S_{T_1}(x) = S_T(x)+t, \qquad \forall\ x \in \Gamma_T(u)\setminus\{v\}.
\end{aligned} \tag{5.9}
$$

Note that $S_T(x) = \deg_T(w) = t+1$ and given that $\deg_T(u) \geq 2$, for any $x \in P_T(w)$. Therefore we have

$$S_{T_1}(x) = \deg_{T_1}(u) = \deg_T(u) + t \geq 2+t > \deg_T(w) = S_T(x). \tag{5.10}$$

Thus from (5.1)-(5.4) and (5.7)-(5.10), we obtain

$$\begin{aligned}
\xi^{ad}(T_1) - \xi^{ad}(T) &= \frac{S_{T_1}(v)}{ec_{T_1}(v)} - \frac{S_T(v)}{ec_T(v)} + \frac{S_{T_1}(w)}{ec_{T_1}(w)} - \frac{S_T(w)}{ec_T(w)} + \frac{S_{T_1}(u)}{ec_{T_1}(u)} - \frac{S_T(u)}{ec_T(u)} \\
&+ \sum_{x\in P_T(w)} \frac{S_{T_1}(x)}{ec_{T_1}(x)} - \sum_{x\in P_T(w)} \frac{S_T(x)}{ec_T(x)} + \sum_{x\in \Gamma_T(u)\setminus\{v\}} \frac{S_{T_1}(x)}{ec_{T_1}(x)} \\
&- \sum_{x\in \Gamma_T(u)\setminus\{v\}} \frac{S_T(x)}{ec_T(x)} \\
&\geq \frac{S_T(v)}{ec_T(v)} - \frac{S_T(v)}{ec_T(v)} + \frac{S_T(w)-t}{ec_T(w)} - \frac{S_T(w)}{ec_T(w)} + \frac{S_T(u)+t}{ec_T(u)} - \frac{S_T(u)}{ec_T(u)} \\
&+ \sum_{x\in P_T(w)} \frac{S_T(x)}{ec_T(x)} - \sum_{x\in P_T(w)} \frac{S_T(x)}{ec_T(x)} + \sum_{x\in \Gamma_T(u)\setminus\{v\}} \frac{S_T(x)+t}{ec_T(x)} \\
&- \sum_{x\in \Gamma_T(u)\setminus\{v\}} \frac{S_T(x)}{ec_T(x)} \\
&= \frac{t}{ec_T(u)} - \frac{t}{ec_T(w)} + \sum_{x\in \Gamma_T(u)\setminus\{v\}} \frac{t}{ec_T(x)}.
\end{aligned}$$

Note that $ec_T(u) \leq ec_T(w)$, equality holds if $\mathrm{d}_T = 4$. Therefore $\xi^{ad}(T_1) \geq \xi^{ad}(T)$. $\square$

Applying Lemma 5.1 repeatedly yields the next theorem.

Theorem 5.2. *The tree $T(n, r, s)$ is the unique tree in $\mathcal{T}(n; r, s)$ which has the smallest eccentric connectivity index among trees in $\mathcal{T}(n; r, s)$, where $n \geq 3$ and $2 \leq r \leq s$.*

Proof. Let $T \in \mathcal{T}(n; r, s)$ be an n-vertex tree. If $T \ncong T(n, r, s)$ then there is a path uvw in T with $\deg_T(u) \geq 2$ and $\Gamma_T(w) = \{v, w_1, w_2, \ldots, w_t\}$, where $w_1, w_2, \ldots, w_t \in P_T(w)$, $t \geq 1$ and also $w_1, w_2, \ldots, w_t$ be the end vertices of a diametrical path in T. By using Lemma 5.1, we construct a tree from T as $T_1 = (T - \{ww_1, \ldots, ww_t\}) \cup \{uw_1, \ldots, uw_t\}$ that satisfies $\xi^c(T_1) \leq \xi^c(T)$. Now if $T_1 \ncong T(n, r, s)$ then there is a path $u'v'w'$ in T_1 with $\deg_{T_1}(u') \geq 2$ and $\Gamma_{T_1}(w') = \{v', w'_1, w'_2, \ldots, w'_t\}$, where $w'_1, w'_2, \ldots, w'_t \in P_{T_1}(w')$, $t \geq 1$ and also $w'_1, w'_2, \ldots, w'_t$ be the end vertices of a diametrical path in T_1. By applying Lemma 5.1, we construct a tree from T_1 as $T_2 = (T_1 - \{w'w'_1, \ldots, w'w'_t\}) \cup \{u'w'_1, \ldots, u'w'_t\}$ that satisfies $\xi^c(T_2) \leq \xi^c(T_1)$. Therefore by using repeatedly Lemma 5.1 on diametrical paths of T we acquire a sequence of trees in $\mathcal{T}(n, r, s)$ with smaller eccentric connectivity index such that $\xi^c(T) \geq \xi^c(T_1) \geq \cdots \geq \xi^c(T_k)$, where $T_k \cong T(n, r, s)$. This shows that $T(n, r, s)$ has the smallest eccentric connectivity index among trees in $T(n, r, s)$. $\square$

By simple determining and using Theorem 5.2, we acquire following result.

Corollary 5.3. *Let $T \in \mathcal{T}(n; r, s)$ with $2 \leq r \leq s$ and $r + s = n$. Then $\xi^c(T) \leq 5n - 6$ with equality if and only if $T \cong T(n, r, s)$.*

By the definition of eccentric adjacency index and a similar interpretation given in Theorem 5.2, we can find the extremal tree with largest eccentric adjacency index in $\mathcal{T}(n; r, s)$ in the next theorem.

Theorem 5.4. *The tree $T(n, r, s)$ is the unique tree in $\mathcal{T}(n; r, s)$ that has the largest eccentric adjacency index among trees in $\mathcal{T}(n; r, s)$, where $n \geq 3$ and $2 \leq r \leq s$.*

By simple assessment and using Theorem 5.4, we acquire next result.

Corollary 5.5. *Let $T \in \mathcal{T}(n; r, s)$ be an n-vertex tree with $2 \leq r \leq s$ and $r + s = n$. Then $\xi^{ad}(T) \leq \frac{1}{3}((r + 1)^2 + (s + 1)^2 - 5)$ with equality if and only if $T \cong T(n, r, s)$.*

5.2 Eccentric connectivity index and eccentric adjacency index of trees with fixed matching number and independence number

Let $\mathcal{T}(n, m)$ be the family of all n-vertex trees with a fixed matching number m and $\mathcal{T}(n, \alpha)$ be the set of all n-vertex trees with independence number α. If $m = 1$, then T is a star S_n with $\xi^c(S_n) = 3(n - 1)$ and $\xi^{ad}(S_n) = \frac{n^2-1}{2}$ for $n \geq 3$. Let $S_{n,m} \in \mathcal{T}(n, m)$ be a tree acquired from star S_{n-m+1} by connecting a pendent edge to each $m - 1$ pendent vertices in S_{n-m+1}. The graph $S_{n,m}$ is shown in Figure 5.2.

In this section, we derive the smallest eccentric connectivity index of trees in $\mathcal{T}(n, m)$ and $\mathcal{T}(n, \alpha)$. Also we find the largest eccentric adjacency index of trees in $\mathcal{T}(n, m)$ and $\mathcal{T}(n, \alpha)$.

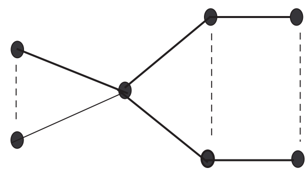

Figure 5.2: The graph $S_{n,m}$.

The following lemmas present the classic properties of a tree with maximum matching m and these lemmas are beneficial in the proofs of main results.

Lemma 5.6 (Hou and Li [56]). *Let $T \in \mathcal{T}(2m, m)$ be a tree with $m \geq 3$. Then T contains at least two pendent vertices such that they are linked to the degree 2 vertices, respectively.*

Lemma 5.7 (Hou and Li [56]). *Let $T \in \mathcal{T}(n, m)$ be a tree with $m \geq 3$ and $n = 2m + 1$. Then T contains a pendent vertex linked to a degree 2 vertex.*

Lemma 5.8 (Hou and Li [56]). *Let $T \in \mathcal{T}(n, m)$ be a tree with $n > 2m$ and $m \geq 3$. Then there exists an m-matching M and $u \in P_T$ such that u does not M-saturated.*

Theorem 5.9 (Xu et al. [95]). *Let $T \in \mathcal{T}(n, m)$ be a tree with $n \geq 2m$ and $m \geq 3$. Then we have $\xi^c(T) \geq 5n + 2m - 7$ with equality if and only if $T \cong S_{n,m}$.*

For an n-vertex tree, it is widely known that $\alpha + m = n$. By Theorem 5.9, it results that

Theorem 5.10. *Let $T \in \mathcal{T}(n, \alpha)$ be an n-vertex tree with $\alpha \leq n - 3$. Then we have $\xi^c(T) \geq 7n - 2\alpha - 7$ with equality if and only if $T \cong S_{n,n-\alpha}$.*

Theorem 5.11 (Akhter and Farooq [1]). *Let $T \in \mathcal{T}(2m, m)$ be an n-vertex tree with $m \geq 3$. Then $\xi^{ad}(T) \leq \dfrac{1}{6}(2m^2 + 11m - 8)$, with equality if and only if $T \cong S_{2m,m}$.*

Theorem 5.12. *Let $T \in \mathcal{T}(n, m)$ be an n-vertex tree with $n \geq 6$ and $m \geq 3$. Then we have $\xi^{ad}(T) \leq \frac{1}{6}(2n^2 + 2m^2 - 4nm + 3n + 5m - 8)$ with equality if and only if $T \cong S_{n,m}$.*

Proof. We establish the result using induction on n. If $n = 2m$, then the required result holds from Theorem 5.11. Assume that $n > 2m$ and the outcome satisfies for trees in $T \in \mathcal{T}(n-1, m)$. Let $T \in \mathcal{T}(n, m)$ and M be a largest matching of T. By Lemma 5.8, there is a pendent vertex w in T such that w is not M-saturated. Let v be the unique neighbor of w in T and $T_1 = T - \{w\}$. Then $T_1 \in \mathcal{T}(n-1, m)$. Since M is a largest matching therefore M contains one edge linked with v. There are $n - 1 - m$ edges of T outside M, therefore $\deg_T(v) \leq n - m$. If $ec_T(w) = 2$, then $T \cong S_n$ with w as a pendent vertex in S_n. Therefore we take $ec_T(w) \geq 3$ and $ec_T(v) \geq 2$.

Now take $x \in P_T(v)$, define $\mathcal{A} = \{y \in \mathcal{V}_T \mid d_T(x, y) = ec_T(y)\}$. It is casual to see that for any $x_1 \in \mathcal{V}_T \setminus (\mathcal{A} \cup P_T(v))$, we have

$$ec_{T_1}(x_1) = ec_T(x_1).$$

There are some vertex $z \in \mathcal{V}_T$ such that $d_{T_1}(y, z) = ec_{T_1}(y)$, for any $y \in \mathcal{A}$. There are two possibilities: either $z = v$ or $z \in \mathcal{V}_T \setminus \{v, w\}$. If $z = v$ then we have

$$ec_{T_1}(y) = d_{T_1}(y, v) < d_T(y, x) = ec_T(y).$$

Now if $z \in \mathcal{V}_T \setminus \{v, w\}$ then we have

$$ec_{T_1}(y) = d_{T_1}(y, z) = d_T(y, z) \leq ec_T(y).$$

By the construction of T_1, we acquire

$$S_{T_1}(v) = S_T(v) - 1.$$

Also, for $x_1 \in \Gamma_T(v) \setminus \{w\}$, we have

$$\begin{aligned} S_{T_1}(x_1) &= \sum_{y \in \Gamma_T(x_1) \setminus \{v\}} \deg_{T_1}(y) + \deg_{T_1}(v) \\ &= \sum_{y \in \Gamma_T(x_1) \setminus \{v\}} \deg_T(y) + (\deg_T(v) - 1) \\ &= S_T(x_1) - 1. \end{aligned}$$

Therefore from the induction hypothesis, we obtain

$$\begin{aligned}
\xi^{ad}(T) &= \sum_{z\in\mathcal{V}_T\setminus(\{v\}\cup\Gamma_T(v))}\frac{S_T(z)}{ec_T(z)}+\frac{S_T(v)}{ec_T(v)}+\sum_{x_1\in\Gamma_T(v)\setminus\{w\}}\frac{S_T(x_1)}{ec_T(x_1)}+\frac{S_T(w)}{ec_T(w)}\\
&\le \sum_{z\in\mathcal{V}_T\setminus(\{v\}\cup\Gamma_T(v))}\frac{S_{T_1}(z)}{ec_{T_1}(z)}+\frac{S_{T_1}(v)+1}{ec_{T_1}(v)}+\sum_{x_1\in\Gamma_T(v)\setminus\{w\}}\frac{S_{T_1}(x_1)+1}{ec_{T_1}(x_1)}+\frac{\deg_{T_1}(v)}{ec_{T_1}(w)}\\
&= \xi^{ad}(T_1)+\frac{1}{ec_{T_1}(v)}+\sum_{x_1\in\Gamma_T(v)\setminus\{w\}}\frac{1}{ec_{T_1}(x_1)}+\frac{\deg_{T_1}(v)}{ec_{T_1}(w)}\\
&\le \frac{2(n-1)^2+2m^2-4(n-1)m+3(n-1)+5m-8)}{6}+\frac{1}{2}\\
&+\sum_{x\in\Gamma_T(v)\setminus\{w\}}\frac{1}{3}+\frac{n-m}{3}\\
&= \frac{2n^2+2m^2-4nm+3n+5m-8)}{6}+\frac{(-4n+4m-1)}{6}+\frac{1}{2}\\
&+\frac{n-m-1}{3}+\frac{n-m}{3}\\
&= \frac{2n^2+2m^2-4nm+3n+5m-8)}{6}.
\end{aligned}$$

The first equality holds if and only if $ec_{T_1}(z) = ec_T(z)$, for all $z \in \mathcal{V}_T$ and second equality proved if and only if $\deg_T(v) = n - 2m$, $|\Gamma_T(v) \setminus \{w\}| = n - m - 1$, $ec_T(v) = 2$ and $ec_T(x) = 3$ for all $x \in \Gamma_T(v) \setminus \{w\}$, that is, $T \cong S_{n,m}$. Therefore, all the equalities proved if and only if $T \cong S_{n,m}$. This completes the proof. □

By using $\alpha + m = n$ in Theorem 5.12, we acquire the next result.

Theorem 5.13. *Let $T \in \mathcal{T}(n,\alpha)$ with $\alpha \le n-3$. Then we have $\xi^{ad}(T) \le \frac{1}{6}(8n + 2\alpha^2 - 5\alpha - 8)$ with equality if and only if $T \cong S_{n,n-\alpha}$.*

5.3 Eccentric connectivity index of trees with domination number

Let $\mathcal{T}(n,\gamma)$ be the family of all the n-vertex trees with domination number γ. If $\gamma = 1$, then T is a star S_n with $\xi^c(S_n) = 3(n-1)$. Let $S_{n,\gamma} \in \mathcal{T}(n,\gamma)$ be a tree acquired from star $K_{1,n}$ by connecting a pendent edge to each $n-\gamma-1$ pendent vertices.

In this section, we find the smallest eccentric connectivity index of trees in $\mathcal{T}(n,\gamma)$.

Lemma 5.14. *Let T be a tree with $n \geq 4$ and $u_1u_2 \in \mathcal{E}_T$ such that $u_1, u_2 \notin P_T$. Let T' be the new tree acquired from T by deleting u_1u_2 and identifying u_1 and u_2, denoted by u_1' and introducing a pendent edge $u_1'u_2'$, where u_2' be a pendent vertex. Then we have $\xi^c(T') < \xi^c(T)$.*

Proof. Let T_1 and T_2 be two components of $T - \{u_1u_2\}$ such that $u_1 \in \mathcal{V}_{T_1}$ and $u_2 \in \mathcal{V}_{T_2}$. For each vertex $w \in \mathcal{V}_{T_1} \setminus \{u_1\}$, we have

$$\begin{aligned} ec_T(w) &= \max\{ec_{T_1}(w), d_{T_1}(w,u_1) + 1 + ec_{T_2}(u_2)\}, \\ ec_{T'}(w) &= \max\{ec_{T_1}(w), d_{T_1}(w,u_1) + ec_{T_2}(u_2), d_{T_1}(w,u_1) + 1\}. \end{aligned} \tag{5.11}$$

For each vertex $w \in \mathcal{V}_{T_2} \setminus \{u_2\}$, we have

$$\begin{aligned} ec_T(w) &= \max\{ec_{T_2}(w), d_{T_2}(w,u_2) + 1 + ec_{T_1}(u_1)\}, \\ ec_{T'}(w) &= \max\{ec_{T_2}(w), d_{T_2}(w,u_2) + ec_{T_1}(u_1), d_{T_2}(w,u_1) + 1\}. \end{aligned} \tag{5.12}$$

Now, it is simply seen that the eccentricities of u_1' and u_2' in T' are as follows:

$$\begin{aligned} ec_{T'}(u_1') &= \max\{ec_{T_1}(u_1), ec_{T_2}(u_2)\}, \\ ec_{T'}(u_2') &= \max\{ec_{T_1}(u_1) + 1, ec_{T_2}(u_2) + 1\}. \end{aligned} \tag{5.13}$$

By the construction of T', we have

$$\deg_{T'}(w) = \deg_T(w), \qquad \forall\ w \in \mathcal{V}_T \setminus \{u_1, u_2\}. \tag{5.14}$$

Also, the degrees of vertices u_1' and u_2' in T' are given by

$$\deg_{T'}(u_1') = \deg_T(u_1) + \deg_T(u_2) - 1, \qquad \deg_{T'}(u_2') = 1. \tag{5.15}$$

Note that from (5.11) and (5.12), we get $ec_{T'}(w) \leq ec_T(w)$ for all $w \in (\mathcal{V}_{T_1} \setminus \{u_1\}) \cup (\mathcal{V}_{T_2} \setminus$

