Mathematical aspects of some graph invariants

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in
Mathematics

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Dedicated

to

my family...

Acknowledgments

> Read: In the name of your Lord who created. Who created man from a clinging entity. Read! Your Lord is the most Noble, Who taught by the pen. Who taught man what he did not know. (Qur′an 96:1-5)

I thank Almighty Allah, the most Gracious and Merciful, for all the blessings in my life and without the help of Whom nothing could be achieved.

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Mehar Ali Malik

Contents

Abstract

A graph invariant is a numerical quantity that remains unchanged under graph isomorphism. Topological indices are graph invariants that represent certain topological features of a graph. For example, connectivity, planarity, girth and diameter are topological features of a graph. Similarly, degrees and distances in a graph are examples of some basic topological features. Some topological indices of a graph can be determined solely in terms of vertex degrees or in terms of distances between the vertices. The former is called a degree-based index and the later is a distance-based index. Another type of topological invariants is the spectrum-based indices that are obtained from the eigenvalues of a graph. Finding an extremal graph with respect to a topological index is the problem of determining a graph maximizing or minimizing the value of that parameter among all graphs of fixed order. Topological descriptors are used in QSAR/QSPR studies to correlate physico-chemical properties of molecules.

Our primary focus in this thesis is the study of extremal graphs with respect to some distance-based topological invariants. The graphs on which we emphasize in this part include connected n-vertex graphs with $n-1$ edges (i.e. trees), connected n-vertex graphs containing n edges (i.e. unicyclic graphs) and connected n-vertex graphs with $n+1$ edges (i.e. bicyclic graphs), where bicyclic graphs may contain two or three cycles. We also study the corresponding extremal conjugated graphs with respect to these indices. We further our investigation to compute closed analytical formulas for some recently defined distance-based indices of join and corona product of any finite number of graphs. Moreover, we compute distance-based indices of some 3-fence graphs and their line graphs. We also compute these indices of the finite square grid and its line graph.

The mathematical concept of estimation can be defined as a process of approximating a desired result with a statistical technique or software tool. The second aim of this thesis is to estimate two spectrum-based indices for the molecular graphs of some nanotubes. More results of such kind are obtained for all nanocones with one arbitrary cycle as the core.

Preface

We start this thesis with a historical note on the origin of graph theory with emphasis on the role of Euler in setting foundation of graph theory. Then we define some basic definitions and set terminologies which are followed throughout the dissertation. In Chapter 2, we define the concept of topological indices and their uses. We introduce some old and new topological indices of graphs and give a survey of important results on their extremal problems. In Chapter 3, we investigate extremal graphs corresponding to total-eccentricity index. We study extremal connected graphs containing k number of cycles, where $0 \leq k \leq 3$, and further extend this study to conjugated graphs in these families. Chapter 4 deals with the study of two newly defined distance-based indices of join and corona product of any finite number of graphs. Chapter 5 deals with the study of distance-based indices of some 3-regular graphs, some molecular graphs of nanotubes and their line graphs. The last chapter is devoted to the calculation of two spectrum-based indices of some nanotubes using computational techniques/softwares. Moreover, these indices are calculated for an infinite family of nanocones.

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List of publications from the thesis

(i) "R. Farooq, M.A. Malik and Juan Rada, Extremal graphs with respect to total-eccentricity index (submitted)."
(ii) "M.A. Malik and R. Farooq, Extremal conjugated unicyclic and bicyclic graphs with respect to total-eccentricity index (submitted)."
(iii) "M.A. Malik, Two degree-distance based topological descriptors of some product graphs, Discrete Appl. Math. 236 (2), 315-328 (2017)."
(iv) "M.A. Malik and R. Farooq, On the eccentric-connectivity index of some 3-fence graphs and their line graphs, Int. J. Appl. Comput. Math. 3(2) 1157-1169 (2017)."
(v) "M.A. Malik and R. Farooq, Some conjectures on energy and Estrada index of nanocones, Optoelectron. Adv. Mater. Rapid Comm. **9** (4) (2015) 415-418." `https://oam-rc.inoe.ro/index.php?option=magazine&op=view&idu=2547&catid=89`
(vi) "M.A. Malik and R. Farooq, Computational results on the energy and Estrada index of nanotubes, Optoelectron. Adv. Mater. Rapid Comm. **9** (2) (2015), 311-313." `https://oam-rc.inoe.ro/index.php?option=magazine&op=view&idu=2527&catid=88`

Chapter 1

Introduction to graph theory

Gottfried Wilhelm von Leibniz was a famous German philosopher who for the first time used the term *analysis situs*, translated as *analysis of positions* [93, 115]. He believed that geometric figures can only be distinguished by their *shapes* [92]. In contrast with his definitions, Leonhard Euler, a Swiss mathematician of the eighteenth century, studied geometric objects and their relationships by ignoring the distances between them, and thus proved to be, as the historians state, a precursor of the theory of graphs.

The first section is devoted to a brief and interesting historical note on the role of Euler in setting foundation of graph theory. In Section 1.2 and 1.3, we will introduce the readers with basic terminologies of modern theory of graphs. Section 1.4 will focus on different methods of graph operations. Then in Section 1.5 and 1.6, we will introduce the notions of distance and matching in graphs. In the last section, we will give a brief account of the modern trend of studying extremal graphs. The notations defined in these sections will be followed throughout the dissertation. For further study, see some text books on graph theory [14, 15, 73].

1.1 Euler's contribution: A historical note

In the mid thirteenth century, the city of Königsberg (now Kaliningrad, Russia) emerged as an important medieval city. There were *seven* bridges connecting the city which was divided into *four* regions by the river Pregel (now Pregolya). It is noted that the citizens of Königsberg used to spend their Sunday afternoons walking around the city. They set themselves a recreational problem to walk around the city and (if possible) return to the starting point after crossing each of the seven bridges exactly once. The problem was called *Königsberg bridge problem* by several notable mathematicians of that era.

Carl Gottlieb Ehler was the mayor of Danzig, situated not far from Königsberg, when this problem attracted his attention. Danzig was situated in Prussia which is now known as Gdansk and it is in Poland. Ehler is believed to be a mathematician. For the solution of this problem, Ehler and one of his fellow Prussian mathematician Heinrich Kühn wrote to Euler in March 1735 (see Figure 1.1 for an original letter and sketch of the bridges). There is no proof of their initial communication on this topic, but from this letter it is clear that they already had discussed this problem.

"You would render to me and our friend Kühn a most valuable service, putting us greatly in your debt, most learned Sir, if you would send us the solution, which you know well, to the problem of the seven Königsberg bridges, together with a proof. It would prove to be an outstanding example of Calculi Situs, worthy of your great genius. I have added a sketch of the said bridges..." [79]

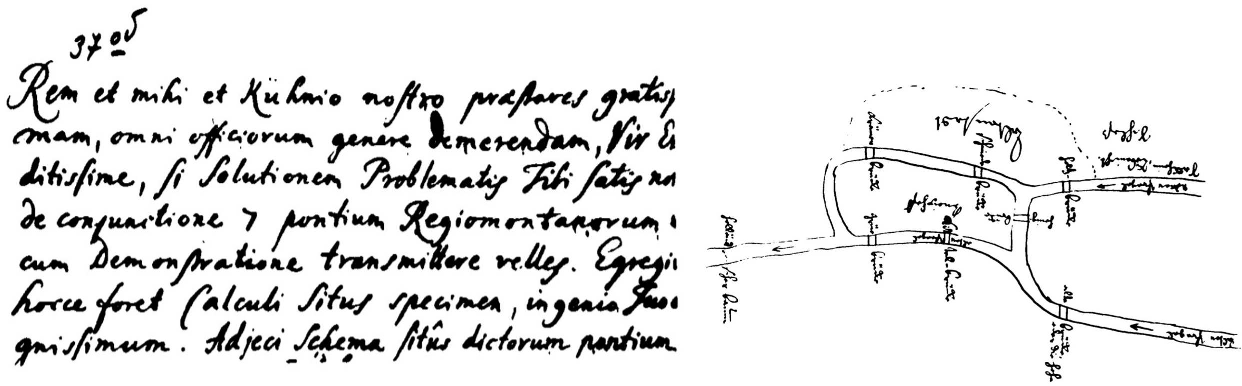

Figure 1.1: Ehler's letter to Euler, March 1735.