$\{u_2\}$). Thus from (5.11)-(5.15), we obtain

$$
\begin{aligned}
\xi^c(T) - \xi^c(T') = & \sum_{w \in \mathcal{V}_{T_1} \setminus \{u_1\}} (\deg_T(w) ec_T(w) - \deg_{T'}(w) ec_{T'}(w)) \\
& + \sum_{w \in \mathcal{V}_{T_2} \setminus \{u_2\}} (\deg_T(w) ec_T(w) - \deg_{T'}(w) ec_{T'}(w)) + \deg_T(u_1) ec_T(u_1) \\
& + \deg_T(u_2) ec_T(u_2) - \deg_{T'}(u_1') ec_{T'}(u_1') - \deg_{T'}(u_2') ec_{T_2}(u_2') \\
& \geq \sum_{w \in V_{T_1} \setminus \{u_1\}} (\deg_T(w) ec_T(w) - \deg_T(w) ec_T(w)) \\
& + \sum_{w \in \mathcal{V}_{T_2} \setminus \{u_2\}} (\deg_T(w) ec_T(w) - \deg_T(w) ec_T(w)) \\
& + \max\{ec_{T_1}(u_1), ec_{T_2}(u_2) + 1\} \deg_T(u_1) \\
& + \max\{ec_{T_1}(u_1) + 1, ec_{T_2}(u_2)\} \deg_T(u_2) - \max\{ec_{T_1}(u_1), ec_{T_2}(u_2)\} \\
& (\deg_T(u_1) + \deg_T(u_2) - 1) - \max\{ec_{T_1}(u_1) + 1, ec_{T_2}(u_2) + 1\}(1) \\
& = \max\{ec_{T_1}(u_1), ec_{T_2}(u_2) + 1\} \deg_T(u_1) + \max\{ec_{T_1}(u_1) + 1, ec_{T_2}(u_2)\} \\
& \deg_T(u_2) - \max\{ec_{T_1}(u_1), ec_{T_2}(u_2)\}(\deg_T(u_1) + \deg_T(u_2) - 1) \\
& - \max\{ec_{T_1}(u_1) + 1, ec_{T_2}(u_2) + 1\}
\end{aligned} \tag{5.16}
$$

Case I: If $ec_{T_1}(u_1) \geq ec_{T_2}(u_2) + 1$, then

$$
\begin{aligned}
\xi^c(T) - \xi^c(T') & \geq ec_{T_1}(u_1) \deg_T(u_1) + (ec_{T_1}(u_1) + 1) \deg_T(u_2) \\
& - ec_{T_1}(u_1)(\deg_T(u_1) + \deg_T(u_2) - 1) - (ec_{T_1}(u_1) + 1) \\
& = \deg_T(u_2) - 1 > 0.
\end{aligned} \tag{5.17}
$$

Case II: If $ec_{T_2}(u_2) \geq ec_{T_1}(u_1) + 1$, then

$$
\begin{aligned}
\xi^c(T) - \xi^c(T') & \geq (ec_{T_2}(u_2) + 1) \deg_T(u_1) + ec_{T_2}(u_2) \deg_T(u_2) \\
& - ec_{T_2}(u_2)(\deg_T(u_1) + \deg_T(u_2) - 1) - (ec_{T_2}(u_2) + 1) \\
& = \deg_T(u_1) - 1 > 0.
\end{aligned} \tag{5.18}
$$

Case III: If $ec_{T_1}(u_1) = ec_{T_2}(u_2)$, then

$$\begin{aligned}\xi^c(T) - \xi^c(T') &\geq (ec_{T_2}(u_2)+1)\deg_T(u_1) + (ec_{T_2}(u_2)+1)\deg_T(u_2) \\ &\quad - ec_{T_2}(u_2)(\deg_T(u_1) + \deg_T(u_2) - 1) - (ec_{T_2}(u_2)+1) \\ &= \deg_T(u_1) + \deg_T(u_2) - 1 > 0.\end{aligned} \tag{5.19}$$

The proof is complete. □

Xu et al. [95] determined that any graph $\mathcal{G}$ without isolated vertices has a subset A of $\mathcal{V}_{\mathcal{G}}$ of cardinality $\gamma_{\mathcal{G}}$ such that for each $u \in A$, there is a vertex in $\mathcal{V}_{\mathcal{G}} \setminus A$ that is only linked to u. Therefore we acquire the following lemma.

Lemma 5.15 (Xu et al. [95])**.** *For any graph $\mathcal{G}$, we have $\gamma_{\mathcal{G}} \leq m_{\mathcal{G}}$.*

Lemma 5.16. *If $T_1 \in \mathcal{T}(n, \gamma)$ has the smallest eccentric connectivity index, then $\gamma_{T_1} = m_{T_1} = \gamma$.*

Proof. By Lemma 5.15, we have $\gamma = \gamma_{T_1} \leq m_{T_1}$. Now it suffices to prove that $\gamma_{T_1} \geq m_{T_1}$. Let $A = \{u_1, u_2, \ldots, u_\gamma\}$ be a dominating set of T_1 with cardinality γ. Then there exists γ edges $u_1u_1', u_2u_2', \ldots, u_\gamma u_\gamma' \in \mathcal{E}_{T_1}$, where $u_1', u_2', \ldots, u_\gamma' \in \mathcal{V}_{T_1} \setminus A$. Note that if $\gamma = \gamma_{T_1} < m_{T_1}$, there exists another edge x_1x_1', that is independent of each edge $u_1u_1', u_2u_2', \ldots, u_\gamma u_\gamma'$.

If $u_i \in A$ dominate both the vertices x_1 and x_2, then a triangle $x_1x_2u_i$ occurs, where $i = 1, 2, \ldots, \gamma$. But we know that T_1 is a tree therefore it is impossible. Thus x_1 and x_2 are dominated by two quit different vertices of A. Without loss of generality we suppose that x_i is dominated by u_i, for $i = 1, 2$, with $\deg_{T_1}(x_1)$, $\deg_{T_1}(x_2) \geq 2$ and $\deg_{T_1}(u_1)$, $\deg_{T_1}(u_2) \geq 2$. Now we can construct a new tree $T_1' \in \mathcal{T}(n, \gamma)$ from T_1 by applying transformation described in Lemma 5.14 on the edge x_1u_1 or x_2u_2 and we get $\xi^c(T_1) > \xi^c(T_1')$. This is the contradiction of our assumption. Therefore $\gamma_{T_1} \geq m_{T_1}$. □

By using Lemma 5.16, Theorem 5.9 and a simple calculation, we acquire next result.

Theorem 5.17. *Let $T \in \mathcal{T}(n, \gamma)$ with $2 \leq \gamma \leq \lfloor \frac{n}{2} \rfloor$. Then we have $\xi^c(T) \geq 5n + 2\gamma - 7$ with equality if and only if $T \cong S_{n,\gamma}$.*

5.4 Conclusion

In this chapter, we focuss on determining the trees with the smallest eccentric connectivity and the largest eccentric adjacency indices among the trees with a given bipartition size. Also we discuss the smallest eccentric adjacency index and the largest eccentric adjacency index of trees among trees with fixed matching number and independence number. In the end, we discuss the smallest trees among all trees with domination number with respect to eccentric connectivity index. Finding extremal graphs with different parameters in general classes of graphs with respect to distance based indices will be an challenging problem.

Chapter 6

Eccentric adjacency index of graphs with a given number of cut edges

In recent years, finding the extremal bounds for certain topological invariants in the form of graph structure parameters has turned out to be a worthwhile direction in extremal graph theory and many results are obtained. In [2], the authors determined the largest unicyclic graphs with fixed girth and the largest tree along a fixed diameter with respect to eccentric adjacency index. Akhter [3] derived the extremal trees for eccentric connectivity and eccentric adjacency indices in form of other graph invariants together with matching number, bipartition size, independence number and domination number. Hua [57] determined the smallest value of Wiener index among connected graphs with fixed cut edges. Motivated by the work referred above, we carry on the research on the eccentric adjacency index of graphs with some given graph invariants. In this chapter, we find the graphs with the largest eccentric adjacency index among the graphs with fixed number of cut edges and characterize the extremal graphs.

The cyclomatic number of an n_G-vertex connected graph G is $c(G) = e_G - n_G + 1$, where e_G is the size of G. In particular, if $c(G) = 0$ then G is a tree. If $c(G) = 1$ then G is a unicyclic graph and if $c(G) = 2$ then G is a bicyclic graph. If an n-vertex connected graph has the cyclomatic number at least one, then the number of its cut edges is at most

$n-3$. Thus, it is obvious from above statement that for any n-vertex connected graph with k cut edges, we always have $0 \leq k \leq n-1$ and $k \neq n-2$.

6.1 The connected graphs with a given number of cut edges

Let $\mathcal{G}(n,k)$ be the set of n-vertex connected graphs with k cut edges, where $0 \leq k \leq n-1$ ($k \neq n-2$). Denote by K_{n-k}^{k} the graph acquired by connecting k pendent vertices with a unique vertex of a complete graph K_{n-k}. In this section, we find an n-vertex connected graph in $\mathcal{G}(n,k)$ with largest eccentric adjacency index. First we prove some lemmas which will be crucial to the proof of our main result.

Lemma 6.1. *Let H_1 and H_2 be two vertex-disjoint connected graphs each of order at least 2 with $u \in \mathcal{V}_{H_1}$ and $v \in \mathcal{V}_{H_2}$. Let G_1 be the graph acquired by connecting u and v by an edge uv and G_2 be the graph acquired by identifying u with v and introducing a pendent edge uw with pendent vertex w, respectively. Then $\xi^{ad}(G_1) < \xi^{ad}(G_2)$.*

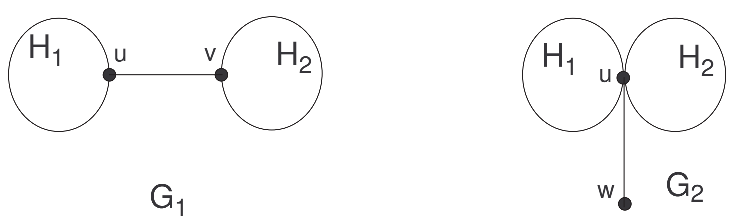

Figure 6.1: The graphs G_1 and G_2 in Lemma 6.1.

Proof. For each vertex $x \in \mathcal{V}_{G_1}$, we have

$$\begin{aligned} ec_{G_1}(x) &= \max\{ec_{H_1}(x),\ d_{H_1}(x,u)+1+ec_{H_2}(v)\}, \quad \text{if } x \in \mathcal{V}_{H_1}, \\ ec_{G_1}(x) &= \max\{ec_{H_2}(x),\ d_{H_2}(x,v)+1+ec_{H_1}(u)\}, \quad \text{if } x \in \mathcal{V}_{H_2}. \end{aligned} \tag{6.1}$$

For each vertex $x \in \mathcal{V}_{G_2} \setminus \{u, w\}$, we have

$$\begin{aligned} ec_{G_2}(x) &= \max\{ec_{H_1}(x),\ d_{H_1}(x,u) + ec_{H_2}(v),\ d_{H_1}(x,u) + 1\}, \quad \text{if } x \in \mathcal{V}_{H_1}, \\ ec_{G_2}(x) &= \max\{ec_{H_2}(x),\ d_{H_2}(x,v) + ec_{H_1}(u),\ d_{H_2}(x,u) + 1\}, \quad \text{if } x \in \mathcal{V}_{H_2}. \end{aligned} \tag{6.2}$$

Now, it is easily seen that the eccentricities of u and w in G_2 are as follows:

$$\begin{aligned} ec_{G_2}(u) &= \max\{ec_{H_1}(u),\ ec_{H_2}(v)\}, \\ ec_{G_2}(w) &= \max\{ec_{H_2}(u) + 1,\ ec_{H_2}(v) + 1\}. \end{aligned} \tag{6.3}$$

Note that from (6.1) and (6.2), we get $ec_{G_1}(x) \geq ec_{G_2}(x)$ for each $x \in \mathcal{V}_{G_1} \setminus \{u, v\}$. By the construction of G_1 and G_2, for each $x \in \mathcal{V}_{G_1} \setminus (\{u, v, w\} \cup \Gamma_{H_1}(u) \cup \Gamma_{H_2}(v))$, we have $S_{G_2}(x) = S_{G_1}(x)$. For each $x \in \Gamma_{H_1}(u)$, we have

$$\begin{aligned} S_{G_1}(x) &= \sum_{y \in \Gamma_{H_1}(x) \setminus \{u\}} \deg_{H_1}(y) + \deg_{H_1}(u) + 1, \\ S_{G_2}(x) &= \sum_{y \in \Gamma_{H_1}(x) \setminus \{u\}} \deg_{H_1}(y) + \deg_{H_1}(u) + \deg_{H_2}(v) + 1. \end{aligned} \tag{6.4}$$

For each $x \in \Gamma_{H_2}(v)$, we have

$$\begin{aligned} S_{G_1}(x) &= \sum_{y \in \Gamma_{H_2}(x) \setminus \{v\}} \deg_{H_2}(y) + \deg_{H_2}(v) + 1, \\ S_{G_2}(x) &= \sum_{y \in \Gamma_{H_2}(x) \setminus \{v\}} \deg_{H_2}(y) + \deg_{H_1}(u) + \deg_{H_2}(v) + 1. \end{aligned} \tag{6.5}$$

Furthermore, the sum of degrees of neighbors of the vertices u, v and w in G_1 and G_2 are given by

$$\begin{aligned} S_{G_1}(u) &= \sum_{y \in \Gamma_{H_1}(u)} \deg_{H_1}(y) + \deg_{H_2}(v) + 1, \\ S_{G_1}(v) &= \sum_{y \in \Gamma_{H_2}(v)} \deg_{H_2}(y) + \deg_{H_1}(u) + 1, \\ S_{G_2}(u) &= \sum_{y \in \Gamma_{H_1}(u)} \deg_{H_1}(y) + \sum_{y \in \Gamma_{H_2}(v)} \deg_{H_2}(y) + 1, \\ S_{G_2}(w) &= \deg_{H_1}(u) + \deg_{H_2}(v) + 1. \end{aligned} \tag{6.6}$$

Therefore, from (6.1)-(6.6), we obtain

$$\begin{aligned}
\xi^c(G_1) - \xi^c(G_2) \leq & \sum_{x\in\Gamma_{H_1}(u)} \left(\frac{\sum\limits_{y\in\Gamma_{H_1}(x)\setminus\{u\}} \deg_{H_1}(y) + \deg_{H_1}(u) + 1}{ec_{G_2}(x)} \right) \\
& - \sum_{x\in\Gamma_{H_1}(u)} \left(\frac{\sum\limits_{y\in\Gamma_{H_1}(x)\setminus\{u\}} \deg_{H_1}(y) + \deg_{H_1}(u) + \deg_{H_2}(v) + 1}{ec_{G_2}(x)} \right) \\
& + \sum_{x\in\Gamma_{H_2}(v)} \left(\frac{\sum\limits_{y\in\Gamma_{H_2}(x)\setminus\{v\}} \deg_{H_2}(y) + \deg_{H_2}(v) + 1}{ec_{G_2}(x)} \right) \\
& - \sum_{x\in\Gamma_{H_2}(v)} \left(\frac{\sum\limits_{y\in\Gamma_{H_2}(x)\setminus\{v\}} \deg_{H_2}(y) + \deg_{H_1}(u) + \deg_{H_2}(v) + 1}{ec_{G_2}(x)} \right) \\
& + \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \deg_{H_2}(v) + 1}{\max\{ec_{H_1}(u),\ ec_{H_2}(v)+1\}} \\
& - \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + 1}{\max\{ec_{H_1}(u),\ ec_{H_2}(v)\}} \\
& + \frac{\sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + \deg_{H_1}(u) + 1}{\max\{ec_{H_2}(v),\ ec_{H_1}(u)+1\}} - \frac{\deg_{H_1}(u) + \deg_{H_2}(v) + 1}{\max\{ec_{H_1}(u)+1,\ ec_{H_2}(v)+1\}} \\
& = -\left(\sum_{x\in\Gamma_{H_1}(u)} \frac{\deg_{H_2}(v)}{ec_{G_2}(x)} + \sum_{x\in\Gamma_{H_2}(v)} \frac{\deg_{H_2}(u)}{ec_{G_2}(x)} \right) \\
& + \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \deg_{H_2}(v) + 1}{\max\{ec_{H_1}(u),\ ec_{H_2}(v)+1\}} \\
& - \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + 1}{\max\{ec_{H_1}(u),\ ec_{H_2}(v)\}} \\
& + \frac{\sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + \deg_{H_1}(u) + 1}{\max\{ec_{H_2}(v),\ ec_{H_1}(u)+1\}} - \frac{\deg_{H_1}(u) + \deg_{H_2}(v) + 1}{\max\{ec_{H_1}(u)+1,\ ec_{H_2}(v)+1\}}
\end{aligned}$$

Case I: If $ec_{H_1}(u) \geq ec_{H_2}(v) + 1$, then

$$\xi^c(G_1) - \xi^c(G_2) \leq -\left(\sum_{x\in\Gamma_{H_1}(u)} \frac{\deg_{H_2}(v)}{ec_{G_2}(x)} + \sum_{x\in\Gamma_{H_2}(v)} \frac{\deg_{H_2}(u)}{ec_{G_2}(x)} \right)$$

$$
\begin{aligned}
&+ \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \deg_{H_2}(v) + 1}{ec_{H_1}(u)} \\
&- \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + 1}{ec_{H_1}(u)} \\
&+ \frac{\sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + \deg_{H_1}(u) + 1}{ec_{H_1}(u) + 1} - \frac{\deg_{H_1}(u) + \deg_{H_2}(v) + 1}{ec_{H_1}(u) + 1}
\end{aligned}
$$

$$
\begin{aligned}
\xi^c(G_1) - \xi^c(G_2) = &- \left(\sum_{x\in\Gamma_{H_1}(u)} \frac{\deg_{H_2}(v)}{ec_{G_2}(x)} + \sum_{x\in\Gamma_{H_2}(v)} \frac{\deg_{H_2}(u)}{ec_{G_2}(x)} \right) \\
&+ \frac{\sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) - \deg_{H_2}(v)}{ec_{H_1}(u) + 1} - \frac{\sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) - \deg_{H_2}(v)}{ec_{H_1}(u)} < 0.
\end{aligned}
$$

Case II: If $ec_{H_2}(v) \geq ec_{H_1}(u) + 1$, then

$$
\begin{aligned}
\xi^c(G_1) - \xi^c(G_2) \leq &- \left(\sum_{x\in\Gamma_{H_1}(u)} \frac{\deg_{H_2}(v)}{ec_{G_2}(x)} + \sum_{x\in\Gamma_{H_2}(v)} \frac{\deg_{H_2}(u)}{ec_{G_2}(x)} \right) \\
&+ \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \deg_{H_2}(v) + 1}{ec_{H_2}(v) + 1} \\
&- \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + 1}{ec_{H_2}(v)} \\
&+ \frac{\sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + \deg_{H_1}(u) + 1}{ec_{H_2}(v)} - \frac{\deg_{H_1}(u) + \deg_{H_2}(v) + 1}{ec_{H_2}(v) + 1} \\
= &- \left(\sum_{x\in\Gamma_{H_1}(u)} \frac{\deg_{H_2}(v)}{ec_{G_2}(x)} + \sum_{x\in\Gamma_{H_2}(v)} \frac{\deg_{H_2}(u)}{ec_{G_2}(x)} \right) \\
&+ \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) - \deg_{H_1}(u)}{ec_{H_2}(v) + 1} - \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) - \deg_{H_1}(u)}{ec_{H_2}(v)} < 0.
\end{aligned}
$$

Case III: If $ec_{H_1}(u) = ec_{H_2}(v)$, then

$$
\begin{aligned}
\xi^c(G_1) - \xi^c(G_2) \leq &- \left(\sum_{x\in\Gamma_{H_1}(u)} \frac{\deg_{H_2}(v)}{ec_{G_2}(x)} + \sum_{x\in\Gamma_{H_2}(v)} \frac{\deg_{H_2}(u)}{ec_{G_2}(x)} \right) \\
&+ \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \deg_{H_2}(v) + 1}{ec_{H_2}(v) + 1}
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + 1}{ec_{H_2}(v)} \\
&+ \frac{\sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + \deg_{H_1}(u) + 1}{ec_{H_2}(v)+1} - \frac{\deg_{H_1}(u) + \deg_{H_2}(v) + 1}{ec_{H_2}(v)+1}
\end{aligned}
$$

$$
\begin{aligned}
\xi^c(G_1) - \xi^c(G_2) = &- \left(\sum_{x\in\Gamma_{H_1}(u)} \frac{\deg_{H_2}(v)}{ec_{G_2}(x)} + \sum_{x\in\Gamma_{H_2}(v)} \frac{\deg_{H_2}(u)}{ec_{G_2}(x)} \right) \\
&+ \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + 1}{ec_{H_2}(v)+1} \\
&- \frac{\sum\limits_{y\in\Gamma_{H_1}(u)} \deg_{H_1}(y) + \sum\limits_{y\in\Gamma_{H_2}(v)} \deg_{H_2}(y) + 1}{ec_{H_2}(v)} < 0.
\end{aligned}
$$

This completes the proof. □

In the following lemma, we prove an elementary result.