At that time, Euler had joined the "Academy of Sciences in St. Petersburg". In August 1735, Euler presented a solution of "Königsberg bridge problem" in the form of a paper to his colleagues and proved that the desired task was impossible. His conclusions are quoted as follows.

"*If there are more than two areas to which an odd number of bridges lead, then such a journey is impossible. If, however, the number of bridges is odd for exactly two areas, then the journey is possible if it starts in either of these two areas. If, finally, there are no areas to which an odd number of bridges lead, then the required journey can be accomplished starting from any area.*" [13]

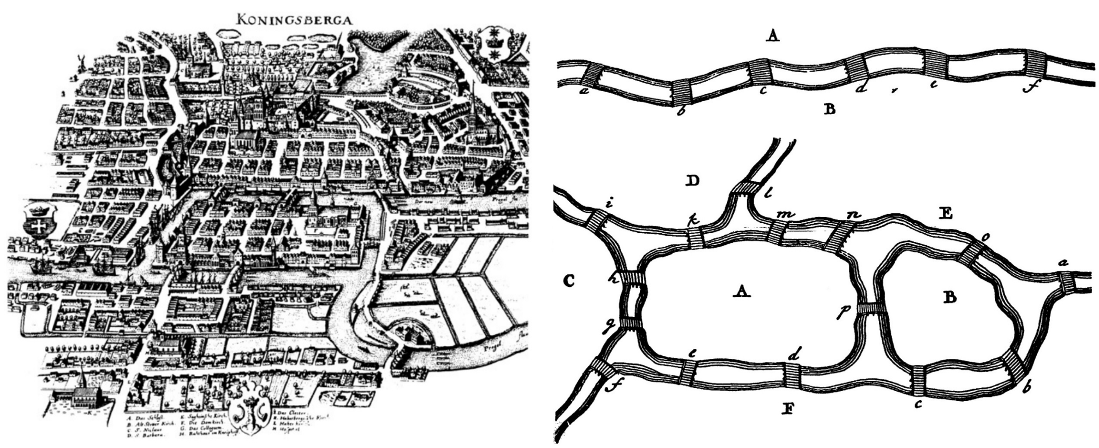

Figure 1.2: A seventeenth century map of Königsberg and Euler's sketches; one for a simpler and one for a more complicated Königsberg bridge problem.

Euler not only solved the problem but also generalized it to any number of islands and bridges. Note that Euler never drew any graph model similar to those which are commonly used today for this problem. He only used sketches of bridges, islands and the river. The graph models made their first appearances after one century. Note that the first recognizable appearance of graphs was drawn by William Higgins [78] in 1789, when he represented chemical structures with points and lines. But it was not widely known for a long time. The problem of Königsberg bridges possessed Euler's mind and so he wrote one of his most celebrated papers on it in 1736, see [47, 79] and Figure 1.2 for the sketches made by Euler. Its complete English translation can be found in [13]. Euler's interest in this new theory can also be understood by one of his letters to an Italian mathematician and philosopher Giovanni Marinoni who was "Court Astronomer" in the court of "Kaiser Leopold I". Some extract of the letter is presented here:

> "*This branch is concerned only with the determination of position and its properties; it does not involve distances, nor calculations made with them.*" [13, 119]

Note that in this letter, by "determination of positions and its properties" Euler refers to objects (or nodes) and their relationships (or adjacencies), and by mentioning that distances are not involved, he refers to the abstract representation of graphs. Thus Euler provided a complete definition of a graph long ago. We will introduce the modern definitions in the next section.

One should not think that Euler's only contribution to graph theory is his solution of "Königsberg bridge problem". Euler presented in 1759 (published in 1766) a paper titled: "Solution d′une question curieuse que ne paroit soumise a aucune analyse (A solution to a curious problem that does not appear to be subjected to any analysis)" [50]. This paper dealt with the solution of a problem known as knight's tour, a problem that gave birth to the notion of Hamiltonian circuits [120]. Further, in [48, 49] one can find the first appearance of "Euler's formula" for polyhedra, which is a relation between the number of faces, vertices, and edges of a planar graph. Euler's first paper on "Königsberg bridge problem" [47] also contains the first known appearance of the famous handshaking lemma of graph theory.

1.2 Graphs and families

The basic idea of a graph and the motivation behind its modern definition as an abstract combinatorial structure can effectively be understood by an example.

Example 1.2.1. *Consider a basket containing four pieces of fruits labeled A, B, C and D. Now suppose there are four children named E, F, G and H. The problem is to give each child a piece of fruit while considering his (or her) choice. The choices are: E likes C and D; F likes A and C; G likes B and C; and H likes A, B and D.*

Clearly, each child dislikes at least one fruit from the basket, so an arbitrary allocation of fruits to children may not be valid. Therefore, for a better understanding of the choices and their comparison, we can use a graphical representation G as shown in Figure 1.3-(a). In this figure, bold edges represent a valid distribution of fruits to the children.

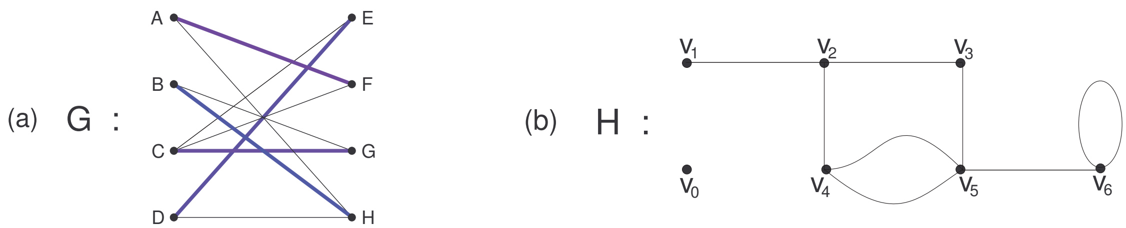

Figure 1.3: (a) The graph described in Example 1.2.1, where bold lines represent a valid distribution of fruits to the children. (b) A graph H used in Example 1.2.2.

A graph, with a conventional name G, can be defined as a pair (V, E) where an element $v \in V$ is named a vertex and an element $e \in E$ is called an edge. Here each element $e \in E$ can be written as (u, v), $\{u, v\}$ or simply uv for $u, v \in V$. A graph without any edges, that is, $E = \emptyset$, is called an empty graph and thus attracts no interest. The sets V and E may also be represented respectively by $V(G)$ and $E(G)$. In a graph, vertices are represented by points and they may represent any object, for example, people, cities, atoms, etc. The edges in a graph are represented by lines or curves connecting the vertices and they may represent acquaintances, roads, chemical bonds, etc. In our study, we only consider finite graphs, that is, graphs with finite vertex and edge sets. In a graph G, if there exists an edge $e \in E(G)$ between two vertices u and $v \in V(G)$ then u and v are *adjacent* or *neighbors* and such edge e is denoted by the labels of its *end-vertices*, that is, $e = uv$. In this case, the edge uv is called *incident* on the vertices u and v. A set of *multiple* edges consists of those edges which have same end-vertices and an edge $uv \in E(G)$ with $u = v$ is called a *loop*. In this thesis, our focus will be on graphs which do not contain any loops or multiple edges. Such graphs are called *simple* graphs. The *order* n (respectively, *size* m) of a graph is its number of vertices (respectively, edges). For $v \in V(G)$, its *neighborhood* is defined by $N_G(v) = \{w \in V(G) \mid vw \in E(G)\}$. The *degree* $d_G(v)$ of a vertex v in G is defined by $|N_G(v)|$. The vertices of degree 0 and 1 in G are respectively called *isolated* (denoted by K_1) and *pendent* vertices. A k-regular graph is one with all vertices of same degree $k \geq 0$. The sum of degrees of all the neighbors of a vertex $v \in V(G)$ is denoted by $S_G(v)$ and is defined as $S_G(v) = \sum_{w \in N_G(v)} d_G(w)$.

Let $S = \{v_1, v_2, \ldots, v_n\}$. A *path* P_n is an n-vertex graph with vertex set S and $v_i v_j \in E(P_n)$ if $j = i + 1$, $1 \leq i \leq n - 1$. A path with vertex set S may also be denoted by $v_1 v_2 \cdots v_n$. A (v_1, v_n)-path is the one starting and ending respectively at v_1 and v_n. A *cycle* C_n with vertex set S is a closed path, that is, a (v_1, v_n)-path with $v_1 = v_n$. The *length* of a path or cycle is naturally defined by the number of edges they contain. The *girth* of a graph is the length of a shortest cycle in it.

Example 1.2.2. *For the graph H shown in Figure 1.3-(b). The neighborhood of v_3 is $\{v_2, v_5\}$ thus $d(v_3) = 2$. The vertex v_0 is isolated and v_1 is pendent. Two multiple edges are shown between v_4 and v_5 and a loop at v_6.*

The *degree* of G is defined by $d(G) = \sum_{v \in V} d_G(v)$. It can be seen that each edge adds 'two' to $d(G)$. Thus, when a graph G has m edges, then degree of G becomes $2m$, that is,

$$\sum_{v \in V(G)} d_G(v) = 2m. \tag{1.1}$$

Equation (1.1) is called the *handshaking lemma* of graph theory.

Apart from paths and cycles, there are special types of graphs which are known by their names. Here we introduce a few such families of n-vertex graphs. An n-vertex graph, denoted by K_n, is the one with every pair of vertices adjacent in it. Such a graph is called *complete.* Consider two disjoint sets V_1 and V_2 with cardinalities r and $n-r$, respectively. The graph $K_{r,n-r}$ is called *complete bipartite* and defined as a graph with vertex set $V_1 \cup V_2$ having maximum size such that no edge of $K_{r,n-r}$ has both of its ends in the same set V_1 or V_2. A star graph S_n is defined by $K_{1,n-1}$. A *molecular graph* is one in which atoms are represented by vertices and the chemical bonds are represented by edges. These graphs represent molecular topology of chemical compounds and will be the topic of our interest in Chapters $5-6$.

1.3 Subgraphs

Since real distances between vertices and the shapes of edges are ignored while studying graphs, there are many possible ways to draw a graph. But all such drawings refer to the same graph and are called isomorphic. Thus two graphs may loosely be defined as isomorphic if one of them can be redrawn exactly as the other. Formally, a pair of graphs G_1 and G_2 are *isomorphic* [14] if there exists a bijection $f : V(G_1) \to V(G_2)$ such that for every edge $uv \in E(G_1)$ we have $f(u)f(v) \in E(G_2)$. In this case, we write $G_1 \cong G_2$. Therefore in graph theory, the family of all graphs isomorphic to a specific graph G is represented by G. A quantity T is a *graph invariant* if and only if $T(G) = T(H)$ whenever $G \cong H$. Thus the order, size and girth are some examples of graph invariants. When two graphs are isomorphic, they are called copies of each other, and thus have the same topological properties. But for large n, there is no easy algorithm for checking graph isomorphism [55]. Two graphs can be shown to be isomorphic by checking a complete set of graph invariants, but no such set is known [73]. When two graphs are not isomorphic, they differ in certain topological features.

Example 1.3.1. *A pair of isomorphic graphs is shown in Figure 1.4-(a). For another pair of graphs shown in Figure 1.4-(b), it is not hard to find out that one of them contains a cycle of length* 8 *but the other does not.*

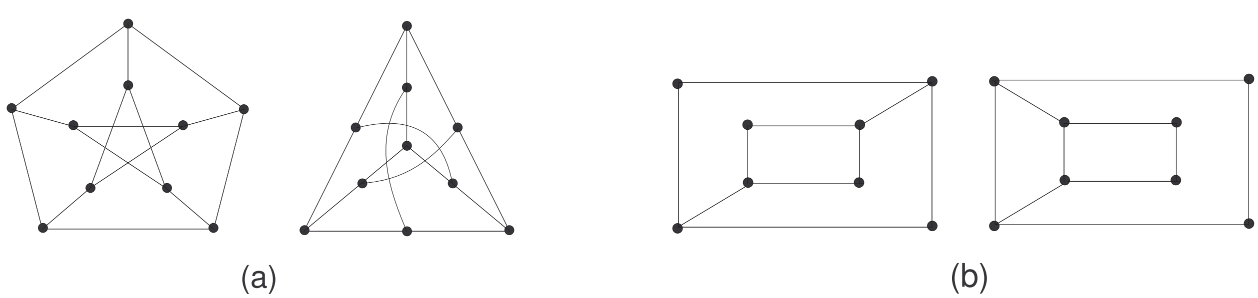

Figure 1.4: (a) A pair of isomorphic graphs. (b) Two non-isomorphic graphs.

A graph is a subgraph of another graph if all of its vertices and edges are contained in the vertex and edge sets of its supergraph. Let $S \subseteq V(G)$. Then the subgraph $G[S]$ of G *induced* by S is a graph with $V(G[S]) = S$ and its edge set contains all edges of G that have both end-vertices in S. A subgraph which contains all the vertices of its supergraph is called *spanning*. Consider the graph G shown in Figure 1.5. For $S = \{v_2, v_3, v_4, v_5\}$, a subgraph H and an induced subgraph $G[S]$ with vertex set S are shown.

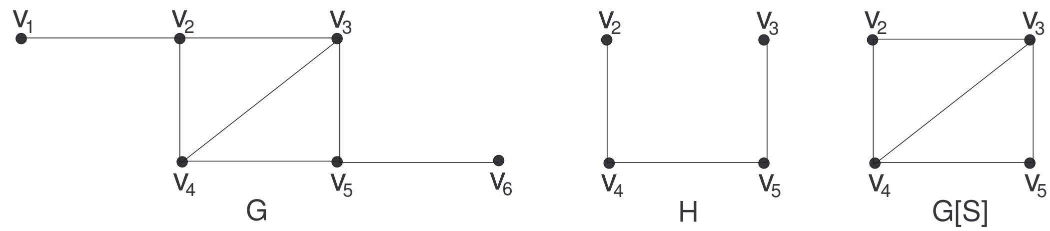

Figure 1.5: The graph G is shown with subgraph H and induced subgraph $G[S]$.