Lemma 6.2. *Let $G \ncong K_n$ be an n-vertex connected graph and $u, v \in \mathcal{V}_G$ be non-adjacent vertices of G. Then $\xi^{ad}(G) < \xi^{ad}(G + uv)$.*

Proof. Observe that $d_G(u, v) \geq 2$ and $d_{G+uv}(u, v) = 1$. Let $x \in \mathcal{V}_G$ and A be the set of eccentric vertices of x in G, such that $ec_G(x) = d_G(x, u) + d_G(u, v) + d_G(v, y)$, for all $y \in A$. Then

$$
\begin{aligned}
ec_{G+uv}(x) &= d_{G+uv}(x, u) + d_{G+uv}(u, v) + d_{G+uv}(v, y) \\
&< d_G(x, u) + d_G(u, v) + d_G(v, y) = ec_G(x).
\end{aligned}
\tag{6.7}
$$

The eccentricities of other vertices of G are same in G and $G + uv$. The sum of degrees of neighbors of the vertices u and v in $G + uv$ are given by

$$
\begin{aligned}
S_{G+uv}(u) &= S_G(u) + \deg_G(v) + 1, \\
S_{G+uv}(v) &= S_G(v) + \deg_G(u) + 1.
\end{aligned}
\tag{6.8}
$$

For each $x \in \Gamma_G(u)$ and $y \in \Gamma_G(v)$, we have

$$
S_{G+uv}(x) = S_G(x) + 1, \qquad S_{G+uv}(y) = S_G(y) + 1. \tag{6.9}
$$

Therefore, from (6.7)-(6.9), we obtain

$$\begin{aligned}
\xi^{ad}(G) - \xi^{ad}(G+uv) \leq\; & \frac{S_G(u)}{ec_{G+uv}(u)} - \frac{S_G(u)+\deg_G(v)+1}{ec_{G+uv}(u)} + \frac{S_G(v)}{ec_{G+uv}(v)} \\
& - \frac{S_G(v)+\deg_G(u)+1}{ec_{G+uv}(v)} + \sum_{x\in\Gamma_G(u)} \left(\frac{S_G(x)}{ec_{G+uv}(x)} - \frac{S_G(x)+1}{ec_{G+uv}(x)}\right) \\
& + \sum_{y\in\Gamma_G(v)} \left(\frac{S_G(y)}{ec_{G+uv}(y)} - \frac{S_G(y)+1}{ec_{G+uv}(y)}\right) \\
& = -\frac{\deg_G(v)+1}{ec_{G+uv}(u)} - \frac{\deg_G(u)+1}{ec_{G+uv}(v)} - \sum_{x\in\Gamma_G(u)} \frac{1}{ec_{G+uv}(x)} \\
& - \sum_{y\in\Gamma_G(v)} \frac{1}{ec_{G+uv}(y)} \\
& < 0.
\end{aligned}$$

This completes the proof. □

Lemma 6.3. *Let H be a complete graph of order $n \geq 2$ and $v_1, \ldots, v_t \in \mathcal{V}_H$ be some distinct vertices of H, where $2 \leq t \leq n$. Let $H_1, H_2, \ldots, H_t$ be the nontrivial connected graphs corresponding to a vertex $v_1, v_2, \ldots, v_t$, respectively and $u_1 \in \mathcal{V}_{H_1}, u_2 \in \mathcal{V}_{H_2}, \ldots, u_t \in \mathcal{V}_{H_t}$. Let G_3 be the graph acquired from H by identifying a vertex $u_j \in \mathcal{V}_{H_j}$ to a vertex $v_j \in \mathcal{V}_H$ for $j = 1, \ldots, t$, respectively. Let G_4 be the graph acquired from H by identifying the vertices $u_1, u_2, \ldots, u_t$ to a vertex, say $v_1 \in \mathcal{V}_H$, of v_j's. Then $\xi^{ad}(G_3) < \xi^{ad}(G_4)$.*

Proof. The order of both G_3 and G_4 is defined as $n = \sum_{j=1}^{t} |H_j| - t + |H|$. For each vertex $u \in \mathcal{V}_{H_j}$, we have

$$\begin{aligned}
ec_{G_3}(u) &= \max\{ec_{H_j}(u),\ d_{H_j}(u,u_j) + 1 + ec_{H_l}(u_l),\ l \neq j\}, \\
ec_{G_4}(u) &= \max\{ec_{H_j}(u),\ d_{H_j}(u,u_j) + ec_{H_l}(u_l),\ l \neq j\}.
\end{aligned} \tag{6.10}$$

For each $w \in \mathcal{V}_H \setminus \{v_1, v_2, \ldots, v_t\}$

$$ec_{G_3}(w) = ec_{G_4}(w) = \max\{1 + ec_{H_j}(v_j),\ j = 1, 2, \ldots, t\}. \tag{6.11}$$

From (6.10) and (6.11), it is obvious that $ec_{G_3}(u) \geq ec_{G_4}(u)$ for each $u \in \mathcal{V}_{H_j}$. Let $A = \mathcal{V}_{H_j} \setminus ((\mathcal{V}_H \cap \mathcal{V}_{H_j}) \cup \Gamma_{H_j}(u_j))$. Note that $S_{G_3}(x) = S_{G_4}(x)$ for each $x \in A$, where

$j = 1, 2, \dots, t$. For each $v_1, v_2, \dots, v_t \in \mathcal{V}_H \cap \mathcal{V}_{H_j}$, $j = 1, \dots, t$,

$$S_{G_3}(v_l) = S_H(v_l) + \sum_{\substack{j=1,\\ j\neq l}}^{t} \deg_{H_j}(u_j) + S_{H_l}(u_l), \quad \text{for } l = 1, 2, \dots, t. \tag{6.12}$$

Also

$$\begin{aligned} &S_{G_3}(x) = S_{G_4}(x) = S_H(x) + \sum_{j=1}^{t} \deg_{H_j}(u_j), && \forall\, x \in \mathcal{V}_H \setminus \{v_1, v_2, \dots, v_t\},\\ &S_{G_3}(x) = S_{H_j}(x) + \deg_H(v_j), && \forall\, x \in \Gamma_{H_j}(u_j), \text{ where } j = 1, 2, \dots, t. \end{aligned} \tag{6.13}$$

From (6.12) and (6.13), we obtain

$$\begin{aligned} \xi^{ad}(G_3) = &\sum_{l=1}^{t} \frac{1}{ec_{G_3}(v_l)} \left(S_H(v_l) + \sum_{\substack{j=1\\ j\neq l}}^{t} \deg_{H_j}(u_j) + S_{H_l}(u_l) \right)\\ &+ \sum_{x\in \mathcal{V}_H\setminus\{v_1,v_2,\dots,v_t\}} \frac{1}{ec_{G_3}(x)} \left(S_H(x) + \sum_{j=1}^{t} \deg_{H_j}(u_j) \right)\\ &+ \sum_{l=1}^{t} \sum_{x\in\Gamma_{H_j}(u_j)} \frac{1}{ec_{G_3}(x)} (S_{H_j}(x) + \deg_H(v_j)) + \sum_{j=1}^{t} \sum_{x\in A} \frac{S_{H_j}(x)}{ec_{G_3}(x)}\\ = &\sum_{x\in\mathcal{V}_H} \frac{S_H(x)}{ec_{G_3}(x)} + \sum_{l=1}^{t} \sum_{\substack{j=1\\ j\neq l}}^{t} \frac{\deg_{H_j}(u_j)}{ec_{G_3}(v_l)} + \sum_{l=1}^{t} \frac{S_{H_l}(u_l)}{ec_{G_3}(v_l)}\\ &+ \sum_{j=1}^{t} \sum_{x\in \mathcal{V}_H\setminus\{v_1,v_2,\dots,v_t\}} \frac{\deg_{H_j}(u_j)}{ec_{G_3}(x)} + \sum_{j=1}^{t} \sum_{x\in\Gamma_{H_j}(u_j)} \frac{S_{H_j}(x)}{ec_{G_3}(x)}\\ &+ \sum_{j=1}^{t} \sum_{x\in\Gamma_{H_j}(u_j)} \frac{\deg_H(v_j)}{ec_{G_3}(x)} + \sum_{j=1}^{t} \sum_{x\in A} \frac{S_{H_j}(x)}{ec_{G_3}(x)}. \end{aligned} \tag{6.14}$$

Furthermore, the sum of the degrees of neighbors of v_1 in G_4 is as follows:

$$S_{G_4}(v_1) = S_H(v_1) + \sum_{j=1}^{t} S_{H_j}(u_j). \tag{6.15}$$

Also

$$\begin{aligned} &S_{G_4}(x) = S_H(x) + \sum_{j=1}^{t} \deg_{H_j}(u_j), && \forall\, x \in \Gamma_H(v_1),\\ &S_{G_4}(x) = S_{H_l}(x) + \deg_H(v_l) + \sum_{\substack{j=1\\ j\neq l}}^{t} \deg_{H_j}(u_j), && \forall\, x \in \Gamma_{H_l}(u_l), \text{ where } l = 1, 2, \dots, t. \end{aligned} \tag{6.16}$$

From (6.15) and (6.16), we obtain

$$\xi^{ad}(G_4) = \sum_{x\in V_H\setminus\{v_1\}} \frac{S_H(x)}{ec_{G_4}(x)} + \frac{1}{ec_{G_4}(v_1)}\left(S_H(v_1) + \sum_{j=1}^{t} S_{H_j}(u_j)\right)$$
$$+ \sum_{x\in\Gamma_H(v_1)} \frac{1}{ec_{G_4}(x)}\left(S_H(x) + \sum_{j=1}^{t}\deg_{H_j}(u_j)\right) + \sum_{l=1}^{t}\sum_{x\in\Gamma_{H_l}(u_l)} \frac{1}{ec_{G_4}(x)}\Bigg(S_{H_l}(x)$$
$$+ \deg_H(v_1) + \sum_{\substack{j=1\\ j\neq l}}^{t}\deg_{H_j}(u_j)\Bigg) + \sum_{j=1}^{t}\sum_{x\in A}\frac{S_{H_j}(x)}{ec_{G_4}(x)}$$
$$= \sum_{x\in V_H}\frac{S_H(x)}{ec_{G_4}(x)} + \sum_{j=1}^{t}\frac{S_{H_j}(u_j)}{ec_{G_4}(v_1)} + \sum_{j=1}^{t}\sum_{x\in\Gamma_H(v_1)}\frac{\deg_{H_j}(u_j)}{ec_{G_4}(x)} + \sum_{l=1}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{S_{H_l}(x)}{ec_{G_4}(x)}$$
$$+ \sum_{l=1}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{\deg_H(v_1)}{ec_{G_4}(x)} + \sum_{l=1}^{t}\sum_{\substack{j=1\\ j\neq l}}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{\deg_{H_j}(u_j)}{ec_{G_4}(x)} + \sum_{j=1}^{t}\sum_{x\in A}\frac{S_{H_j}(x)}{ec_{G_4}(x)}.$$

Since H is a complete graph therefore $\Gamma_H(v_1) = \mathcal{V}_H \setminus \{v_1\}$ and the degree of every vertex is same.

$$\xi^{ad}(G_4) = \sum_{x\in\mathcal{V}_H}\frac{S_H(x)}{ec_{G_4}(x)} + \sum_{j=1}^{t}\frac{S_{H_j}(u_j)}{ec_{G_4}(v_1)} + \sum_{j=1}^{t}\sum_{x\in\mathcal{V}_H\setminus\{v_1\}}\frac{\deg_{H_j}(u_j)}{ec_{G_4}(x)} + \sum_{l=1}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{S_{H_l}(x)}{ec_{G_4}(x)}$$
$$+ \sum_{l=1}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{\deg_H(v_1)}{ec_{G_4}(x)} + \sum_{l=1}^{t}\sum_{\substack{j=1\\ j\neq l}}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{\deg_{H_j}(u_j)}{ec_{G_4}(x)} + \sum_{j=1}^{t}\sum_{x\in A}\frac{S_{H_j}(x)}{ec_{G_4}(x)}$$
$$= \sum_{x\in\mathcal{V}_H}\frac{S_H(x)}{ec_{G_4}(x)} + \sum_{j=1}^{t}\frac{S_{H_j}(u_j)}{ec_{G_4}(v_1)} + \sum_{l=1}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{S_{H_l}(x)}{ec_{G_4}(x)} \tag{6.17}$$
$$+ \sum_{l=1}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{\deg_H(v_1)}{ec_{G_4}(x)} + \sum_{j=1}^{t}\left(\sum_{x\in\mathcal{V}_H\setminus\{v_1,v_2,\ldots,v_t\}}\frac{\deg_{H_j}(u_j)}{ec_{G_4}(x)} + \sum_{x\in\{v_2,\ldots,v_t\}}\frac{\deg_{H_j}(u_j)}{ec_{G_4}(x)}\right)$$
$$+ \sum_{l=1}^{t}\sum_{\substack{j=1\\ j\neq l}}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{\deg_{H_j}(u_j)}{ec_{G_4}(x)} + \sum_{j=1}^{t}\sum_{x\in A}\frac{S_{H_j}(x)}{ec_{G_4}(x)}.$$

Thus from (6.14) and (6.17), we obtain

$$\xi^{ad}(G_3) - \xi^{ad}(G_4) \leq \sum_{j=2}^{t}\left(\frac{S_{H_j}(u_j)}{ec_{G_4}(v_j)} - \frac{S_{H_j}(u_j)}{ec_{G_4}(v_1)}\right) + \sum_{j=2}^{t}\sum_{x\in\Gamma_{H_j}(u_j)}\left(\frac{\deg_H(v_j)}{ec_{G_4}(x)} - \frac{\deg_H(v_1)}{ec_{G_4}(x)}\right)$$

$$+\sum_{j=2}^{t}\left(\frac{\deg_{H_j}(u_j)}{ec_{G_4}(v_1)}-\frac{\deg_{H_j}(u_j)}{ec_{G_4}(v_j)}\right)-\sum_{l=1}^{t}\sum_{\substack{j=1\\ j\neq l}}^{t}\sum_{x\in\Gamma_{H_l}(u_l)}\frac{\deg_{H_j}(u_j)}{ec_{G_4}(x)}$$

$$< 0.$$

This completes the proof. □

By elementary calculations, one can easily derive the following lemma.

Lemma 6.4. *Let K_{n-k}^k be an n-vertex connected graph as described above, where $0 \leq k \leq n-1$ $(k \neq n-2)$. Then*

$$\xi^{ad}(K_{n-k}^k) = \begin{cases} n(n-1)^2 & \text{for } k=0, \\ \frac{1}{2}((n-k-1)^2(n-k)+(n-1)^2+2k) & \text{for } k \geq 1. \end{cases}$$

Proof. If $k = 0$ then $K_{n-k}^k \cong K_n$ and $\xi^{ad}(K_{n-k}^k) = n(n-1)^2$. Since there are $n-k-1$ vertices of eccentricity 2 and the sum of degrees of its neighbors $((n-k-2)(n-k-1)+(n-1))$, one vertex of eccentricity 1 and the sum of degrees of its neighbors $(n-k-1)^2+k$, and k pendent vertices of eccentricity 2 and the sum of degrees of its neighbor $n-1$ in K_{n-k}^k, $k \geq 1$. Therefore we obtain the following:

$$\begin{aligned}\xi^{ad}(K_{n-k}^k) &= \frac{(n-k-1)[(n-k-2)(n-k-1)+(n-1)]}{2} \\ &+ \frac{(n-k-1)^2+k}{1} + \frac{k(n-1)}{2} \\ &= \frac{1}{2}(n-k-1)^2(n-k-2+2) + \frac{1}{2}(n-1)(n-k-1+k)+k \\ &= \frac{1}{2}((n-k-1)^2(n-k)+(n-1)^2+2k).\end{aligned}$$

This completes the proof. □

The following theorem gives the n-vertex connected graph with larger eccentric adjacency index among all the graphs in $\mathcal{G}(n,k)$, where $0 \leq k \leq n-1$ $(k \neq n-2)$.