1.4 Graph operations

In this section, we describe several graph operations that will be used frequently throughout this dissertation. First we define some graph operations performed on one graph. Consider a graph G and $X \subseteq E(G)$. The subgraph $G - X$ of G, called the *edge-deleted* subgraph of G, is constructed by deleting the edges in X from G. When X contains a single element, say e, then the notation $G - e$ is used instead of $G - X$. Now consider a subset Y of $V(G)$. By deleting elements of Y from G along with their incident edges, we obtain a subgraph denoted by $G - Y$. It is called *vertex-deleted* subgraph of G. Analogously, when Y contains a single element, say v, then the notation $G - v$ is used instead of $G - Y$. For an edge $uv \in E(G)$, the operation of *edge contraction* $G|_{uv}$ can be performed by deleting the edge uv from G and merging u and v into an new vertex w (that is, $w \notin V(G)$), such that w becomes incident with all the edges (except uv) incident on u and v. Similar to edge contraction, we have another operation called *edge subdivision*, which is performed, for $uv \in E(G)$, by replacing uv with a path uwv, where $w \notin V(G)$. For a graph G, another graph $L(G)$ can be constructed which has vertex set $V(L(G)) = E(G)$ and $e_1, e_2 \in E(L(G))$ if and only if an end-vertex is shared by both e_1 and e_2 in G. Then $L(G)$ is called the *line* graph of G. For given G, a new graph can be obtained with vertex set $V(G)$ and containing all edges that are not present in G. It is called the *complement* $\overline{G}$ of G. The *self-complementary* graphs are those which are identical with their complements. It is known [15] that an n-vertex self-complementary graph satisfies $n \equiv 0 \pmod 4$ or $n \equiv 1 \pmod 4$.

Now we define some more advanced graph operations which may be performed between one or more graphs. Two graphs G_1 and G_2 are said to be disjoint if their vertex and edge sets are disjoint. Let G_1, G_2 be disjoint graphs, then $G_1 \cup G_2$ is their *disjoint union* with vertex set $V(G_1) \cup V(G_2)$ and $E(G_1 \cup G_2) = E(G_1) \cup E(G_2)$. When $G_1 \cong G_2$, we first replace $V(G_1)$ and $V(G_2)$ by two disjoint sets of the same cardinalities and then obtain their disjoint union in the same way as described before. Thus the disjoint union of G_1 and G_2 is obtained by placing the two graphs together without adding any vertex or edge. We will denote by kG the disjoint union $G \cup G \cup \ldots \cup G$ (k-times). There is another operation on graphs known as join of graphs. The *join* of two disjoint graphs G_1 and G_2 denoted by $G_1 + G_2$ is a graph on $|V(G_1) \cup V(G_2)|$ vertices and contains all edges in $E(G_1 \cup G_2)$ and the edges joining vertices of G_1 with vertices of G_2 [152]. That is, $E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{uv \mid u \in V(G_1) \text{ and } v \in V(G_2)\}$. For example, $K_{m,n} = mK_1 + nK_1$, where K_1 denotes an isolated vertex.

Let a graph G with vertex set $\{v_1, v_2, \ldots, v_n\}$. Let nH denotes n copies of a graph H, that is, $H_i \cong H$ for $1 \leq i \leq n$. Then *corona product* $G \odot H$ is the graph on vertex set $V(G) \cup \{\cup_{i=1}^{n} V(H_i)\}$ and edge set $E(G) \cup \{\cup_{i=1}^{n} E(H_i)\} \cup \{v_i w \mid w \in E(H_i), 1 \leq i \leq n\}$. The corona product of three graphs G_1, G_2 and G_3 is defined as $G_1 \odot G_2 \odot G_3 = (G_1 \odot G_2) \odot G_3$. As an example, consider three graphs G_1, G_2 and G_3 respectively defined as C_4, P_2 and C_3. Then the corona product $G_1 \odot G_2 \odot G_3$ is presented in Figure 1.6.

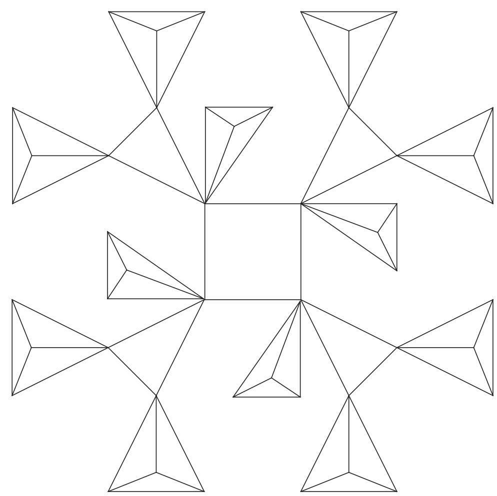

Figure 1.6: Corona product $G_1 \odot G_2 \odot G_3$, where $G_1 = C_4$, $G_2 = P_2$ and $G_3 = C_3$.

Many more operations on graphs can be found in Harary and Wilcox [75]. For advanced contents on graph operations, reader is referred to a handbook on product graphs [70].

1.5 Distance and connectivity

Theoretical and application perspectives derived mathematicians to study the discrete analog of distance studied in Euclidean geometry. Thus the study of distances in graphs is lead by the fact that discrete structures are modeled by a graph [16].

In a *connected* graph G, for every pair of vertices we can find a path connecting them. In G, a *component* is a subgraph that is not contained in any other connected subgraph of G. When G has more than one components, it is called *disconnected*. For a connected graph G, a *cut-vertex* $v \in V(G)$ has the property that $G - v$ is disconnected, and a *cut-edge* $e \in E(G)$ is such that $G - e$ is disconnected. A cut-edge is also called a *bridge*. It can be noticed that an edge is a bridge if and only if it does not belong to a cycle [15]. A connected subgraph of G that does not contain any cut-vertex and is not contained in a larger such subgraph of G is known as a *block*. The length of a shortest path between two vertices u and v in a connected graph G is defined as the *distance* $d_G(u, v)$ between u and v. The *status* of a vertex v in G is defined as $D_G(v) = \sum_{w \in V(G)} d(v, w)$. The largest distance from a vertex $v \in V(G)$ to any other vertex in G is called the *eccentricity* of v, denoted by $e_G(v)$. Alternatively,

$e_G(v) = \max\{d_G(v, w) \mid w \in V(G)\}$. The *diameter* $\operatorname{diam}(G)$ and *radius* $\operatorname{rad}(G)$ of graph G are defined as:

$$\operatorname{diam}(G) = \max_{v \in V(G)} \{e_G(v)\}, \quad \operatorname{rad}(G) = \min_{v \in V(G)} \{e_G(v)\}.$$

When $\operatorname{rad}(G) = \operatorname{diam}(G)$, then G is called a *self-centered* graph. A vertex v in G is said to be *central* (respectively, *peripheral*) if $e_G(v) = \operatorname{rad}(G)$ (respectively, $e_G(v) = \operatorname{diam}(G)$). The *center* $C(G)$ of a graph G denotes the subgraph of G induced by the set $\{c \in V(G) \mid e_G(c) = \operatorname{rad}(G)\}$.

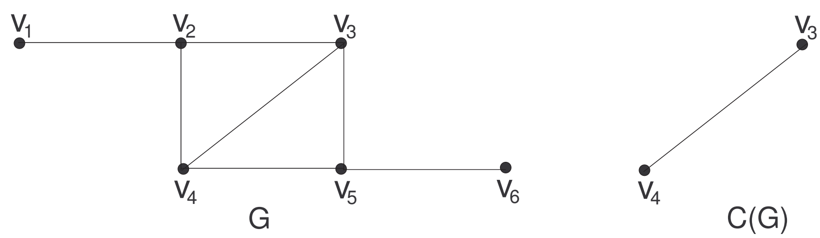

Figure 1.7: The center $C(G)$ of a graph G.

An *acyclic* graph is the one not containing any cycle. A connected graph that is also acyclic is known as a *tree*. There are some families of graphs which are called tree-like structures because they become a tree after deletion of a few edges. For example, an n-vertex unicyclic (respectively, bicyclic) graph is a connected graph which contains n (respectively, $n+1$) edges. For an n-vertex tree T with m edges, we have $m = n - 1$ [15]. The three properties that are fundamental for a tree T are its connectedness, $m = n - 1$ and being acyclic. Note that any two of these three properties of T imply the third. Moreover, a tree T has the following properties [15].

(a) A unique path exists between every pair of vertices in T.

(b) Every edge in T is a bridge and every vertex $w \in V(T)$ with $d_T(w) \geq 2$ is a cut-vertex.

(c) When $m \geq 1$ then T has more than one pendent vertices.

Also observe that the center of a tree is either K_1 or K_2. The proofs are elementary and may be found in any text book of graph theory (see [15, 57]).

1.6 Matching

An *independent* set of edges in a graph G contains those edges which do not share any end-vertex [127]. A *matching* in a graph G is an independent set of edges of G. A matching with maximum number of edges is called a *maximum matching*. In Example 1.2.1, where the objective was to give each child a fruit of his or her choice, the problem is to find a maximum matching 1.3. Such a matching is shown by bold edges in the same figure. Another application of matching occurs in scheduling problems where the objective is to assign workers to jobs. When G has a matching M, a vertex v of G is called M-saturated if there exists $e \in M$ such that e is incident on v, otherwise v is called M-unsaturated. A matching M of G is called *perfect* if it saturates every vertex of G. Clearly, a perfect matching in an n-vertex graph will have size $\frac{n}{2}$, requiring n to be an even number. An M-alternating path in G is a path whose edges alternate between M and $\overline{M}$, where $\overline{M}$ denotes complement of M. An M-augmenting path in G is an M-alternating path starting and ending at M-unsaturated vertices. It can be observed that a matching M in a graph containing an M-augmenting path cannot be maximum. A graph with a perfect matching is called *conjugated* graph or *Kekulé* structure. In graphs representing organic compounds, the stability and analysis of resonance energy of hydrocarbons are studied by the help of Kekulé structures [66].

1.7 Extremal graph theory

It is the analysis of comparison between global parameters and local substructures of a graph [29]. Some simple examples of extremal problems in graphs are given as follows.

Example 1.7.1. *Consider a connected graph G of size m, then $m \leq \binom{n}{2}$, where equality occurs for a complete graph.*

Example 1.7.2. *Denote the number of triangles required to cover all edges of a graph G by $f(n)$. Then $f(n) \leq \binom{n}{2}/3$, where the equality holds for a complete graph G.*

In Example 1.7.1, the complete graph K_n plays the role of an extremal (maximal) graph when the function which is desired to be maximized is the size of the graph. Similarly, the empty graph, the one that contains no edges, will serve as the minimal graph in this case.

In 1941, Turán [135] initiated studying extremal graphs. The forerunner of this subject is the following problem of Turán which he completely solved in the same paper.

Theorem 1.7.1 (Turán [135])**.** *For a given $r \in \{3, 4, \ldots, n\}$, what is the maximal size graph that does not contain K_r.*

Other motivational work on extremal graphs can be found in [36–39, 72].

Chapter 2

Graph theory and topological indices: Literature review

Over the past two centuries, many confluences are evident in the development of graph theory and modern chemistry. Graph-theoretical notions have never stopped cropping up in a chemical context and chemical problems have been studied by mathematicians using graph-theoretical tools. Here we mention in a chronological order some famous mathematicians from the past who have studied chemical problems. This includes Sylvester [130] who observed the similarity between a chemical constitutional formula and a graph in 1878. Then, in 1896, Cayley [18] worked on the enumeration of some chemical trees. In 1970, Read and Harary [114] studied the famous “polyhex problem” of enumerating polycyclic aromatic molecules.

There is a method for binding a drug target that searches for small molecules from a large database of molecules. This method is known as virtual screening. The purpose of this process is to search more than 10^{60} molecules and give a small number of molecules that fulfill a specific purpose. Then these molecules are purchased and tested. This filtration process generates a group of similar molecules, where the similarity of these molecular structures is described by certain common features which may be physico-chemical, biological or merely topological in nature. In this thesis, we will only be interested in topological properties. Since molecular similarity is an intuitive notion, there does not exist a unique unambiguous measure for it. Molecular description used in molecular similarity analysis is performed by using molecular descriptors or indices. Such descriptors measuring only some topological features of a molecule are called topological descriptor or *topological indices*. For applications of topological indices in drug design, we refer to a book published by Kier and Hall [90].

We give formal definition of a topological index in Section 2.1 followed by some more details on their applications. Then in Section 2.2, we give details on some of the oldest reported topological indices. In Section 2.3, we introduce the reader with some spectrum-based topological descriptors. In the last section, we give known results relevant to our study.

2.1 Topological indices

A topological index can be defined as a number defined by graph theoretic expressions and which represents some topological feature of a chemical structure. Since a topological index describes the topology of molecules, identical values are obtained for isomorphic graphs by any topological index and that is why we call these indices 'graph invariants'. Alternatively, we define a topological index as a function of type $T : \mathbb{G} \to \mathbb{R}$, where $\mathbb{G}$ denotes the set of all graphs such that $T(G) = T(H)$ if and only if graphs G and H are isomorphic. Wide applications have been found for such invariants in the correlation of many physico-chemical properties of molecules [9, 118] and also in the similarity and isomorphism tests [111, 112]. Topological indices are used for comparison between the physico-chemical and/or biological properties of molecules in QSAR/QSPR studies [134]. Using topological descriptors, QSAR/QSPR studies search and propose new chemicals which can serve as candidates for safer and potent drugs [59, 121, 122, 125]. To date, over 1000 papers on the subject have appeared, see the reviews [8, 116] and a book [7].

Topological indices may be classified into several categories depending upon the specific topological feature from which they are measured or calculated. Some basic topological features include degrees of vertices, distances between vertices, matchings of different sizes in a graph, etc. These features categorize topological indices into degree-based, distance-based, counting-polynomials based indices and into some other types as well.

Some indices defined in terms of degrees and distances can also be calculated by some matrices associated with a graph, a detailed discussion on this topic can be found in a review article by Rouvray [117]. A fundamental matrix associated with a graph and some important parameters calculated from this matrix are discussed in Section 2.3 and Chapter 6.

2.2 Some old and new topological indices

Consider an n-vertex simple connected graph G. For the first time, a topological index was used by Hosoya [80] in 1971. The main idea, however, was used earlier by Harold Wiener. Thus, the oldest reported topological index was the one introduced by Wiener [138] in 1947 to calculate the boiling points of paraffins. Later on, in 1971, Hosoya [80] defined the notion of Wiener index for G as:

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

In the same paper [138], another index W_p known as "Wiener polarity index" was also introduced. It is defined as the quantity of unordered pairs of vertices $\{u, v\}$ in G such that $d_G(u, v) = 3$. Alternatively, it can be defined for $\{u, v\} \subseteq V(G)$ as:

$$W_p(G) = \big|\big\{\{u,v\} \mid d_G(u,v) = 3\big\}\big|, \tag{2.1}$$

To calculate boiling points of paraffins a linear formula was used in terms of W and W_p.