Theorem 6.5. *Let $G \in \mathcal{G}(n,k)$ be an n-vertex connected graph with k cut edges. Then*

$$\xi^{ad}(G) \leq \begin{cases} n(n-1)^2 & \text{for } k=0, \\ \frac{1}{2}((n-k-1)^2(n-k)+(n-1)^2+2k) & \text{for } k \geq 1, \end{cases}$$

quality hold if and only if $G \cong K_{n-k}^k$.

Proof. Let $G_{max} \in \mathcal{G}(n,k)$ be a graph with the largest eccentric adjacency index among all n-vertex connected graphs with k cut edges. Let $\mathcal{E}' = \{e_1, e_2, \ldots, e_k\} \subseteq \mathcal{E}_{G_{max}}$ be the set of all cut edges of G_{max}. Then all edges in $\mathcal{E}'$ must be pendent edges and incident at a common vertex of G_{max}, say w. For $k = 0$, the graph G_{max} has no cut edges and its each component is a clique or a single vertex. If G_{max} is not the graph as described above, then we can add an edge e between two non-adjacent vertices of G_{max} and obtain a new graph $G_{max} + uv$ having no cut edges. But by Lemma 6.2, we get $\xi^c(G_{max}) < \xi^c(G_{max} + uv)$ and it contradict our assumption.

Therefore now we have $1 \leq k \leq n-1$ and $k \neq n-2$. If G_{max} has an internal cut edge uv, then we can construct a new graph by identifying u with v and introducing a pendent edge uw with pendent vertex w and denote it by G_2. It is obvious that G_2 has k cut edges. Thus by Lemma 6.3, we obtain $\xi^c(G_{max}) < \xi^c(G_2)$, which is a contradiction. When $k = n-1$ we have G_{max} is a tree, and thus we have $G_{max} \cong S_n = K_1^{n-1}$.

Next we suppose that $1 \leq k \leq n-3$. Now let 2-edge-connected graph G_3 with order $n-k$ and k pendent edges is an induced subgraph of G_{max}. If $G_3 \ncong K_{n-k}$ then we can add edges into G_3. Similar to above argument, we can deduce a new graph with a larger eccentric adjacency index than G_{max}; therefore $G_3 \cong K_{n-k}$ in G_{max}. Moreover, we can conform that all k pendent edges in G_{max} must be attached at the same vertex of K_{n-k}. Let $G_4 \ncong G_{max}$ be a graph with k pendent edges and these vertices attached at v_i vertices of G_4. Then we can transform the k pendent edges to exactly one vertex of clique K_{n-k} of G_4. Therefore by Lemma 6.1, we construct a new graph with a larger eccentric adjacency index than that of G_{max}, which is a contradiction.

Therefore from all above discussion, we must have $G_{max} \cong K_{n-k}^k$. By Lemma 6.4, we have $\xi^{ad}(K_{n-k}^k) = n(n-1)^2$ for $k = 0$, and $\xi^{ad}(K_{n-k}^k) = \frac{1}{2}((n-k-1)^2(n-k)+(n-1)^2+2k)$ for $k \geq 1$ and this completes the proof. □

Following result is the consequence of Theorem 6.5 for $k = n-1$.

Theorem 6.6. *Let G be an n-vertex connected graph, $n \geq 2$. Then $\xi^{ad}(G) \leq \frac{n^2-1}{2}$ with* *equality if and only if* $G \cong S_n$.

6.2 Conclusion

This chapter center on a family $\mathcal{G}(n,k)$ of those n-vertex graphs which contain k cut edges. We acquired the graphs in $\mathcal{G}(n,k)$ which have the largest eccentric adjacency index and characterized the extremal graphs. It will be worthwhile to consider other distance and eccentricity based topological indices for the class $\mathcal{G}(n,k)$ of graphs and compute their respective extremal graphs.

Chapter 7

Total eccentricity index of trees with fixed pendent vertices and trees with fixed diameter

The importance of trees is evident from their implementations in various diverse fields, for example, computer science, the computation of saturated hydrocarbons, the electrical circuits, etc [49]. Samith et al. [82] determined the trees that minimizes and maximizes total eccentricity index among all trees along a given degree sequence.

Let $\mathcal{T}(n,p)$, $2 \leq p \leq n-1$, be the family of n-vertex trees with p pendent vertices. In this chapter, we find trees in $\mathcal{T}(n,p)$ with the smallest and the largest total eccentricity index. We propose three algorithms to transform given trees into trees with smaller or larger total eccentricity indices. We also define a class $\mathcal{T}(n,\mathrm{d})$ of n-vertex trees with a fixed diameter d and determine trees in this class with the smallest and the largest total eccentricity index.

7.1 Smallest total eccentricity index of trees with fixed pendent vertices

A tree $T \in \mathcal{T}(n,p)$ is called a starlike tree if there exists a vertex $v \in \mathcal{V}_T$ with $\deg_T(v) = \triangle_T = p$. Let $\mathcal{S}(n,p) \subset \mathcal{T}(n,p)$ be the family of all n-vertex starlike trees with p pendent vertices. Thus, if T is a tree in $\mathcal{S}(n,p)$ with a vertex v satisfying $\deg_T(v) = p$, then corresponding to each edge xv incident on v, there is exactly one pendent vertex reachable from v by a path containing the edge xv. A starlike tree $T \in \mathcal{S}(n,p)$ is called balanced if $|d_T(v,x) - d_T(v,y)| \leq 1$ for all $x, y \in P_T$, where $\deg_T(v) = \triangle_T = p$. The family of all balanced starlike trees is presented by $\widetilde{\mathcal{S}}(n,p)$.

In this section, we find the trees with smallest total eccentricity index among trees in $\mathcal{T}(n,p)$. We propose two Algorithms; namely Algorithm A and Algorithm B. In Algorithm A, we transform a given tree in $\mathcal{T}(n,p)$ into a tree in $\mathcal{S}(n,p)$. In Algorithm B, we construct a tree in $\widetilde{\mathcal{S}}(n,p)$ from a given tree in $\mathcal{S}(n,p)$.

Let $T \in \mathcal{T}(n,p) \setminus \mathcal{S}(n,p)$ and take a diametrical path in T with end vertices x_{d} and y_{d}. Let $c \in \mathcal{V}_{C(T)}$ and $uv \in \mathcal{E}_T$ satisfying:

(c_1) $\deg_T(u) \geq 3$.

(c_2) $u \neq c$.

(c_3) u lies on c, v-path.

(c_4) v does not lie on $x_{\mathrm{d}}, y_{\mathrm{d}}$-path.

Our purpose is to construct a new tree $T' \in \mathcal{T}(n,p)$ from any given tree $T \in \mathcal{T}(n,p)$ by removing an edge $uv \in \mathcal{E}_T$ and attaching v to a central vertex c of T. The condition (c_1) ensures that new tree T' has p pendent vertices. The condition (c_2) guarantees that degree of c increases in T'. The condition (c_3) ensures that T' remains a tree and condition (c_4) ensures that $x_{\mathrm{d}}, y_{\mathrm{d}}$-path is also diametrical in T'.

We notice that if $T \in \mathcal{S}(n,p)$ with a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path then there is no $uv \in \mathcal{E}_T$ satisfying $(c_1) - (c_4)$. The following result will be useful in the sequel.

Lemma 7.1. [36] *Let T be an n-vertex tree and take a diametrical u, v-path in T. Then* *for any* $x \in \mathcal{V}_T$*, either* $ec_T(x) = d_T(x,u)$ *or* $ec_T(x) = d_T(x,v)$*.*

In next lemma, we construct a tree in $\mathcal{T}(n,p)$ from any given tree in $\mathcal{T}(n,p)$ such that the new tree has equal or smaller total eccentricity index.

Lemma 7.2. *Let* $T \in \mathcal{T}(n,p)$ *and* $c \in \mathcal{V}_{C(T)}$*. Take a diametrical* $x_{\mathrm{d}}, y_{\mathrm{d}}$*-path and* $uv \in \mathcal{E}_T$ *satisfying* $(c_1) - (c_4)$*. Construct a new tree* $T' = \{T - \{uv\}\} \cup \{cv\}$*. Then* $T' \in \mathcal{T}(n,p)$ *and* $\tau(T') \leq \tau(T)$*.*

Proof. Let P be the diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path in T. By (c_1) and (c_3), we see that

$$d_T(c,v) = d_T(c,u) + d_T(u,v).$$

Note that $d_T(u,v) = 1$ and by (c_2), we have $d_T(c,u) \geq 1$. Thus

$$d_T(c,v) \geq 2. \tag{7.1}$$

Let H be the component of $T - u$ containing the vertex v and $y \in \mathcal{V}_H$. Then

$$d_T(c,y) = d_T(c,v) + d_T(v,y).$$

This along with (7.1) gives

$$d_T(c,y) \geq 2 + d_T(v,y). \tag{7.2}$$

Also

$$d_{T'}(c,y) = d_{T'}(c,v) + d_{T'}(v,y).$$

By construction of T', we have $d_{T'}(c,v) = 1$ and $d_{T'}(v,y) = d_T(v,y)$. Thus by (7.2), we obtain

$$d_{T'}(c,y) < d_T(c,y). \tag{7.3}$$

By (c_4), the vertex v does not lie on P, so P is also contained in T'. Moreover, by the construction of T', $d_{T'}(c,x) = d_T(c,x)$ for all $x \in \mathcal{V}_T \setminus \mathcal{V}_H$. This along with (7.3) implies that P is a diametrical path in T'. Thus for each $x \in \mathcal{V}_T \setminus \mathcal{V}_H$, we have

$$ec_T(x) = ec_{T'}(x). \tag{7.4}$$

As $y \in \mathcal{V}_H$ and P is a diametrical path in T', either $ec_{T'}(y) = d_{T'}(y, x_{\text{d}})$ or $ec_{T'}(y) = d_{T'}(y, y_{\text{d}})$ by Lemma 7.1. Without loss of generality, suppose that $ec_{T'}(y) = d_{T'}(y, x_{\text{d}})$. But $d_{T'}(y, x_{\text{d}}) = d_{T'}(y, c) + d_{T'}(c, x_{\text{d}})$. This gives

$$ec_{T'}(c) = d_{T'}(c, x_{\text{d}}) \leq d_{T'}(c, y_{\text{d}}) + 1.$$

But $d_{T'}(c, x_{\text{d}}) = d_T(c, x_{\text{d}})$ and $d_{T'}(c, y_{\text{d}}) = d_T(c, y_{\text{d}})$. Then the above inequality can be written as

$$ec_{T'}(c) = d_T(c, x_{\text{d}}) \leq d_T(c, y_{\text{d}}) + 1. \tag{7.5}$$

Thus by (7.3), we obtain

$$\begin{aligned} ec_{T'}(y) &= d_{T'}(y, c) + d_{T'}(c, x_{\text{d}}) \\ &< d_T(y, c) + d_T(c, x_{\text{d}}). \end{aligned} \tag{7.6}$$

By Lemma 7.1, either $ec_T(y) = d_T(y, x_{\text{d}})$ or $ec_T(y) = d_T(y, y_{\text{d}})$. Let $ec_T(y) = d_T(y, x_{\text{d}})$. But $d_T(y, x_{\text{d}}) = d_T(y, c) + d_T(c, x_{\text{d}})$. Then (7.6) implies that

$$ec_{T'}(y) < ec_T(y). \tag{7.7}$$

If $ec_T(y) = d_T(y, y_{\text{d}})$, then (7.5) and (7.6) give

$$\begin{aligned} ec_{T'}(y) &< d_T(y, c) + d_T(c, x_{\text{d}}) \\ &\leq d_T(y, c) + d_T(c, y_{\text{d}}) + 1 \\ &= ec_T(y) + 1. \end{aligned}$$

That is

$$ec_{T'}(y) \leq ec_T(y). \tag{7.8}$$

By (7.4), (7.7) and (7.8), we obtain

$$\begin{aligned} \tau(T) &= \sum_{z \in \mathcal{V}_T \setminus \mathcal{V}_H} ec_T(z) + \sum_{z \in \mathcal{V}_H} ec_T(z) \\ &> \sum_{z \in \mathcal{V}_T \setminus \mathcal{V}_H} ec_{T'}(z) + \sum_{z \in \mathcal{V}_H} ec_{T'}(z) \\ &= \sum_{z \in \mathcal{V}_{T'}} ec_{T'}(z) \\ &= \tau(T'). \end{aligned}$$

As given that $\deg_T(u) \geq 3$, we have $\deg_{T'}(u) \geq 2$. Also $\deg_{T'}(c) = \deg_T(c) + 1$ and $\deg_{T'}(x) = \deg_T(x)$ for all $x \in \mathcal{V}_T \setminus \{u, c\}$. Therefore, T' is also a tree with p number of pendent vertices. The proof is complete. $\square$

Now we device an algorithm to convert any given tree in $\mathcal{T}(n,p)$ into a starlike tree in $\mathcal{S}(n,p)$.

Algorithm A

Step 0: Take a tree $T \in \mathcal{T}(n,p) \setminus \mathcal{S}(n,p)$, find a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path in T, $c \in \mathcal{V}_{C(T)}$ and $uv \in \mathcal{E}_T$ satisfying $(c_1) - (c_4)$.

Step 1: If $\deg_T(c) = p$ then stop.

Step 2: Set $T := \{T - \{uv\}\} \cup \{cv\}$. Find $uv \in \mathcal{E}_T$ satisfying $(c_1) - (c_4)$; go to Step 1.

In next theorem, we discuss the termination and correctness of Algorithm A.

Theorem 7.3. (Termination and Correctness) *The Algorithm A terminates after a finite number of iterations and outputs a tree in $\mathcal{S}(n,p)$.*

Proof. In each iteration of the Algorithm A, the degree of the vertex c increases strictly at Step 2. The Algorithm A stops at Step 1 when $\deg_T(c) = p$. Since p is finite, the Algorithm A terminates after a finite number of iterations.

By Lemma 7.2, we see that before and after modification of T at Step 2 of Algorithm A, the number of pendent vertices of the tree T remain the same. Also, corresponding to each edge cx incident on c, there is at least one pendent vertex reachable from c by a path containing the edge cx. When Algorithm A stops at Step 1, we have $\deg_T(c) = p$. This implies that corresponding to each edge cx incident on c, there is exactly one pendent vertex reachable from c by a path containing the edge cx, that is, $T \in \mathcal{S}(n,p)$. $\square$

Theorem 7.4. *Corresponding to a tree T in $\mathcal{T}(n,p) \setminus \mathcal{S}(n,p)$, there exists a tree T_1 in $\mathcal{S}(n,p)$ with $\tau(T) > \tau(T_1)$.*

Proof. Let $T \in \mathcal{T}(n,p) \setminus \mathcal{S}(n,p)$. By Theorem 7.3, we see that Algorithm A outputs a tree $T_1 \in \mathcal{S}(n,p)$ corresponding to the tree T. Lemma 7.2 guaranties that $\tau(T) > \tau(T_1)$. $\square$

In next lemma, we construct a tree in $\widetilde{\mathcal{S}}(n,p)$ from a given tree in $\mathcal{S}(n,p)$ such that the new tree has smaller total eccentricity index.

Lemma 7.5. *Let $T \in \mathcal{S}(n,p)$, $x_{\mathrm{d}}, v \in P_T$ and $c \in \mathcal{V}_T$ satisfying:*

$$\deg_T(c) = p, \tag{7.9}$$

$$d_T(x_{\mathrm{d}}, c) = \max\{d_T(x,c) \mid \; x \in P_T\}, \tag{7.10}$$

$$d_T(v, c) = \min\{d_T(x,c) \mid \; x \in P_T\}, \tag{7.11}$$

$$d_T(x_{\mathrm{d}}, c) - d_T(v,c) \geq 2. \tag{7.12}$$

Take $x_{\mathrm{d}-1}x_{\mathrm{d}} \in \mathcal{E}_T$ and construct a new tree T' obtained from T as $T' = \{T - \{x_{\mathrm{d}-1}x_{\mathrm{d}}\}\} \cup \{vx_{\mathrm{d}}\}$. Then $T' \in \widetilde{\mathcal{S}}(n,p)$ and $\tau(T) > \tau(T')$.