Another topological index amongst the first few topological indices is the Hosoya index. It was put forward by Hosoya [80] in 1971. Let $\rho(G, \kappa)$ is the number of ways of choosing κ

independent edges from G then $\rho(G,\kappa)$ denotes the number of matchings of size κ in G. Then the Hosoya index $H(G)$ is defined in terms of $\rho(G,\kappa)$ as:

$$H(G) = \sum_{\kappa} \rho(G,\kappa).$$

The boiling points and other similar physico-chemical properties largely depend on the interactions of large number of identical molecules in liquid phase and are determined by space-filling characteristics of molecules. This property is, to some extent, exhibited by several topological indices, and Hosoya index is one of such kind. This index has shown excellent correlations with the boiling points of a wide range of organic molecules. In the case of Hosoya index, a number of other uses have been found. It was shown that the sorting of large databases of chemical structures can be done by using this index. Moreover, it gives a good reflection of the nature of a species with regard to its degree of branching and cyclization.

Randić [110] in 1975, defined the first "degree-based topological index" and named it as "branching index". After some time, it was renamed to "connectivity index", but now a days it is known as Randić index. It was designed to reflect the amount of branching present in a chemical species. Using this index, very good correlations were obtained with a wide range of physico-chemical properties, such as vapor pressure and chromatographic retention times. The suitability of the Randić index for drug design was immediately recognized. The Randić index $R(G)$ is defined as:

$$R(G) = \sum_{xy\in E(G)} \frac{1}{\sqrt{d_G(x)d_G(y)}}. \tag{2.2}$$

For further details on degree-based indices, readers are referred to a feature article [62] and review articles [9, 94].

Gutman and Trinajstic [68] observed that the total π-electron energy depends upon the structure of corresponding molecular graph. In this study, they obtained the following expressions.

$$M_1 = \sum_{u\in V(G)} d_G(u)^2 = \sum_{xy\in E(G)} (d_G(x) + d_G(y)), \tag{2.3}$$

$$M_2 = \sum_{xy\in E(G)} d_G(x)d_G(y). \tag{2.4}$$

These indices were later called the Zagreb group indices. It was immediately recognized that these terms provide quantitative measures of molecular branching [62]. Another old index defined by Randić [113] is the "hyper-Wiener index" of graph G denoted by $WW(G)$ and defined as follows.

$$WW(G) = \frac{1}{2} \sum_{x,y\in V(G)} (d_G(x,y) + d_G(x,y)^2). \tag{2.5}$$

In this thesis, we emphasize on those topological indices which are defined in terms of degrees and distances in G, except in Chapter 6 where approximation of spectrum-based indices by using software tools is explored. Now we discuss some degree and distance-based topological indices, whereas the spectrum-based indices are discussed in Section 2.3 and 2.5. The average-eccentricity of G was defined in 1988 by Skorobogatov and Dobrynin [128] as:

$$avec(G) = \frac{1}{n} \sum_{u\in V(G)} e_G(u). \tag{2.6}$$

For recent results on average-eccentricity, we refer to [33, 95]. In the recent literature, a modification of $avec(G)$ is used and cited as total-eccentricity index $\tau(G)$. It is defined as:

$$\tau(G) = \sum_{u \in V(G)} e_G(u). \tag{2.7}$$

Sharma et al. [125] defined the "eccentric-connectivity index" $\xi(G)$ of G as defined by the following expression.

$$\xi(G) = \sum_{x \in V(G)} d_G(x) e_G(x). \tag{2.8}$$

It has been shown in the literature that the predictability of "Eccentric-connectivity index" is very high for pharmaceutical properties of chemicals. Thus pharmaceutical companies can use such indices to development new safer and cheaper drugs [122]. Since "Eccentric connectivity index" is defined in terms of degrees of vertices, thus it can be used in measuring branching in alkanes [85].

Dobrynin and Kochetova [31] introduced "degree-distance" index $DD(G)$ of G. It is the product of the sum of distances starting from each vertex and its degree. This index is mathematically defined as follows.

$$DD(G) = \sum_{x \in V(G)} d_G(x) D_G(x).$$

The indices ξ^{sv} and ξ^{ad} were respectively introduced for a graph G by Sardana and Madan [122] and Gupta et al. [58] as:

$$\xi^{sv}(G) = \sum_{x \in V(G)} \frac{e_G(x) D_G(x)}{d_G(x)} \tag{2.9}$$

$$\xi^{ad}(G) = \sum_{x \in V(G)} \frac{S_G(x)}{e_G(x)}. \tag{2.10}$$

The power of prediction of ξ^{sv} was highlighted by the authors in [122] for anti-HIV activity of TIBO derivatives. Moreover, the authors compared the properties of $\xi^{sv}(G)$ with $\xi(G)$ and observed excellent correlations. The antioxidant activity of some chemicals like nitroxides were well correlated by W and ξ^{sv} [121]. Interestingly, the results of "adjacent-eccentric distance sum index" were found to be more efficient than the results of Wiener index. Similarly, ξ^{ad} was used for predicting the anti-HIV activity of 107 "1-[(2-hydroxyethoxy)methyl]-6-(phenylthio)thymine" (HEPT) derivatives. Prediction accuracy of ξ^{ad} exceeded ninety percent.

2.3 Some spectrum-based topological indices

Let $\{v_1, v_2, \ldots, v_n\}$ be the vertex set of a graph G. Then the adjacencies between the vertices of G can be represented in the form of an $n \times n$ matrix known as the *adjacency matrix* of G and denoted by $A(G)$ or simply A. The (i, j)-th entry a_{ij} of A is 1 if v_i is adjacent to v_j in G, and 0 otherwise. Let I_n denotes the identity matrix of dimension n and A be the adjacency matrix of G then the polynomial associated with graph G called the *characteristic polynomial* is defined by

$$\Phi(G, \lambda) = \det(\lambda \mathrm{I_n} - \mathrm{A}).$$

The *eigenvalues* and *spectrum* of G are respectively the roots and spectrum of $\Phi(G, \lambda)$. When G represents a molecular graph, the matrix A is real and symmetric. Thus all eigenvalues of G are real. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of G. The *energy* $\mathcal{E}(G)$ of G is given by the following expression.

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{2.11}$$

The notion of energy for graphs was introduced in 1978 by Gutman [60]. The basic idea however was originated from Hückel theory. The quantity $\mathcal{E}$ is in good correlation with total π-electron energy of conjugated hydrocarbon [64]. More details on energy and its applications can be found in [22, 69, 143].

The *Estrada index* $\mathcal{EE}(G)$ of graph G was introduced in 2000 by Estrada [41] as:

$$\mathcal{EE}(G) = \sum_{i=1}^{n} \exp^{\lambda_i}. \tag{2.12}$$

It has noteworthy applications in chemical sciences. It has been used in quantifying degree of folding of proteins as well as in long-chain biomolecules [41–43]. This index is also considered as a measure for bipartivity and centrality of graphs and complex networks [46]. Some general topological features of complex networks are also characterized by using $\mathcal{EE}$ [44]. Ashrafi [3] studied $\mathcal{E}$ and $\mathcal{EE}$ of some nanotubes composed of C_5 and C_7. Ashrafi and Sadati [5] studied $\mathcal{E}$ and $\mathcal{EE}$ by using numerical techniques for the graphs of carbon nanocones containing one pentagon at their center. In the continuation of this study, Malik and Farooq [98] studied these indices of nanotubes and nanocones. For more details in this direction, we refer to [3–5, 44, 63, 134, 142].

2.4 Known results

In the following, we give several results giving maximal and minimal graphs, with given parameters such as size, diameter, cut-edges, etc., with respect to some Wiener-type indices. We start with an elementary result.

Theorem 2.4.1 (Xua et al. [141]). *Let G be an n-vertex connected graph. Then*

(i) $W(G) \geq W(K_n)$, *where the equality is satisfied iff* $G \cong K_n$;

(ii) $WW(G) \geq WW(K_n)$, *such that the equality holds iff* $G \cong K_n$.