Proof. Let Q be the x_{d}, v-path in T. By construction, we note that $T' \in \mathcal{S}(n,p)$ and $\mathcal{V}_T = \mathcal{V}_{T'}$. Consider the next two cases:

Case 1. If $d_T(x_{\mathrm{d}}, v) = \mathrm{d}_T$ then $x_{\mathrm{d}-1}, x_{\mathrm{d}}$-path is diametrical in T' and

$$\sum_{x \in \mathcal{V}_Q} ec_T(x) = \sum_{x \in \mathcal{V}_Q} ec_{T'}(x). \tag{7.13}$$

Let $x \in \mathcal{V}_T \setminus \mathcal{V}_Q$. Then $ec_T(x) = d_T(x, x_{\mathrm{d}})$. By Lemma 7.1, either $ec_{T'}(x) = d_{T'}(x, x_{\mathrm{d}-1})$ or $ec_{T'}(x) = d_{T'}(x, x_{\mathrm{d}})$. Also, by (7.12), we obtain $d_T(x_{\mathrm{d}}, c) - 1 \geq d_T(v,c) + 1$. Thus, by the construction of T', we obtain

$$\begin{aligned}
d_{T'}(x, x_{\mathrm{d}}) &= d_{T'}(x,c) + d_{T'}(c, x_{\mathrm{d}}) \\
&= d_{T'}(x,c) + d_{T'}(c,v) + 1 \\
&= d_{T'}(x,c) + d_T(c,v) + 1 \\
&\leq d_{T'}(x,c) + d_T(x_{\mathrm{d}}, c) - 1 \\
&= d_{T'}(x,c) + d_T(c, x_{\mathrm{d}-1}) \\
&= d_{T'}(x,c) + d_{T'}(c, x_{\mathrm{d}-1}) \\
&= d_{T'}(x, x_{\mathrm{d}-1}).
\end{aligned}$$

This shows that $ec_{T'}(x) = d_{T'}(x, x_{\mathrm{d}-1})$. Therefore

$$\begin{aligned} ec_T(x) &= d_T(x, x_{\mathrm{d}}) \\ &= d_{T'}(x, x_{\mathrm{d}-1}) + 1 \\ &= ec_{T'}(x) + 1. \end{aligned} \tag{7.14}$$

Thus from (7.13) and (7.14), we obtain

$$\begin{aligned} \tau(T) &= \sum_{z \in \mathcal{V}_Q} ec_T(z) + \sum_{z \in \mathcal{V}_T \setminus \mathcal{V}_Q} ec_T(z) \\ &= \sum_{z \in \mathcal{V}_Q} ec_{T'}(z) + \sum_{z \in \mathcal{V}_T \setminus \mathcal{V}_Q} (ec_{T'}(z) + 1) \\ &> \sum_{z \in \mathcal{V}_Q} ec_{T'}(z) + \sum_{z \in \mathcal{V}_T \setminus \mathcal{V}_Q} ec_{T'}(z) \\ &= \tau(T'). \end{aligned}$$

Case 2. When $d_T(x_{\mathrm{d}}, v) < \mathrm{d}_T$. Let $y_{\mathrm{d}} \in P_T$ such that $x_{\mathrm{d}}, y_{\mathrm{d}}$-path is diametrical in T. Then by Lemma 7.1, either $ec_T(x) = d_T(x, x_{\mathrm{d}})$ or $ec_T(x) = d_T(x, y_{\mathrm{d}})$ for each $x \in \mathcal{V}_T$. Define

$$\widetilde{V} = \{x \in \mathcal{V}_T \mid ec_T(x) = d_T(x, y) \text{ for some } y \in P_T \setminus \{x_{\mathrm{d}}\}\}.$$

Let $z \in \widetilde{V} \setminus \{x_{\mathrm{d}}\}$. Then there exists $y' \in P_T \setminus \{x_{\mathrm{d}}\}$ such that

$$ec_T(z) = d_T(z, y') \geq d_T(z, y) \tag{7.15}$$

for all $y \in P_T$. Given that $\mathrm{d}_T > d_T(x_{\mathrm{d}}, v)$. This along with Lemma 7.1 implies that v is not an eccentric vertex of any vertex of T. Thus

$$ec_T(z) = d_T(z, y') > d_T(z, v). \tag{7.16}$$

By the construction of T', we have $d_{T'}(z, y') = d_T(z, y')$, $d_{T'}(z, x_{\mathrm{d}}) = d_T(z, v) + 1$ and $d_{T'}(z, x_{\mathrm{d}-1}) = d_T(z, x_{\mathrm{d}-1})$. From (7.16), we obtain

$$\begin{aligned} d_{T'}(z, y') = d_T(z, y') &\geq d_T(z, v) + 1 \\ &\geq d_{T'}(z, x_{\mathrm{d}}). \end{aligned} \tag{7.17}$$

From (7.15), it is obvious to see that

$$\begin{aligned} d_{T'}(z, y') = d_T(z, y') &\geq d_T(z, x_{\mathrm{d}}) \\ &> d_T(z, x_{\mathrm{d}-1}) = d_{T'}(z, x_{\mathrm{d}-1}). \end{aligned} \tag{7.18}$$

From (7.15), (7.17) and (7.18), we get $d_{T'}(z, y') \geq d_{T'}(z, y)$ for all $y \in P_{T'}$. Thus

$$ec_{T'}(z) = d_{T'}(z, y') = d_T(z, y') = ec_T(z). \tag{7.19}$$

Now let $z \in \mathcal{V}_T \setminus \widetilde{V}$. Since $\mathrm{d}_T > d_T(x_{\mathrm{d}}, v)$, it holds that $d_T(c, y_{\mathrm{d}}) \geq d_T(c, v) + 1$. Also by definition of $\widetilde{V}$, we obtain $d_T(z, x_{\mathrm{d}}) > d_T(z, y_{\mathrm{d}})$. Now if z lies on c, x_{d}-path in T then

$$\begin{aligned} d_T(z, x_{\mathrm{d}-1}) + 1 &= d_T(z, x_{\mathrm{d}}) \\ &> d_T(z, y_{\mathrm{d}}) \\ &= d_T(z, c) + d_T(c, y_{\mathrm{d}}) \\ &\geq d_T(z, c) + d_T(c, v) + 1 \\ &= d_T(z, v) + 1. \end{aligned}$$

That is,

$$d_T(z, x_{\mathrm{d}-1}) \geq d_T(z, v) + 1. \tag{7.20}$$

If z does not lie on c, x_{d}-path in T then $d_T(z, c) + d_T(c, v) \geq d_T(z, v)$. Also (7.12) gives $d_T(c, x_{\mathrm{d}}) \geq d_T(c, v) + 2$. Therefore

$$\begin{aligned} d_T(z, x_{\mathrm{d}-1}) + 1 &= d_T(z, x_{\mathrm{d}}) \\ &= d_T(z, c) + d_T(c, x_{\mathrm{d}}) \\ &\geq d_T(z, c) + d_T(c, v) + 2 \\ &\geq d_T(z, v) + 2. \end{aligned}$$

That is,

$$d_T(z, x_{\mathrm{d}-1}) \geq d_T(z, v) + 1. \tag{7.21}$$

But by the construction of T', we have $d_{T'}(z, x_{\mathrm{d}-1}) = d_T(z, x_{\mathrm{d}-1})$ and $d_{T'}(z, x_{\mathrm{d}}) = d_T(z, v) + 1$. Thus from (7.20) and (7.21), we have

$$d_{T'}(z, x_{\mathrm{d}-1}) \geq d_{T'}(z, x_{\mathrm{d}}). \tag{7.22}$$

Also as $z \in \mathcal{V}_T \setminus \widetilde{V}$, we have $d_T(z, x_{\rm d}) > d_T(z, y)$ for all $y \in P_T \setminus \{x_{\rm d}\}$. Thus

$$d_T(z, x_{\rm d-1}) = d_T(z, x_{\rm d}) - 1 \geq d_T(z, y)$$

for all $y \in P_T \setminus \{x_{\rm d}\}$. But $d_{T'}(z, x_{\rm d-1}) = d_T(z, x_{\rm d-1})$ and $d_T(z, y) = d_{T'}(z, y)$ for all $y \in P_T \setminus \{x_{\rm d}\}$. Therefore

$$d_{T'}(z, x_{\rm d-1}) \geq d_{T'}(z, y) \tag{7.23}$$

for all $y \in P_T \setminus \{x_{\rm d}\}$. From (7.22) and (7.23), we obtain $d_{T'}(z, x_{\rm d-1}) \geq d_{T'}(z, y)$ for all $y \in P_{T'}$. Thus

$$\begin{aligned} ec_{T'}(z) &= d_{T'}(z, x_{\rm d-1}) \\ &< d_{T'}(z, x_{\rm d-1}) + 1 \\ &= d_T(z, x_{\rm d}) = ec_T(z). \end{aligned} \tag{7.24}$$

Now if $v \in \widetilde{V}$ then (7.19) gives $ec_{T'}(v) = ec_T(v)$. Also, by (7.12), we get

$$\begin{aligned} ec_T(v) = d_T(v, y_{\rm d}) &= d_T(v, c) + d_T(c, y_{\rm d}) \\ &\leq d_T(x_{\rm d}, c) + d_T(c, y_{\rm d}) - 2 \\ &= d_T(x_{\rm d}, y_{\rm d}) - 2 \\ &= ec_T(x_{\rm d}) - 2, \end{aligned} \tag{7.25}$$

By construction of T', we have $ec_{T'}(x_{\rm d}) = ec_{T'}(v) + 1$. This together (7.25) implies

$$ec_{T'}(x_{\rm d}) = ec_T(v) + 1 \leq ec_T(x_{\rm d}) - 1 < ec_T(x_{\rm d}). \tag{7.26}$$

Now let $v \in \mathcal{V}_T \setminus \widetilde{V}$. Then obviously v does not lie on $c, x_{\rm d}$-path. Thus by (7.23), we have $d_{T'}(v, x_{\rm d-1}) \geq d_{T'}(v, y)$ for all $y \in P_{T'}$. Also, since $d_T(x_{\rm d}, v) < {\rm d}_T$, it holds that

$$ec_T(v) < ec_T(x_{\rm d}). \tag{7.27}$$

Thus $ec_{T'}(v) = d_{T'}(v, x_{\rm d-1})$. By construction of T', we have $ec_{T'}(x_{\rm d}) = ec_{T'}(v) + 1$ and $d_{T'}(v, x_{\rm d-1}) = d_T(v, x_{\rm d-1})$, that is, $ec_{T'}(x_{\rm d}) = d_T(v, x_{\rm d-1}) + 1$. Therefore using (7.27) we get

$$\begin{aligned} ec_{T'}(x_{\rm d}) &= d_T(v, x_{\rm d-1}) + 1 = d_T(v, x_{\rm d}) \\ &= ec_T(v) < ec_T(x_{\rm d}). \end{aligned} \tag{7.28}$$

From (7.19), (7.25), (7.26) and (7.28), we obtain

$$\begin{aligned}\tau(T) &= \sum_{z\in\widetilde{V}\setminus\{x_{\rm d}\}} ec_T(z) + \sum_{z\in\mathcal{V}_T\setminus\widetilde{V}} ec_T(z) + ec_T(x_{\rm d}) \\ &> \sum_{z\in\widetilde{V}\setminus\{x_{\rm d}\}} ec_{T'}(z) + \sum_{z\in\mathcal{V}_T\setminus\widetilde{V}} ec_{T'}(z) + ec_{T'}(x_{\rm d}) \\ &= \sum_{z\in\mathcal{V}_{T'}} ec_{T'}(z) \\ &= \tau(T').\end{aligned}$$

The proof is complete. □

We device an algorithm to construct a tree in $\widetilde{\mathcal{S}}(n,p)$ from a given tree in $\mathcal{S}(n,p)$.

Algorithm B

Step 0: Take a tree $T \in \mathcal{S}(n,p) \setminus \widetilde{\mathcal{S}}(n,p)$, find set of pendent vertices P_T and fix a vertex $c \in \mathcal{V}_T$ with $\deg_T(c) = \triangle_T$. Find $x_{\rm d}, v \in P_T$ satisfying (7.10) and (7.11).

Step 1: If $|d_T(c, x_{\rm d}) - d_T(c, v)| \leq 1$ then stop.

Step 2: Take $x_{{\rm d}-1}x_{\rm d} \in \mathcal{E}_T$ and set $T := \{T - \{x_{{\rm d}-1}x_{\rm d}\}\} \cup \{vx_{\rm d}\}$. Find the set of pendent vertices P_T and $x_{\rm d}, v \in P_T$ satisfying (7.10) and (7.11) for the modified T. Go to Step 1.

Next, we discuss the termination and correctness of Algorithm B.

Theorem 7.6. (Termination and Correctness) *The Algorithm B terminates after a finite number of iterations and outputs a tree in* $\widetilde{\mathcal{S}}(n,p)$.

Proof. Let T be a tree in $\mathcal{S}(n,p)$, $x_{\rm d}, v \in P_T$, $c \in \mathcal{V}_T$ satisfying (7.10) and (7.11), and $x_{{\rm d}-1} \in \Gamma_T(x_{\rm d})$ before the execution of Step 2 and T' be the modified tree at Step 2 in any iteration of the Algorithm B. Then $x_{{\rm d}-1}, x_{\rm d} \in P_{T'}$ and

$$\begin{aligned}d_{T'}(c, x_{{\rm d}-1}) - d_{T'}(c, x_{\rm d}) &= d_T(c, x_{\rm d}) - 1 - (d_T(c, v) + 1) \\ &= d_T(c, x_{\rm d}) - d_T(c, v) - 2.\end{aligned} \tag{7.29}$$

This shows that the difference between distances of two pendent vertices of T' from the vertex c strictly decreases. Also, as $d_T(c, x_{\mathrm{d}}) - d_T(c, v) \geq 2$, we have

$$\begin{aligned} d_{T'}(c, x_{\mathrm{d}-1}) &= d_T(c, x_{\mathrm{d}}) - 1 \\ &\geq d_T(c, v) + 1 \\ &= d_{T'}(c, x_{\mathrm{d}}). \end{aligned}$$

This shows that x_{d} satisfies (7.10) for T' if and only if $d_{T'}(c, x_{\mathrm{d}-1}) = d_{T'}(c, x_{\mathrm{d}})$. But if $d_{T'}(c, x_{\mathrm{d}-1}) = d_{T'}(c, x_{\mathrm{d}})$ then the Algorithm B will stop at Step 1 in the next iteration. This shows that the newly added edge vx_{d} will not be removed in the subsequent iterations. Thus once an edge is added at Step 2, it will not be removed in the subsequent iterations. This along with (7.29) ensures that the Algorithm B stops after a finite number of iterations.

By Lemma 7.5, it is evident that the modified tree T at Step 2 belongs to $\mathcal{S}(n, p)$ in each iteration of the Algorithm B. When the Algorithm B terminates, T satisfies $|d_T(c, x_{\mathrm{d}}) - d_T(c, v)| \leq 1$ and thus belongs to $\widetilde{\mathcal{S}}(n, p)$. □

Theorem 7.7. *Corresponding to a tree T in $\mathcal{S}(n, p) \setminus \widetilde{\mathcal{S}}(n, p)$, there exists a tree S in $\widetilde{\mathcal{S}}(n, p)$ with $\tau(T) > \tau(S)$.*

Proof. Let $T \in \mathcal{S}(n, p) \setminus \widetilde{\mathcal{S}}(n, p)$. By Theorem 7.6, the Algorithm B outputs a tree $S \in \widetilde{\mathcal{S}}(n, p)$. Lemma 7.5 implies that $\tau(T) > \tau(S)$. □

Remark 7.8. Let $S_1, S_2 \in \widetilde{\mathcal{S}}(n, p)$. Then from the structure of S_1 and S_2, one can easily see that $\tau(S_1) = \tau(S_2)$.

We finally state our main result of this section. We compute the tree with smallest total eccentricity indices among the trees in $\mathcal{T}(n, p)$ by using Theorems 7.4 and 7.7.

Theorem 7.9. *Any tree in $\widetilde{\mathcal{S}}(n, p)$ has smallest total eccentricity index among the trees in $\mathcal{T}(n, p)$. That is, for any $S \in \widetilde{\mathcal{S}}(n, p)$, we have $\tau(S) \leq \tau(T)$ for all $T \in \mathcal{T}(n, p)$.*

Proof. Let $T \in \mathcal{T}(n,p) \setminus \mathcal{S}(n,p)$. Then by Theorem 7.4, there is a tree $T' \in \mathcal{S}(n,p)$ with $\tau(T) > \tau(T')$. Now if $T' \notin \widetilde{\mathcal{S}}(n,p)$ then by Theorem 7.7, there exists a tree S in $\widetilde{\mathcal{S}}(n,p)$ such that $\tau(T') > \tau(S)$. If $T' \in \widetilde{\mathcal{S}}(n,p)$ then by Remark 7.8, $\tau(T') = \tau(S)$. Therefore $\tau(T) \geq \tau(S)$. □

By Lemma 7.2, we note that when Step 2 to Step 1 is executed in Algorithm A, the total eccentricity index of the modified tree strictly decreases. Thus for a given tree $T \in \mathcal{T}(n,p) \setminus \mathcal{S}(n,p)$, if Algorithm A terminates after l iterations, it generates a sequence of trees $T, T_1, T_2, \ldots, T_l$ satisfying $\tau(T) > \tau(T_1) > \tau(T_2) > \cdots > \tau(T_l)$, where $T_l \in \mathcal{S}(n,p)$.

By Lemma 7.5, we see that when Algorithm B goes from Step 2 to Step 1, the total eccentricity index of the modified tree strictly decreases. Thus the Algorithm B generates a sequence of trees $T_l, T_{l+1}, \ldots, T_k$ satisfying $\tau(T_l) > \tau(T_{l+1}) > \cdots > \tau(T_k)$, where $T_k \in \widetilde{\mathcal{S}}(n,p)$.

Example 7.10. Consider a tree $T \in \mathcal{T}(14,6)$ shown in Figure 7.1. The Algorithm A will generate a sequence of trees T, T_1, T_2, T_3, T_4, where $T_4 \in \mathcal{S}(14,6)$ satisfying the following:

$$\tau(T) > \tau(T_1) > \tau(T_2) > \tau(T_3) > \tau(T_4).$$

This sequence of trees is shown in Figure 7.1. We observe that the sequence of trees is not unique because the modification of any tree at Step 2 in Algorithm A depends upon the choice of edge uv.

Now we apply Algorithm B on T_4 to get a tree in $\widetilde{\mathcal{S}}(14,6)$. By the use of Algorithm B we get a sequence of trees T_4, T_5, T_6, T_7, where $T_7 \in \widetilde{\mathcal{S}}(14,6)$. This sequence of trees is shown in Figure 7.2. We remark that this sequence of trees is not unique. The sequence of modified trees at Step 2 in Algorithm B depends upon the choice of edge $x_{\mathrm{d}-1}x_{\mathrm{d}}$ and vertex v. The relation among the total eccentricity indices of T_4, T_5, T_6, T_7 is as follows:

$$\tau(T_4) > \tau(T_5) > \tau(T_6) > \tau(T_7).$$

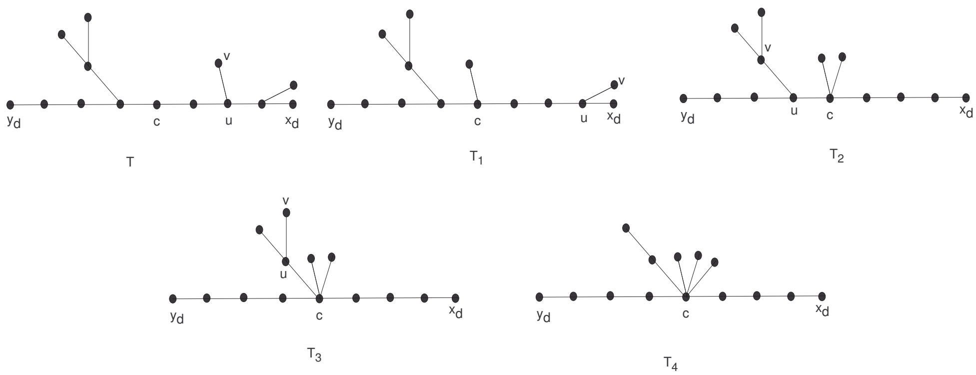

Figure 7.1: A sequence of trees generated by Algorithm A in each iteration.