Consider $PK_{n,m}$ to be a family of path-complete graphs, constructed by $P_{n-m} \cup K_m$ by adding some edges between one end-vertex of the path and some vertices of K_m. The path-complete graph $PK_{10,5}$ can be seen in Figure 2.1-(a). The following result gives, with fixed order and size, the graphs which are maximal and minimal for W.

Theorem 2.4.2 (Harary [71]). *For an n-vertex connected graph G, the path-complete graph G' with m edges and diameter d in $PK_{n,m}$ is the unique graph with maximal Wiener index.*

Theorem 2.4.3 (Šlotés [136]). *For an n-vertex connected graph G. The path-complete graph G' with m edges in $PK_{n,m}$ is the unique graph with maximal Wiener index.*

Theorem 2.4.4 (Xua et al. [141]). *Let G be an n-vertex connected graph having m edges. Then any graph G with diameter at most 2 has minimal Wiener index.*

Theorem 2.4.5 (Khalifeh et al. [89]). *Let $a \geq 2$ be a positive integer and G be any connected graph with m edges, where $\binom{a}{2} \leq m \leq \binom{a+1}{2}$. Then*

$$a(a+1) - m \leq W(G),$$

with equality holding iff $G \ncong G_0$, where G_0 is the graph obtained by deleting $\binom{a+1}{2} - m$ edges from the complete graph K_{a+1} that are incident with a fixed vertex in it.

A *cactus* is a connected graph such that each block is either an edge or a cycle. Let $Cat(n,t)$ denote all cacti with n vertices and t cycles. A cactus $Cat(15,4)$ is shown in Figure 2.1-(b). Let $C_0(n,t)$ be a cactus obtained by adding t independent edges between the leaves of S_n. In the following, it is shown that $C_0(n,t)$ is the unique minimal graph for Wiener and hyper-Wiener index.

Theorem 2.4.6 (Liu and Lu [96], Feng et al. [54]). *Among all graphs in $Cat(n,t)$, the unique graph with minimal Wiener and hyper-Wiener indices is the graph $C_0(n,t)$.*

Consider attaching k leaves to a vertex of K_{n-k}, the resultant graph is denoted by K_n^k, for $1 \leq k < n$. The graph K_8^3 is shown in Figure 2.2-(a). The graph K_n^k is the unique minimal graph corresponding to Wiener and hyper-Wiener index for all n-vertex graphs with k cut-edges, as shown in the following result.

Theorem 2.4.7 (Hua [81], Wu and Liu [139]). *The graph K_n^k is the unique graph with minimal Wiener index for all n-vertex connected graphs having k bridges.*

Theorem 2.4.8 (Wu and Trinajstić [140]). *For all n-vertex connected graphs having k bridges, K_n^k is the unique minimal graph for WW.*

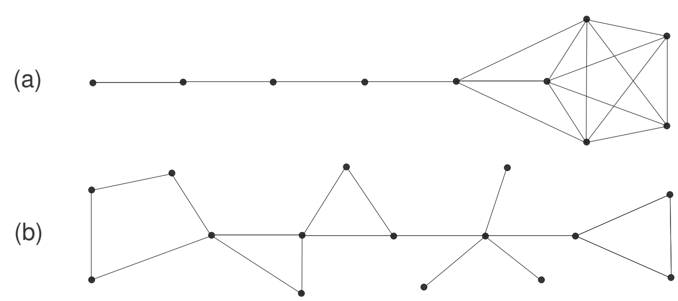

Figure 2.1: (a) A path-complete graph $PK_{10,5}$ obtained by joining an end-vertex of P_5 with three vertices of K_5. (b) A cactus $Cat(15,4)$.

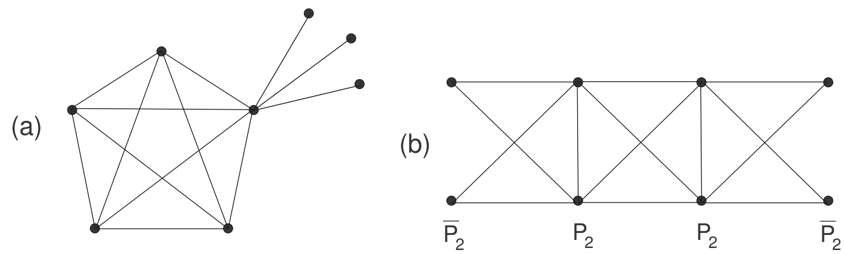

Figure 2.2: (a) The graph K_8^3. (b) A graph in $\mathcal{H}_{4n}$ with $G \cong P_2$.

Let G be n-vertex graph and $\overline{G}$ be its complement, and let G_1, G_2, G_3, G_4 denote four copies of G. Let $\mathcal{G}_{4n}$ represent the all graphs such that $V(\mathcal{G}_{4n}) = \cup_{i=1}^{4} V(G_i)$ and $E(\mathcal{G}_{4n}) = \cup_{i=1}^{4} E(G_i) \cup \{vw \mid v \in V(G_i) \text{ and } w \in V(G_{i+1}),\ 1 \leq i \leq 3\}$. Let $\mathcal{H}_{4n}$ denote the collection of those graphs in $\mathcal{G}_{4n}$ which are obtained by replacing G_1 and G_4 with $\overline{G}$. Similarly, $\mathcal{H}_{4n+1}$ denotes the graphs which are obtained from $\mathcal{H}_{4n}$ by adding a new vertex which is adjacent with all vertices of G_2 and G_3. In the following theorem, all self-complementary graphs with extremal average distance are determined.

Theorem 2.4.9 (Hendry [77])**.** *Let G be a self-complementary graph of order n.*

(i) *If* $n \equiv 0 \pmod 4$*, then*

$$\frac{3n(n-1)}{4} \leq W(G) \leq \frac{n(n-1)(13n-12)}{16n-16},$$

where left equality holds iff G is a graph with diameter 2, and the right equality holds iff $G \in \mathcal{H}_{4n}$.

(ii) *If* $n \equiv 1 \pmod 4$*, then*

$$\frac{3n(n-1)}{4} \leq W(G) \leq \frac{n(n-1)(13n-1)}{16n},$$

where left equality holds iff G has diameter 2, and equality on the right holds iff $G \in \mathcal{H}_{4n+1}$.

For graphs G and H, the graph G is said to be $\{H\}$-free (or simply H-free) if there is no subgraph of G isomorphic to H. In the following, minimal graphs corresponding to Wiener and Wiener-polarity index are determined amongst all n-vertex connected $\{C_3, C_4\}$-free graphs having size m.

Theorem 2.4.10 (Zhou and Gutman [150])**.** *Let G be an n-vertex connected triangle- and quadrangle-free graph having m edges. Then*

$$W(G) \geq \frac{3n(n-1)}{2} - \frac{1}{2}M_1(G) - m,$$

where equality holds iff G is a graph of diameter $d \leq 3$.

Theorem 2.4.11 (Zhou et al. [147]). *Let G be an n-vertex connected triangle- and quadrangle-free graph having m edges. Then*

$$WW(G) \geq 3n(n-1) - \frac{3}{2}M_1(G) - 2m,$$

where equality holds iff diamG ≤ 3.

The following proposition give the increasing property of $W(G)$ and $WW(G)$ with respect to edge addition.

Proposition 1 (Xua et al. [141]). *Let G be a connected graph with $e \notin E(G)$. Then we have $W(G) > W(G+e)$ and $WW(G) > WW(G+e)$.*

In the following theorems, the path P_n and star S_n are proved, by several authors, to be the maximal and minimal graphs for $W(G)$ and $WW(G)$, respectively.