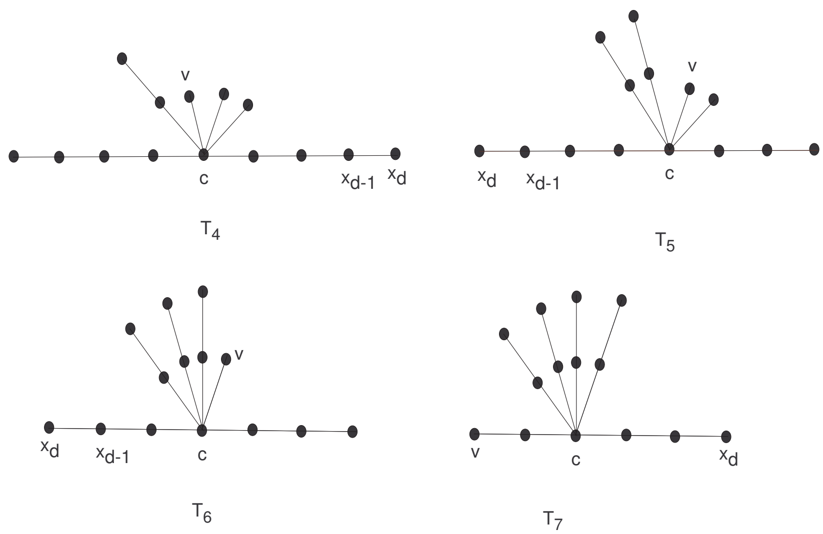

Figure 7.2: A sequence of trees generated by Algorithm B in each iteration.

7.2 Largest total eccentricity index of trees with fixed pendent vertices

Take a tree $T \in \mathcal{T}(n, p)$ with a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path and let $x_{\mathrm{d}-1}$ and $y_{\mathrm{d}-1}$ be neighbors of x_{d} and y_{d}, respectively, in T. Assume that T satisfies the following:

(m_1) $\mathrm{d}_T = n - p + 1$.

(m_2) $\deg_T(y_{\mathrm{d}-1}) + \deg_T(x_{\mathrm{d}-1}) = p + 2$.

A tree $T \in \mathcal{T}(14, 6)$ satisfying (m_1) and (m_2) is shown in Figure 7.3. Denote by

$\widetilde{\mathcal{T}}(n,p)$, the family of those trees in $\mathcal{T}(n,p)$ that satisfy (m_1) and (m_2).

Remark 7.11. Let $T_1, T_2 \in \widetilde{\mathcal{T}}(n,p)$. Then from the structure of T_1 and T_2, one can easily see that $\tau(T_1) = \tau(T_2)$.

In this section, we find those trees in $\mathcal{T}(n,p)$ which have larger total eccentricity index. We will prove that if T is a tree in $\mathcal{T}(n,p) \setminus \widetilde{\mathcal{T}}(n,p)$ and $\widetilde{T} \in \widetilde{\mathcal{T}}(n,p)$ then $\tau(T) < \tau(\widetilde{T})$.

Let $T \in \mathcal{T}(n,p) \setminus \widetilde{\mathcal{T}}(n,p)$ and take a diametrical path in T with end vertices x_{d} and y_{d}. Let $x_{\mathrm{d}-1} \in \Gamma_T(x_{\mathrm{d}})$, $y_{\mathrm{d}-1} \in \Gamma_T(y_{\mathrm{d}})$ and $uv \in \mathcal{E}_T$ satisfying:

(d_1) $\deg_T(u) \geq 3$.

(d_2) u lies on $x_{\mathrm{d}}, y_{\mathrm{d}}$-path.

(d_3) v does not lie on $x_{\mathrm{d}}, y_{\mathrm{d}}$-path.

(d_4) $u \neq x_{\mathrm{d}-1}$ and $u \neq y_{\mathrm{d}-1}$.

Observe that if $T \in \widetilde{\mathcal{T}}(n,p)$ with a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path then there is no $uv \in \mathcal{E}_T$ satisfying $(d_1) - (d_4)$. In next result, we construct a new tree in $\mathcal{T}(n,p)$ from a given tree in $\mathcal{T}(n,p)$ with larger total eccentricity index.

Lemma 7.12. *Let $T \in \mathcal{T}(n,p) \setminus \widetilde{\mathcal{T}}(n,p)$. Take a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path and $uv \in \mathcal{E}_T$ satisfying $(d_1) - (d_4)$. Construct a new tree $T' = \{T - \{uv\}\} \cup \{y_{\mathrm{d}-1}v\}$. Then $T' \in \mathcal{T}(n,p)$ and $\tau(T') > \tau(T)$.*

Proof. Let Q be the diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path in T. By (d_1) and (d_3), we have

$$d_T(v, x_{\mathrm{d}}) = d_T(v, u) + d_T(u, x_{\mathrm{d}}),$$

$$d_T(v, y_{\mathrm{d}}) = d_T(v, u) + d_T(u, y_{\mathrm{d}}).$$

Note that $d_T(u,v) = 1$ and by (d_2) and (d_4), we see that

$$d_T(u, x_d) \geq 2, \quad d_T(u, y_d) \geq 2. \tag{7.30}$$

By (d_4), it holds that $d_T(y_{\mathrm{d}-1}, u) \geq 1$ and $d_{T'}(y_{\mathrm{d}-1}, u) = d_T(y_{\mathrm{d}-1}, u)$ by the construction of T'. Thus

$$\begin{aligned} d_{T'}(v,u) &= d_{T'}(v,y_{\mathrm{d}-1}) + d_{T'}(y_{\mathrm{d}-1},u) \\ &= 1 + d_T(y_{\mathrm{d}-1},u) \\ &\geq 2. \end{aligned} \tag{7.31}$$

Let H be the component of $T-u$ containing the vertex v. Define $R = \{z \in \mathcal{V}_T \mid ec_T(z) = d_T(z, y_{\mathrm{d}})\}$ and take $w \in \mathcal{V}_H$ with $ec_H(v) = d_H(v,w)$. By the choice of w, we have $\mathrm{d}_{T'} = d_{T'}(x_{\mathrm{d}}, w)$ and thus

$$\begin{aligned} \mathrm{d}_{T'} &= d_{T'}(x_{\mathrm{d}},y_{\mathrm{d}-1}) + d_{T'}(y_{\mathrm{d}-1},v) + d_{T'}(v,w) \\ &= d_T(x_{\mathrm{d}},y_{\mathrm{d}-1}) + 1 + d_T(v,w) \\ &\geq d_T(x_{\mathrm{d}},y_{\mathrm{d}}) = \mathrm{d}_T. \end{aligned}$$

Let $x \in \mathcal{V}_T \setminus (\mathcal{V}_H \cup R)$. Then $ec_T(x) = d_T(x, x_{\mathrm{d}})$. By Lemma 7.1, either $ec_{T'}(x) = d_{T'}(x, x_{\mathrm{d}})$ or $ec_{T'}(x) = d_{T'}(x,w)$. If $ec_{T'}(x) = d_{T'}(x, x_{\mathrm{d}})$ then

$$ec_{T'}(x) = d_{T'}(x,x_{\mathrm{d}}) = d_T(x,x_{\mathrm{d}}) = ec_T(x). \tag{7.32}$$

Now if $ec_{T'}(x) = d_{T'}(x,w)$ then obviously $d_{T'}(x,w) \geq d_{T'}(x,x_{\mathrm{d}})$. Thus

$$\begin{aligned} ec_{T'}(x) &\geq d_{T'}(x,x_d) \\ &= d_T(x,x_d) \\ &= ec_T(x). \end{aligned} \tag{7.33}$$

From (7.32) and (7.33), we have

$$ec_{T'}(x) \geq ec_T(x). \tag{7.34}$$

Now let $x \in R \setminus \mathcal{V}_H$. Then $ec_T(x) = d_T(x, y_{\mathrm{d}-1}) + 1$ and $ec_{T'}(x) = d_{T'}(x,w)$ by the construction of T'. Thus

$$\begin{aligned} ec_{T'}(x) = d_{T'}(x,w) &= d_{T'}(x,y_{\mathrm{d}-1}) + d_{T'}(y_{\mathrm{d}-1},v) + d_{T'}(v,w) \\ &= d_T(x,y_{\mathrm{d}-1}) + 1 + d_T(v,w) \\ &= ec_T(x) + d_T(v,w) \\ &\geq ec_T(x). \end{aligned} \tag{7.35}$$

Finally, let $x \in \mathcal{V}_H$. It is evident that $ec_T(x) = d_T(x,u) + ec_T(u)$ and from (7.31) we have $d_{T'}(v,u) \geq 2$. If $x \in \mathcal{V}_H \setminus R$ then $ec_T(u) = d_T(u, x_{\mathrm{d}})$. Also

$$\begin{aligned} ec_{T'}(x) &= d_{T'}(x, x_{\mathrm{d}}) \\ &= d_{T'}(x,v) + d_{T'}(v,u) + d_{T'}(u, x_{\mathrm{d}}) \\ &= d_T(x,v) + d_{T'}(v,u) + d_T(u, x_{\mathrm{d}}) \\ &\geq d_T(x,v) + 2 + ec_T(u) \\ &= ec_T(x) + 1. \end{aligned} \tag{7.36}$$

Now if $x \in \mathcal{V}_H \cap R$ then $ec_T(u) = d_T(u, y_{\mathrm{d}}) = d_T(u, y_{\mathrm{d}-1}) + 1$. From (7.30), it holds that $d_T(u, x_{\mathrm{d}}) \geq 2$. Thus

$$\begin{aligned} ec_{T'}(x) &= d_{T'}(x, x_{\mathrm{d}}) \\ &= d_{T'}(x,v) + d_{T'}(v, y_{\mathrm{d}-1}) + d_{T'}(y_{\mathrm{d}-1}, u) + d_{T'}(u, x_{\mathrm{d}}) \\ &= d_T(x,v) + 1 + d_T(y_{\mathrm{d}-1}, u) + d_T(u, x_{\mathrm{d}}) \\ &\geq d_T(x,v) + ec_T(u) + 2 \\ &= ec_T(x) + 1. \end{aligned} \tag{7.37}$$

From (7.36) and (7.37), we obtain

$$ec_{T'}(x) \geq ec_T(x) + 1. \tag{7.38}$$

Thus from (7.34), (7.35) and (7.38), we obtain

$$\begin{aligned} \tau(T) &= \sum_{z \in \mathcal{V}_T \setminus (\mathcal{V}_H \cup R)} ec_T(z) + \sum_{z \in R \setminus \mathcal{V}_H} ec_T(z) + \sum_{z \in \mathcal{V}_H} ec_T(z) \\ &\leq \sum_{z \in \mathcal{V}_T \setminus (\mathcal{V}_H \cup R)} ec_{T'}(z) + \sum_{z \in R \setminus \mathcal{V}_H} ec_{T'}(z) + \sum_{z \in \mathcal{V}_H} (ec_{T'}(z) - 1) \\ &< \sum_{z \in \mathcal{V}_T \setminus (\mathcal{V}_H \cup R)} ec_{T'}(z) + \sum_{z \in R \setminus \mathcal{V}_H} ec_{T'}(z) + \sum_{z \in \mathcal{V}_H} ec_{T'}(z) \\ &= \tau(T'). \end{aligned}$$

The proof is complete. □

Algorithm C

Step 0: Take a tree $T \in \mathcal{T}(n,p) \setminus \widetilde{\mathcal{T}}(n,p)$, find a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path in T and $uv \in \mathcal{E}_T$ satisfying $(d_1)-(d_4)$. Let $\{x_{\mathrm{d}-1}\} = \Gamma_T(x_{\mathrm{d}})$ and $\{y_{\mathrm{d}-1}\} = \Gamma_T(y_{\mathrm{d}})$.

Step 1: If $\deg_T(y_{\mathrm{d}-1}) = p + 2 - \deg_T(x_{\mathrm{d}-1})$ then stop.

Step 2: Take the component H of $T - u$ containing the vertex v and let $w \in \mathcal{V}_H$ with $ec_H(v) = d_H(v,w)$. Modify T by $T := \{T - \{uv\}\} \cup \{y_{\mathrm{d}-1}v\}$.

Step 3: Set $\{y_{\mathrm{d}-1}\} := \Gamma_T(w)$ and $y_{\mathrm{d}} := w$. Find an edge $u'v' \in \mathcal{E}_T$ satisfying $(d_1)-(d_4)$ and set $u := u'$, $v := v'$; go to Step 1.

We device an algorithm to transform a given tree in $\mathcal{T}(n,p)$ into a tree in $\widetilde{\mathcal{T}}(n,p)$. The termination and correctness of Algorithm C is discussed below.

Theorem 7.13. (Termination and Correctness) *The Algorithm C terminates after a finite number of iterations and outputs a tree $\widetilde{T} \in \widetilde{\mathcal{T}}(n,p)$.*

Proof. Let T be a tree before modification at Step 2 and T' be the tree after modification at Step 2 in any iteration of the Algorithm C. There are two possible cases at Step 2.

Case 1. When $\mathcal{V}_H = \{v\}$. In this case, $v = w$ and hence $ec_H(v) = 0$ at Step 2. Therefore $\mathrm{d}_T = \mathrm{d}_{T'}$ and $\deg_{T'}(y_{\mathrm{d}-1}) = \deg_T(y_{\mathrm{d}-1}) + 1$ at Step 2. Moreover, $y_{\mathrm{d}-1}$ will remain same after modifications at Step 3.

Case 2. When $\mathcal{V}_H \neq \{v\}$. In this case, $ec_H(v) > 0$ and $\mathrm{d}_{T'} = \mathrm{d}_T + ec_H(v)$ at Step 2, that is, diameter of the modified tree strictly increases.

From Case 1 and Case 2, we observe that d_T increases or remains the same in any iteration of the Algorithm C. If Case 2 occurs in any iteration of the Algorithm C then diameter of the modified tree strictly increases. Since $\mathrm{d}_T \leq n-1$, the Case 2 will occur finite number of times. If Case 1 occurs then d_T remains the same but $\deg_T(y_{\mathrm{d}-1})$ increases. Since $\deg_T(y_{\mathrm{d}-1})$ can be increased in at most $n-3$ consecutive iterations of the Algorithm C, it follows that Case 1 will successively occur at most $n-3$ times.

From the above, we conclude that Algorithm C will stop after a finite number of iterations. □

Theorem 7.14. (Correctness) *If Algorithm C terminates then its outputs a tree $\widetilde{T} \in \widetilde{\mathcal{T}}(n,p)$.*

Proof. By Lemma 7.12, we note that before and after the modification at Step 2 in each iteration of Algorithm C, the tree T belongs to $\mathcal{T}(n,p)$ and diameter increases or remains same. When Algorithm C stops at Step 1, T satisfies $\deg_T(y_{\mathrm{d}-1}) = p + 2 - \deg_T(x_{\mathrm{d}-1})$. Also T has no edge uv satisfying $(d_1) - (d_4)$, that is, all pendent vertices are incident with $x_{\mathrm{d}-1}$ or $y_{\mathrm{d}-1}$. This shows that $T \in \widetilde{\mathcal{T}}(n,p)$. □

Theorem 7.15. *Corresponding to a tree T in $\mathcal{T}(n,p) \setminus \widetilde{\mathcal{T}}(n,p)$, there exists a tree $\widetilde{T}$ in $\widetilde{\mathcal{T}}(n,p)$ with $\tau(T) < \tau(\widetilde{T})$.*

Proof. Let $T \in \mathcal{T}(n,p) \setminus \widetilde{\mathcal{T}}(n,p)$. By Theorem 7.14, the Algorithm C outputs a tree $\widetilde{T} \in \widetilde{\mathcal{T}}(n,p)$. Thus by Lemma 7.12, we obtain $\tau(T) < \tau(\widetilde{T})$. □

In next theorem, we find the trees with largest total eccentricity index among the trees in $\mathcal{T}(n,p)$.

Theorem 7.16. *Any tree in $\widetilde{\mathcal{T}}(n,p)$ has largest total eccentricity index among all the trees in $\mathcal{T}(n,p)$. That is, for any $\widetilde{T} \in \widetilde{\mathcal{T}}(n,p)$, we have $\tau(\widetilde{T}) \geq \tau(T)$ for all $T \in \mathcal{T}(n,p)$.*

Proof. Let $T \in \mathcal{T}(n,p)$ and $\widetilde{T} \in \widetilde{\mathcal{T}}(n,p)$. If $T \in \widetilde{\mathcal{T}}(n,p)$ then by Remark 7.11, $\tau(T) = \tau(\widetilde{T})$. If $T \in \mathcal{T}(n,p) \setminus \widetilde{\mathcal{T}}(n,p)$ then by Theorem 7.15, there exists a tree $\widetilde{T}$ in $\widetilde{\mathcal{T}}(n,p)$ such that $\tau(T) < \tau(\widetilde{T})$. Therefore $\tau(T) \leq \tau(\widetilde{T})$. □

Corollary 7.17. *For any tree $T \in \mathcal{T}(n,p)$, we have*

$$\tau(T) \leq \begin{cases} \frac{3}{4}n^2 - \left(\frac{p-1}{2}\right)n - \left\lfloor \frac{(p-1)^2}{4} \right\rfloor & \text{if } n \text{ is even,} \\ \frac{3}{4}n^2 - \left(\frac{p-1}{2}\right)n - \frac{(p-1)^2-1}{4} & \text{if } n \text{ is odd and } p \text{ is even,} \\ \frac{3}{4}n^2 - \left(\frac{p-1}{2}\right)n - \frac{(p-1)^2}{4} & \text{if } n \text{ and } p \text{ are odd,} \end{cases}$$

equality holds when $T \in \widetilde{\mathcal{T}}(n,p)$.

Proof. Let $\widetilde{T} \in \widetilde{\mathcal{T}}(n,p)$. After simple computation, we obtain

$$\tau(\widetilde{T}) = \begin{cases} \frac{3}{4}n^2 - \left(\frac{p-1}{2}\right)n - \left\lfloor \frac{(p-1)^2}{4} \right\rfloor & \text{if } n \text{ is even,} \\ \frac{3}{4}n^2 - \left(\frac{p-1}{2}\right)n - \frac{(p-1)^2-1}{4} & \text{if } n \text{ is odd and } p \text{ is even,} \\ \frac{3}{4}n^2 - \left(\frac{p-1}{2}\right)n - \frac{(p-1)^2}{4} & \text{if } n \text{ and } p \text{ are odd,} \end{cases}$$

Now by Theorem 7.16, we have $\tau(T) \leq \tau(\widetilde{T})$ for all $T \in \mathcal{T}(n,p)$. □

By Lemma 7.12, we note that when Step 3 to Step 1 is executed in Algorithm C, the total eccentricity index of the modified tree strictly increases. Thus for a given tree $T \in \mathcal{T}(n,p)$, if the Algorithm C terminates after k iterations, it generates a sequence of trees $T_1, T_2, \ldots, T_k$ in $\mathcal{T}(n,p)$ satisfying $\tau(T) < \tau(T_1) < \tau(T_2) < \cdots < \tau(T_k)$, where $T_k \in \widetilde{\mathcal{T}}(n,p)$.

Example 7.18. Consider a tree $T \in \mathcal{T}(14,6)$ shown in Figure 7.3. The Algorithm C will generate a sequence of trees T, T_1, T_2, T_3, T_4 such that

$$\tau(T) < \tau(T_1) < \tau(T_2) < \tau(T_3) < \tau(T_4).$$

This sequence of trees is shown in Figure 7.3. Then note that $T_4 \in \widetilde{\mathcal{T}}(n,p)$. The modification of tree at Step 2 in Algorithm C depends upon the choice of uv edge. We remark that this sequence of trees is not unique.

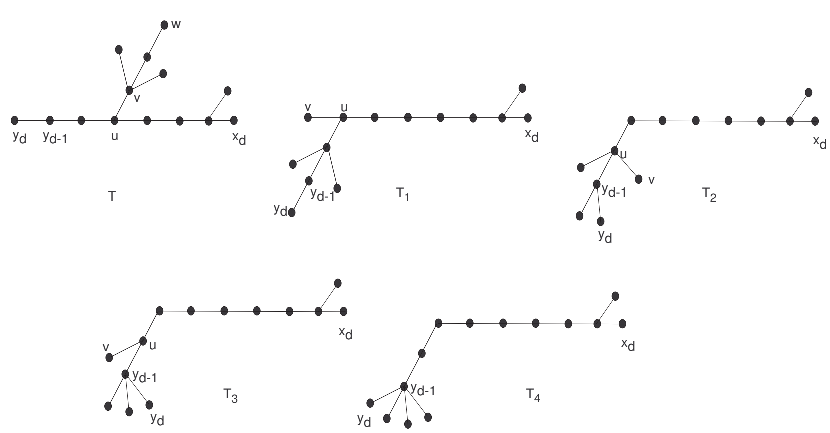

Figure 7.3: A sequence of trees generated by Algorithm C in each iteration.

7.3 Smallest and largest total eccentricity index of trees with fixed diameter

Let $\mathcal{T}(n, \mathrm{d})$ be the family of n-vertex trees with a fixed diameter d. Then we have the following result.

Theorem 7.19. [61] *If* $T \in \mathcal{T}(n, \mathrm{d})$*, then*

$$C(T) = \begin{cases} K_1 & \text{if } \mathrm{d} = 2\mathrm{r}_T, \\ K_2 & \text{if } \mathrm{d} = 2\mathrm{r}_T - 1. \end{cases}$$

Let $\mathcal{T}_1(n, \mathrm{d})$ be the subfamily of $\mathcal{T}(n, \mathrm{d})$ consisting of those trees obtained from a path of length d by connecting $n - \mathrm{d} - 1$ pendent vertices to the central vertices of the path.

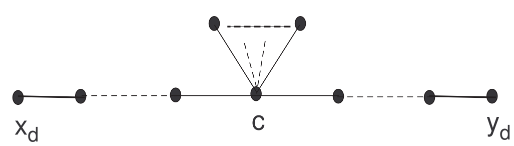

Figure 7.4: The tree $T' \in \mathcal{T}_1(n, \mathrm{d})$.

Remark 7.20. From the structure of trees in $\mathcal{T}_1(n, \mathrm{d})$, it is obvious to see that all trees in $\mathcal{T}_1(n, \mathrm{d})$ have equal total eccentricity index.

In this section, we will prove that the trees in $\mathcal{T}_1(n, \mathrm{d})$ have the smallest total eccentricity index among the trees in $\mathcal{T}(n, \mathrm{d})$. To show this, we will use mathematical technique used in Section 7.1.

Let $T \in \mathcal{T}(n, \mathrm{d}) \setminus \mathcal{T}_1(n, \mathrm{d})$ and take a diametrical $x_\mathrm{d}, y_\mathrm{d}$-path in T. Let $c \in \mathcal{V}_{C(T)}$ and $uv \in \mathcal{E}_T$ satisfying:

(f_1) $u \neq c$.

(f_2) $v \in P_T \setminus \{x_\mathrm{d}, y_\mathrm{d}\}$.

Condition (c_1) is not required to construct a tree in $\mathcal{T}_1(n, \mathrm{d})$ and condition (c_2) and (f_1) are the same. Condition (f_2) implies conditions (c_3) and (c_4). We notice that if

$T \in \mathcal{T}_1(n, \mathrm{d})$ with a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path then there is no $uv \in \mathcal{E}_T$ satisfying (f_1) and (f_2).

The proof of the following lemma follows from the proof of Lemma 7.2 with minor modifications.

Lemma 7.21. *Let $T \in \mathcal{T}(n, \mathrm{d}) \setminus \mathcal{T}_1(n, \mathrm{d})$ and $c \in \mathcal{V}_{C(T)}$. Take a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path in T and $uv \in \mathcal{E}_T$ satisfying (f_1) and (f_2). Construct a new tree $T' = \{T - \{uv\}\} \cup \{cv\}$. Then $T \in \mathcal{T}(n, \mathrm{d})$ and $\tau(T') < \tau(T)$.*

Let $T \in \mathcal{T}_1(n, \mathrm{d})$. Then by Theorem 7.19, $C(T) = K_1$ or $C(T) = K_2$. If $C(T) = K_1$ then one can easily compute that the sum of degrees of the vertices in $C(T)$ is $n - \mathrm{d} + 1$. Similarly, if $C(T) = K_2$ then the sum of degrees of vertices in $C(T)$ is $n - \mathrm{d} + 3$. However, maximum degree of any central vertex of T is $n - \mathrm{d} + 1$. In next algorithm, we convert a given tree in $\mathcal{T}(n, \mathrm{d}) \setminus \mathcal{T}_1(n, \mathrm{d})$ into a starlike tree in $\mathcal{T}_1(n, \mathrm{d})$. This algorithm is an analogue of Algorithm A.

Algorithm AA

Step 0: Take a tree $T \in \mathcal{T}(n, \mathrm{d}) \setminus \mathcal{T}_1(n, \mathrm{d})$, find a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path in T, $c \in \mathcal{V}_{C(T)}$ and $uv \in \mathcal{E}_T$ satisfying (f_1) and (f_2).

Step 1: If $\deg_T(c) = n + 1 - \mathrm{d}$, then stop.

Step 2: Set $T := \{T - \{uv\}\} \cup \{cv\}$. Find $uv \in \mathcal{E}_T$ satisfying (f_1) and (f_2); go to Step 1.

The proof of the following theorem follows from the proof of Theorem 7.3.

Theorem 7.22. (Termination and Correctness) *The Algorithm AA terminates after a finite number of iterations and outputs a tree T in $\mathcal{T}_1(n, \mathrm{d})$.*

Using Remark 7.20, Lemma 7.21 and Theorem 7.22, we have the following result.

Theorem 7.23. *Any tree in $\mathcal{T}_1(n, \mathrm{d})$ has the smallest total eccentricity index among the trees in $\mathcal{T}(n, \mathrm{d})$.*

Following corollary gives lower bound of total eccentricity index of trees in $\mathcal{T}(n,d)$.

Corollary 7.24. *For any tree $T \in \mathcal{T}(n,\mathrm{d})$, we have*

$$\tau(T) \geq \begin{cases} \left(\frac{\mathrm{d}+2}{2}\right)n + \frac{\mathrm{d}^2-2\mathrm{d}-4}{4} & \text{if d is even,} \\ \left(\frac{\mathrm{d}+3}{2}\right)n + \frac{\mathrm{d}^2-4\mathrm{d}-5}{4} & \text{if d is odd,} \end{cases}$$

with equality if and only if $T \in \mathcal{T}_1(n,\mathrm{d})$.

Proof. Let $T' \in \mathcal{T}_1(n,\mathrm{d})$. If d is even then $C(T') = K_1$ and let c be the central vertex of T'. Then $ec_{T'}(c) = \frac{d}{2}$. Thus the sum of eccentricities of vertices on the diametrical path is given by

$$\frac{\mathrm{d}}{2} + 2\left[\left(\frac{\mathrm{d}}{2}+1\right) + \left(\frac{\mathrm{d}}{2}+2\right) + \cdots + \left(\frac{\mathrm{d}}{2}+\frac{\mathrm{d}}{2}\right)\right] = \frac{3\mathrm{d}^2+4\mathrm{d}}{4}.$$

Also, if u is any pendent vertex attached with c then $ec_{T'}(u) = \frac{\mathrm{d}}{2}+1$. Since there are $n-(\mathrm{d}+1)$ pendent vertices attached with c, the sum of eccentricities of these vertices is given by $(n-(\mathrm{d}+1))(\frac{\mathrm{d}}{2}+1)$. Therefore

$$\begin{aligned} \tau(T') &= \left(\frac{\mathrm{d}}{2}+1\right)(n-(\mathrm{d}+1)) + \frac{3\mathrm{d}^2+4\mathrm{d}}{4} \\ &= \left(\frac{\mathrm{d}+2}{2}\right)n + \frac{\mathrm{d}^2-2\mathrm{d}-4}{4}. \end{aligned}$$

If d is odd then $C(T') = K_2$ and let c_1 and c_2 be the central vertices of T'. Then $ec_{T'}(c_1) = ec_{T'}(c_2) = \frac{\mathrm{d}+1}{2}$. Thus the sum of eccentricities of vertices on the diametrical path is given by

$$2 \times \frac{\mathrm{d}+1}{2} + 2\left[\left(\frac{\mathrm{d}+1}{2}+1\right) + \left(\frac{\mathrm{d}+1}{2}+2\right) + \cdots + \left(\frac{\mathrm{d}+1}{2}+\frac{\mathrm{d}-1}{2}\right)\right] = \frac{3\mathrm{d}^2+4\mathrm{d}+1}{4}.$$

Also, if u is any pendent vertex attached with c_1 or c_2 then $ec_{T'}(u) = \frac{\mathrm{d}+1}{2}+1$. Since there are $n-(\mathrm{d}+1)$ pendent vertices attached with central vertices, the sum of the eccentricities of these vertices is given by $(n-(\mathrm{d}+1))(\frac{\mathrm{d}+1}{2}+1)$. Therefore

$$
\begin{aligned}
\tau(T') &= \left(\frac{\mathrm{d}+3}{2}\right)(n-\mathrm{d}-1) + \frac{3\mathrm{d}^2+4\mathrm{d}+1}{4} \\
&= \left(\frac{\mathrm{d}+3}{2}\right)n + \frac{\mathrm{d}^2-4\mathrm{d}-5}{4}.
\end{aligned}
$$

By Theorem 7.23, we have $\tau(T) \geq \tau(T')$ for each $T \in \mathcal{T}(n, \mathrm{d})$. This gives the required inequalities. □

Now we find the trees in $\mathcal{T}(n, \mathrm{d})$ that have the largest total eccentricity index by employing the mathematical technique used in Section 7.2. Let $\mathcal{T}_2(n, \mathrm{d})$ be the subfamily of those n-vertex trees which are obtained from two stars by attaching the centers of stars by a path of length $\mathrm{d}-2$. Then obviously $\mathcal{T}_2(n, \mathrm{d}) \subseteq \mathcal{T}(n, \mathrm{d})$. A tree $T \in \mathcal{T}_2(n, \mathrm{d})$ is shown in Figure 7.5. Also, we note that $\deg_T(y_{\mathrm{d}-1}) + \deg_T(x_{\mathrm{d}-1}) = n - \mathrm{d} + 3$.

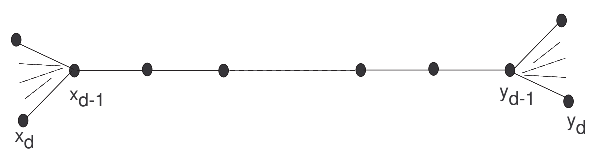

Figure 7.5: The tree $T \in \mathcal{T}_2(n, \mathrm{d})$.

Let $T \in \mathcal{T}(n, \mathrm{d}) \setminus \mathcal{T}_2(n, \mathrm{d})$ and take a diametrical path in T with end vertices x_{d} and y_{d}. Let $x_{\mathrm{d}-1} \in \Gamma_T(x_{\mathrm{d}})$, $y_{\mathrm{d}-1} \in \Gamma_T(y_{\mathrm{d}})$ and $uv \in \mathcal{E}_T$ satisfying:

(g_1) $v \in P_T$.

(g_2) $u \neq x_{\mathrm{d}-1}$ and $u \neq y_{\mathrm{d}-1}$.

We notice that if $T \in \mathcal{T}_2(n, \mathrm{d})$ then there is no $uv \in \mathcal{E}_T$ with $v \in P_T$ and $u \neq x_{\mathrm{d}-1}$, $u \neq y_{\mathrm{d}-1}$.

Next lemma follows from Lemma 7.12.

Lemma 7.25. *Let $T \in \mathcal{T}(n, \mathrm{d}) \setminus \mathcal{T}_2(n, \mathrm{d})$ with a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path in T. Take $x_{\mathrm{d}-1} \in \Gamma_T(x_{\mathrm{d}})$, $y_{\mathrm{d}-1} \in \Gamma_T(y_{\mathrm{d}})$ and $uv \in \mathcal{E}_T$ satisfying (g_1) and (g_2). Construct a new tree $T' = \{T - \{uv\}\} \cup \{y_{\mathrm{d}-1}v\}$. Then $T' \in \mathcal{T}_2(n, \mathrm{d})$ and $\tau(T) < \tau(T')$.*

Now we device an algorithm to transform a given tree in $\mathcal{T}(n,p)$ into a tree in $\mathcal{T}_2(n,\mathrm{d})$. This algorithm is analogue of Algorithm C.

Algorithm CC

Step 0: Take a tree $T \in \mathcal{T}(n,\mathrm{d}) \setminus \mathcal{T}_2(n,\mathrm{d})$, find a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path in T. Let $\{x_{\mathrm{d}-1}\} = \Gamma_T(x_{\mathrm{d}})$, $\{y_{\mathrm{d}-1}\} = \Gamma_T(y_{\mathrm{d}})$ and $uv \in \mathcal{E}_T$ satisfying (g_1) and (g_2).

Step 1: If $\deg_T(y_{\mathrm{d}-1}) = n - \mathrm{d} + 3 - \deg_T(x_{\mathrm{d}-1})$ then stop.

Step 2: Set $T := \{T - \{uv\}\} \cup \{y_{\mathrm{d}-1}v\}$.

Step 3: Find an edge $uv \in \mathcal{E}_T$ satisfying (g_1) and (g_2); go to Step 1.

The proof of next theorem follows from the proof of Theorem 7.14.

Theorem 7.26. (Termination and Correctness) *The Algorithm CC terminates after a finite number of iterations and outputs a tree in* $\mathcal{T}_2(n,\mathrm{d})$.

Remark 7.27. From the structure of trees in $\mathcal{T}_2(n,\mathrm{d})$, it is obvious to observe that all trees in $\mathcal{T}_2(n,\mathrm{d})$ have equal total eccentricity index.

Using Lemma 7.25, Theorem 7.26 and Remark 7.27, we can prove the following theorem.

Theorem 7.28. *Any tree in* $\mathcal{T}_2(n,\mathrm{d})$ *has largest total eccentricity index among trees in* $\mathcal{T}(n,\mathrm{d})$.

Next corollary gives upper bounds on total eccentricity index of trees in $\mathcal{T}(n,\mathrm{d})$

Corollary 7.29. *For any tree* $T \in \mathcal{T}(n,\mathrm{d})$ *we have*

$$\tau(T) \leq \begin{cases} \mathrm{d}n - \frac{\mathrm{d}^2}{4} & \text{if } \mathrm{d} \text{ is even,} \\ \mathrm{d}n - \frac{\mathrm{d}^2-1}{4} & \text{if } \mathrm{d} \text{ is odd,} \end{cases}$$

with equality if and only if $T \in \mathcal{T}_2(n,\mathrm{d})$.

Proof. Let $T' \in \mathcal{T}_2(n, \mathrm{d})$ and take a diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path in T'. Let $x_{\mathrm{d}-1} \in \Gamma_{T'}(x_{\mathrm{d}})$ and $y_{\mathrm{d}-1} \in \Gamma_{T'}(y_{\mathrm{d}})$. Then $ec_{T'}(x_{\mathrm{d}-1}) = ec_{T'}(y_{\mathrm{d}-1}) = \mathrm{d} - 1$. Also, if u is any pendent vertex attached with $x_{\mathrm{d}-1}$ or $y_{\mathrm{d}-1}$ then $ec_{T'}(u) = \mathrm{d}$. Since there are $n - (\mathrm{d} - 1)$ pendent vertices attached with $x_{\mathrm{d}-1}$ and $y_{\mathrm{d}-1}$, the sum of the eccentricities of these vertices is given by $(n - (\mathrm{d} - 1))\mathrm{d}$.

If d is even then $C(T') = K_1$ and the sum of eccentricities of vertices on diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path other then x_{d} and y_{d} is given by

$$\frac{\mathrm{d}}{2} + 2\left[\left(\frac{\mathrm{d}}{2} + 1\right) + \left(\frac{\mathrm{d}}{2} + 2\right) + \cdots + \left(\frac{\mathrm{d}}{2} + \frac{\mathrm{d} - 2}{2}\right)\right] = \frac{3\mathrm{d}^2 - 4\mathrm{d}}{4}.$$

Therefore

$$\begin{aligned} \tau(T') &= \mathrm{d}(n - \mathrm{d} + 1) + \frac{3\mathrm{d}^2 - 4\mathrm{d}}{4} \\ &= \mathrm{d}n - \frac{\mathrm{d}^2}{4}. \end{aligned}$$

If d is odd then $C(T') = K_2$ and the sum of the eccentricities of vertices on diametrical $x_{\mathrm{d}}, y_{\mathrm{d}}$-path other then x_{d} and y_{d} is given by

$$2 \times \frac{\mathrm{d} + 1}{2} + 2\left[\left(\frac{\mathrm{d} + 1}{2} + 1\right) + \left(\frac{\mathrm{d} + 1}{2} + 2\right) + \cdots + \left(\frac{\mathrm{d} + 1}{2} + \frac{\mathrm{d} - 3}{2}\right)\right] = \frac{3\mathrm{d}^2 - 4\mathrm{d} + 1}{4}.$$

Therefore

$$\begin{aligned} \tau(T') &= \mathrm{d}(n - \mathrm{d} + 1) + \frac{3\mathrm{d}^2 - 4\mathrm{d} + 1}{4} \\ &= \mathrm{d}n - \frac{\mathrm{d}^2 - 1}{4}. \end{aligned}$$

By Theorem 7.23, we have $\tau(T) \leq \tau(T')$ for each $T \in \mathcal{T}(n, \mathrm{d})$. □

7.4 Conclusion

In this chapter, we determine the trees with smallest and largest total eccentricity index among the class of trees with given pendent vertices. We propose three algorithms to transform given trees into trees with smaller or larger total eccentricity indices. Also we define a family of trees with a fixed diameter and investigate the trees with the smallest and the largest total eccentricity index in this class. Further work in this course is to find the extremal graphs with different parameters for examples bipartition size, independence number, domination number, fixed blocks, etc, in general classes of graphs with reference to total eccentricity index.

References

[1] S. Akhter, R. Farooq, *Computing the eccentric connectivity index and eccentric adjacency index of conjugated trees*, Util. Math., (to appear).

[2] S. Akhter, R. Farooq, *On the eccentric adjacency index of unicyclic graphs and trees*, Asian-European Journal of Mathematics, 13(1) (2020), 2050028.

[3] S. Akhter, *Two degree distance based topological indices of chemical trees*, IEEE access, 7 (2019), 95653–95658.

[4] S. Akhter, R. Farooq, *Eccentric adjacency index of graphs with a given number of cut edges*, Bull. Malays. Math. Sci. Soc., (2019), 1–14, DOI: 10:1007=s40840-019-00820-x.

[5] N. Alon, S. Hoory, N. Linial, *The Moore bound for irregular graphs*, Graphs Combin., 18(1) (2002), 53–57.

[6] A. T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, *Topological indices for structure-activity correlations*, Topics Curr. Chem., 114 (1983), 21–55.

[7] N. Biggs, E. K. Lloyd, R. J. Wilson, *Graph Theory*, Clarendon Press, Oxford, (1976), 1736–1936.

[8] B. Bollobás, P. Erdős, *Graphs of extremal weights*, Ars Comb., 50 (1998), 225–233.

[9] B. Bollobás, *Modern Graph Theory*, Graduate Texts in Mathematics, New York: Springer-Verlag, (1998).

[10] A. Bondy, M. R. Murty, *Graph Theory*, Graduate Texts in Mathematics, Springer, New York, (2008).

[11] F. Buckley, F. Harary, *Distance in graphs*, Addison-Wesley, Redwood, (1990).

[12] A. Cayley, *On the mathematical theory of isomers*, Philos. Mag., 47 (1874), 444–446.

[13] A. Cayley, *On the theory of the analytical forms called trees*, Philos. Mag., 13 (1857), 172–176.

[14] G. Chartrand, P. Zhang, *Introduction to graph theory*, Tata McGraw-Hill, New Delhi, (2005).

[15] P. Dankelmann, M. J. Morgan, S. Mukwembi, H. C. Swart, *On the eccentric connectivity index and Wiener index of a graph*, Quaest. Math., 37(1) (2014), 39–47.

[16] K. C. Das, D. W. Lee, A. Graovac, *Some properties of Zagreb eccentricity indices*, Ars Math. Contemp., 6 (2013), 117–125.

[17] N. De, *Bounds for the connective eccentric index*, Int. J. Contemp. Math. Sciences, 7(44) (2012), 2161–2166.

[18] N. De, A. Pal, Sk. Md. Abu Nayeem, *Connective eccentric index of some graph operations*, arXiv preprint arXiv:1406.0378, (2014).

[19] N. De, Sk. Md. Abu Nayeem, A. Pal, *Total eccentricity index of the generalized Hierarchical poroduct of graphs*, Int. J. Appl. Comput. Math., 1 (2015), 503–511.

[20] N. De, A. Pal, Sk. Md. Abu Nayeem, *Total eccentricity index of some composite graphs*, Malaya J. Math., 3(4) (2015), 523–529.

[21] A. A. Dobrynin, R. Entringer, I. Gutman, *Wiener index of trees: Theory and applications*, Acta Appl. Math., 66(3) (2001), 211–249.

[22] H. Dureja, S. Gupta, A. K. Madan, *Predicting anti-HIV-1 activity of 6-arylbenzonitriles: Computational approach using super augmented eccentric connectivity topochemical indices*, J. Mol. Graph. Model., 26 (2008), 1020–1029.

[23] Z. Du, A. Ilic, *A proof of the conjecture regarding the sum of domination number and average eccentricity*, Discrete Appl. Math., 201 (2016), 105-113.

[24] Z. Du, B. Zhou, N. Trinajstić, *Extremal properties of the Zagreb eccentricity indices*, Croat. Chem. Acta, 85(3) (2012), 359–362.

[25] Z. Du, B. Zhou, *Minimum Wiener indices of trees and unicyclic graphs of given matching number*, MATCH Commun. Math. Comput. Chem., 63(1) (2010), 101–112.

[26] S. Ediz, *On the Ediz eccentric connectivity index of a graph*, Optoelectron. Adv. Mater. Rapid Commun., 5(11) (2011), 1263–1264.

[27] S. Ediz, *Computing Ediz eccentric connectivity index of an infinite class of nanostar dendrimers*, Optoelectron. Adv. Mater. Rapid Commun., 4 (2010), 1847–1848.

[28] S. Ediz, *The Ediz eccentric connectivity index of one pentagonal carbon nanocones*, Fullerenes, Nanotubes and Carbon Nanostructures, 21(2) (2013), 113–116.

[29] R. C. Entringer, D. E. Jackson, D. A. Snyder, *Distance in graphs*, Czech. Math. J., 26(2) (1976), 283–296.

[30] P. Erdős, A. H. Stone, *On the structure of linear graphs*, Bull. Amer. Math. Soc., 52 (1946), 1087-1091.

[31] P. Erdős, T. Gallai, *On maximal paths and circuits of graphs*, Acta Math. Acad. Sci. Hungar., 10 (1959), 337-356.

[32] P. Erdős, *On the graph theorem of Turán*, Mat. Lapok, 21 (1970), 249-251.

[33] L. Euler, *Solutio problematis ad geometriam situs pertinentiss*, Commentarii academiae scientiarum Petropolitanae, 8 (1736), 128-140.

[34] M. R. Farahani, *The Ediz eccentric connectivity index and the total eccentricity index of a benzenoid system*, J. Chem. Acta, 2(1) (2013), 22–25.

[35] R. Farooq, S. Akhter, J. Rada, *Total eccentricity index of trees with fixed pendent vertices and trees with fixed diameter*, (submitted).

[36] R. Farooq, M. A. Malik, J. Rada, *Extremal graphs with respect to the total eccentricity index*, arXiv preprint arXiv:1711.07021, (2017).

[37] R. Farooq, M. A. Malik, *Extremal conjugated unicyclic and bicyclic graphs with respect to total eccentricity index*, arXiv preprint arXiv:1905.08630, (2019).

[38] K. Fathalikhani, *Total Eccentricity of some graph operations*, Electron. Notes Discret. Math., 45 (2014), 125–131.

[39] M. Ghorbani, M. A. Hosseinzadeh, *A new version of Zagreb indices*, Filomat 26(1) (2012), 93–100.

[40] J. L. Gross, J. Yellen, *Graph Theory and its Applications*, Chapman and Hall/CRC, USA, (2005).

[41] I. Gribkovskaia, Ø. Halskau Sr., G. Laporte, *The bridges of Königsberg: a historical perspective*, Networks, 49(3) (2007), 199–203.

[42] S. Gupta, M. Singh, A. K. Madan, *Connective eccentricity index: A novel topological descriptor for predicting biological activity*, J. Mol. Graph. Model., 18 (2000), 18–25.

[43] S. Gupta, M. Singh, A. K. Madan, *Predicting anti-HIV activity: computational approach using a novel topological descriptor*, J. Comput. Aided. Mol. Des., 15(7) (2001), 671–678.

[44] S. Gupta, M. Singh, A. K. Madan, *Application of graph theory: Relationship of eccentric connectivity index and Wieners index with anti-inflammatory activity*, J. Math. Anal. Appl., 266 (2002), 259-268.

[45] I. Gutman, N. Trinajstić, *Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett., 17 (1972), 535–538.

[46] I. Gutman, *Degree-based topological indices*, Croat. Chem. Acta, 86 (2013), 351-361.

[47] I. Gutman, *A property of the Wiener number and its modifications*, Indian J. Chem., 36A (1997), 128–132.

[48] F. Harary, *A Seminar on Graph Theory, Chapter 8: Extremal problems in graph theory (P Erdős)*, Holt, Rinehart and Winston, New York, (1967).

[49] F. Harary, *Graph Theory*, Addison-Wesley Pub. Co., (1969).

[50] F. Harary, R. C. Read, *The enumeration of tree-like polyhexes*, Proc. Edinburgh Math. Soc., 17(1) (1970), 1–13.

[51] B. Hedman, *Another extremal problem for Turán graphs*, Discrete Math., 65(2) (1987), 173–176.

[52] W. Higgins, *A Comparative View of the Phlogistic and Anti-Phlogistic Theories*, J. Murray, London, (1789).

[53] B. Hopkin, R. Wilson, *The truth about Königsberg*, The College Mathematics journal, 35(3) (2004), 198-207.

[54] H. Hosoya, *Topological index. a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons*, Bull. Chem. Soc. Jpn., 44(9) (1971), 2332–2339.

[55] H. Hosoya, Y. Gao, *Mathematical and chemical analysis of Wieners polarity number, in: D. H. Rouvray, R. B. King (Eds.)*, Topology in Chemistry–Discrete Mathematics of Molecules, Horwood, Chichester, (2002), 38–57.

[56] Y. P. Hou, J. S. Li, *Bounds on the largest eigenvalues of trees with a given size of matching*, Linear Algebra Appl., 342 (2002), 203–217.

[57] H. Hua, *Wiener and Schultz molecular topological indices of graphs with specified cut edges*, MATCH Commun. Math. Comput. Chem., 61 (2009), 643–651.

[58] H. Hua, K. Ch. Das, *The relationship between the eccentric connectivity index and Zagreb indices*, Discrete Appl. Math., 161 (2013), 2480–2491.

[59] H. Hua, S. Zhang, K. Xu, *Further results on the eccentric distance sum*, Discrete Appl. Math., 160 (2012), 170–180.

[60] A. Ilić, I. Gutman, *Eccentric connectivity index of chemical trees*, MATCH Commun. Math. Comput. Chem., 65 (2011), 731–744.

[61] C. Jordan, *Sur les assemblages de lignes*, Journal für die reine und angewandte Mathematik, 70 (1869), 185–190.

[62] L. B. Kier, L. H. Hall. *Molecular connectivity in chemistry and drug research*, Academic Press, New York and London, (1976).

[63] D. Köing, *Theorie der endlichen and unendlichen graphen*, Akademische Verlasgesllschaft, Leipzing 1936, reprinted by Chelsea, New York, (1950).

[64] D. König, *Graphs and matrices*, Mat. Fiz. Lapok, (in Hungarian), 38 (1931), 116–119.

[65] H. Kopp, *Über den Zusammenhang zwischen der chemischen Constitution und einigen physikalischen Eigenschaften bei flüssigen Verbindungen*, Ann. Chem. Pharm., 50 (1844), 71–144.

[66] V. Kumar, S. Sardana, A. K. Madan, *Predicting anti-HIV activity of 2,3-diary l-1,3-thiazolidin-4-ones:computational approaches using reformed eccentric connectivity index*, J. Mol. Model., 10 (2004), 399–407.

[67] X. Li, I. Gutman, *Mathematical aspects of Randić type molecular structure descriptors*, Mathematical Chemistry Monographs No. 1, Kragujevac, (2006).

[68] X. Li, Y. Shi, *Chemical indices, mean distance and radius*, MATCH Commun. Math. Comput. Chem., 75(1) (2016), 57–70.

[69] I. Lukovits, W. Linert, *Polaritynumbers of cyclecontaining structures*, J. Chem. Inf. Comput. Sci., 38(4) (1998), 715–719.

[70] W. Mantel, *Problem 28 (Solution by H. Gouwentak, W. Mantel, J. Teixeira de Mattes, F. Schuh and W. A. Wythoff)*, Wiskundige Opgaven, 10 (1907), 60–61.

[71] M. J. Morgan, S. Mukwembi, H. C. Swart, *On the eccentric connectivity index of a graph*, Discrete Math., 311 (2011), 1229–1234.

[72] M. J. Morgan, S. Mukwembi, H. C. Swart, *A lower bound on the eccentric connectivity index of a graph*, Discrete Appl. Math., 160 (2012), 248–258.

[73] Y. Nacaroğlu, A. D. Maden, *On the eccentric connectivity index of unicyclic graphs*, Iran. J. Math. Chem., 9(1) (2018), 47–56.

[74] X. Qi, Z. Du, *On Zagreb eccentricity indices of trees*, MATCH Commun. Math. Comput. Chem., 78 (2017), 241–256.

[75] M. Randić, *On characterization of molecular branching*, J. Amer. Chem. Soc., 97 (1975), 6609–6615.

[76] M. Randić, *Novel molecular descriptor for structure-property studies*, Chem. Phys. Lett., 211(4-5) (1993), 478–483.

[77] D. H. Rouvray, *The search for useful topological indices in chemistry: Topological indices promise to have far-reaching applications in fields as diverse as bonding theory, cancer research, and drug design*, Amer. Sci., 61(6) (1973), 729-735.

[78] S. Sardana, A. K. Madan, *Application of graph theory: Relationship of molecular connectivity index, Wieners index and eccentric connectivity index with diuretic activity*, MATCH Commun. Math. Comput. Chem., 43 (2001), 85–98.

[79] S. Sardana, A. K. Madan, *Application of graph theory: Relationship of antimycobacterial activity of quinolone derivatives with eccentric connectivity index and Zagreb group parameters*, MATCH Commun. Math. Comput. Chem., 45 (2002), 35–53.

[80] R. Sharafdini, M. Safazadeh, *On eccentric adjacency index of several infinite classes of fullerenes*, British J. Math. Comput. Sci., 12(5) (2016), 1–11.

[81] V. Sharma, R. Goswami, A. K. Madan, *Eccentric connectivity index: a novel highly discriminating topological descriptor for structure-property and structure-activity studies*, J. Chem. Inf. Comput. Sci., 37(2) (1997), 273–282.

[82] H. Smith, L. Székely, H. Wang, *Eccentricity sums in trees*, Discrete Appl. Math., 207 (2016), 120–131.

[83] V. A. Skorobogatov, A. A. Dobrynin, *Metric analysis of graphs*, MATCH Commun. Math. Comput. Chem., 23 (1988), 105–151.

[84] D. Stevanović, *Maximizing Wiener index of graphs with fixed maximum degree*, MATCH Commun. Math. Comput. Chem., 60(1) (2008), 71–83.

[85] J. Sylvester, *On an application of the new atomic theory to the graphical representation of the invariants and covariants of binary quantics, with three appendices*, American J. Math., 1(1) (1878), 64–104.

[86] Y. Tang, B. Zhou, *On average eccentricity*, MATCH Commun. Math. Comput. Chem., 67(2) (2012), 405–423.

[87] L. Tang, X. Wang, W. Liu, L. Feng, *The extremal values of connective eccentricity index for trees and unicyclic graphs*, International Journal of Computer Mathematics, 94(3) (2017), 437–453.

[88] A. Thackray, *Atoms and Powers: an essay on Newtonian matter-theory and the development of chemistry*, Harvard University Press, Cambridge, Massachusetts, (1970).

[89] N. Trinajstić, *Chemical graph theory*, CRC Press, Boca Raton, (1983).

[90] P. Turán, *Eine extremalaufgabe aus der graphentheorie*, Mat. Fiz. Lapok, 48 (1941), 435–452.

[91] D. Vukičević, A. Graovac, *Note on the comparison of the first and second normalized Zagreb eccentricity indices*, Acta Chim. Slov., 57 (2010), 524–538.

[92] H. Wiener, *Structural determination of the paraffin boiling points*, J. Amer. Chem. Soc., 69(1) (1947), 17–20.

[93] Y. Wu, Y. Chen, *On the extremal eccentric connectivity index of graphs*, Appl. Math. Comput., 331 (2018), 61–68.

[94] R. Xing, B. Zhou, N. Trinajstić, *On Zagreb eccentricity indices*, Croat. Chem. Acta, 84(4) (2011), 493–497.

[95] K. Xu, K. C. Das, H. Liu, *Some extremal results on the connective eccentricity index of graphs*, J. Math. Anal. Appl., 433(2) (2016), 803–817.

[96] G. Yu, L. Feng, *On the Wiener index of unicyclic graphs with given girth*, Ars Combin., 94 (2010), 361–369.

[97] G. Yu, L. Feng, *On connective eccentricity index of graphs*, MATCH Commun. Math. Comput. Chem., 69(3) (2013), 611–628.

[98] G. Yu, H. Qu, L. Tang, L. Feng, *On the connective eccentricity index of trees and unicyclic graphs with given diameter*, J. Math. Anal. Appl., 420(2) (2014), 1776–1786.

[99] B. Zhou, N. Trinajstić, *On a novel connectivity index*, J. Math. Chem., 46(4) (2009), 1252–1270.

[100] B. Zhou, N. Trinajstić, *On general sum connectivity index*, J. Math. Chem., 47(1) (2010), 210–218.

[101] B. Zhou, Z. Du, *On eccentric connectivity index*, MATCH Commun. Math. Comput. Chem., 63(1) (2010), 181–198.

[102] J. Zhang, B. Zhou, Z. Liu, *On the minimal eccentric connectivity indices of graphs*, Discrete Math., 312(5) (2012), 819–829.

[103] J. Zhang, Z. Liu, B. Zhou, *On the maximal eccentric connectivity indices of graphs*, Appl. Math. J. Chinese Univ., 29(3) (2014), 374–378.