Theorem 2.4.12 (Entringer et al. [35], Gutman et al. [65], Rada [109]). *Let T be an n-vertex tree. Then $W(S_n) \leq W(T) \leq W(P_n)$, where left equality is satisfied iff $T \cong S_n$ and right equality is satisfied iff T is a path.*

Theorem 2.4.13 (Gutman et al. [65]). *Let T be an n-vertex tree. We have $WW(S_n) \leq WW(T) \leq WW(P_n)$, where left equality holds iff $T \cong S_n$ and right equality holds iff T is a path.*

The extremal graphs with maximal Wiener and hyper-Wiener index among all graphs are determined in the following.

Corollary 2.4.1 (Entringer et al. [35]). *Let G be an n-vertex connected. Then $W(G) \leq W(P_n)$, where the equality holds iff G is a path.*

Corollary 2.4.2 (Xua et al. [141]). *Let G be a connected graph of order n. Then $WW(G) \leq WW(P_n)$, where the equality holds iff G is a path.*

The dumbbell $D(n,p,q)$ consists of a path P_{n-p-q} with p mutually non-adjacent vertices adjacent to one pendent vertex of P_{n-p-q} and rest of q mutually non-adjacent vertices adjacent to other pendent vertex of P_{n-p-q}.

Deng [28] determined the maximal values for Wiener polarity for chemical trees, but he did not characterize the corresponding extremal trees.

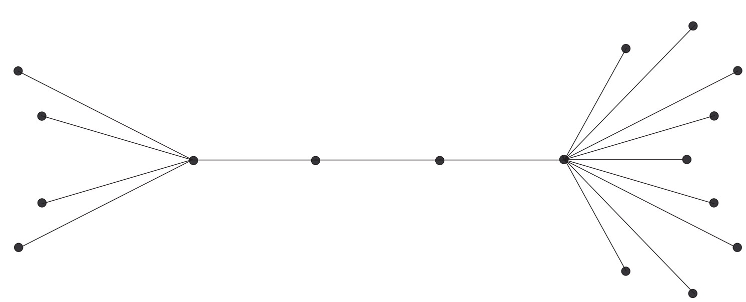

Figure 2.3: The dumbbell graph $D(17,4,9)$.

Theorem 2.4.14 (Liu and Liu [97]). *Let T be an n-vertex tree different from S_n. Then $W_P(T) \geq W_P(D(n, n-k-b, b))$, where the equality holds iff $T \cong D(n, n-k-b, b)$ with $k \geq 3$ and $n-k \geq b \geq 0$.*

Arockiraj et al. [2] developed a new technique based on the cut-method to compute WW for silicate and oxide networks. They also obtained the analytical expressions of Wiener polarity indices for these networks. Chen et al. [21] studied the Wiener polarity index of lattice networks, which include square, hexagonal, triangular lattices and the $3^3 \cdot 4^2$-lattices. For more results on extremal graphs for distance-based indices, see [141].

Next, we discuss some indices based on eccentricities and the corresponding graph extremals. For a graph G, Zhou and Du [148] studied the mathematical properties of $\xi^c(G)$.

Theorem 2.4.15. *Let G be a connected graph of size m. Then*

$$2m \cdot \mathrm{rad}(G) \leq \xi^c(G) \leq 2m \cdot \mathrm{diam}(G),$$

where both equalities hold iff G is a self-centered graph.

Theorem 2.4.16 (Zhou and Du [148] and Morgan et al. [101]). *Let G be a connected n-vertex graph with n at least 4, we have $\xi^c(G) \geq 3(n-1)$, where equality holds iff G is the star S_n.*

Corollary 2.4.3 (Zhou and Du [148]). *For a unicyclic graph G having order at least 4. Then $\xi^c(G) \geq 3n+1$, such that the equality holds iff G can be obtained by joining two non-adjacent vertices of S_n by an edge.*

Theorem 2.4.17 (Morgan et al. [101]). *For an n-vertex tree T with $n \geq 2$. We have*

$$\xi^c(T) \leq \xi^c(P_n) = \begin{cases} \frac{1}{2}(3n^2 - 6n + 4) & \text{for } n \cong 0 \pmod 2 \\ \frac{3}{2}(n-1)^2 & \text{for } n \cong 1 \pmod 2. \end{cases}$$

Corollary 2.4.4 (Zhou and Du [148]). *For a bicyclic graph G having order at least 5. We have $\xi^c(G) \geq 3n+5$, such that the equality holds iff G can be constructed by joining two pairs of non-adjacent vertices of S_n.*

Following result gives a relationship between ξ^c and DD.

Proposition 2 (Zhou and Du [148]). *Consider a connected graph G having order at least 2. We have $\xi^c(G) \geq \frac{1}{n-1} DD(G)$, with equality iff G is a complete graph.*

Eskender and Vumar [40] studied ξ^c of generalized hierarchical product [11] of graphs and some F-sum graphs [34]. The maximal and minimal values of $\xi^c(G)$ and corresponding graphs are obtained in [101, 145]. For further details on eccentric-connectivity index, see [102, 148].

Shi [126] proved some conjectures relating the Wiener and Randić index of graphs for trees. Qi and Du [106] studied the eccentricity version of Zagreb indices for trees. The maximal and minimal values of ξ^c and graphs corresponding to these values in several graph families are obtained in [102, 103, 145].

Liang and Liu [95] proved a conjecture on the relation between the average-eccentricity and Randić index. Dankelmann and Mukwembi [24] obtained upper bounds on the average-eccentricity in terms of several graph parameters. Smith et al. [129] studied the extremal values of total-eccentricity index in trees. Ilić [84] studied some maximal and minimal graphs corresponding to average-eccentricity. Farooq et al. [53] studied the extremal trees, unicyclic and bicyclic graphs and extremal conjugated trees for total-eccentricity index. Farooq and Malik [52] studied the extremal conjugated unicyclic and bicyclic graphs for total-eccentricity index.

Vukićević and Gašperov [137] tested some special and interesting discrete adriatic indices. These indices were shown to have very good predictive properties. The inverse sum indeg index (ISI index) is one of these indices defined as follows.

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)}. \tag{2.13}$$

Sedlar et al. [124] studied graph-theoretical properties of the ISI index and determined its extremal values in several classes of graphs. In [20] the authors derived some bounds and corresponding extremal graphs for ISI in terms of vertex (edge) connectivity, chromatic number, vertex bipartiteness, etc.

The inverse degree $r(G)$ of G is the sum of reciprocals of the vertex degrees in G. It was first introduced in the conjectures generated by a computer program Graffiti [51]. This index is given by

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

The relationship of $r(G)$ with other graph parameters has been studied by various authors. Mukwembi [104] studied lower and upper bounds for inverse degree $r(G)$ in terms of several graph parameters. Sardana and Madan [123] studied relation between of W and ξ^{sv} to detect the activities of some chemicals. Qu and Cao [107] gave some elementary bounds on $\xi^{sv}(G)$ and also discussed the increasing property of $\xi^{sv}(G)$ for graphs.

Lemma 2.4.5 (Qu and Cao [107]). *Let $G \ncong K_n$ be an n-vertex connected graph and $e \in E(\overline{G})$. Then $\xi^{sv}(G) > \xi^{sv}(G+e)$.*

Theorem 2.4.18 (Qu and Cao [107]). *Let G be an n-vertex connected graph. Then $\xi^{sv}(G) \geq n$, with equality holding iff $G \cong K_n$. If $G \ncong K_n$, then*

$$\xi^{sv}(G) \geq n - 2 + \frac{4n}{n-2},$$

where equality holds iff $G \cong K_n - e$, where $e \in E(K_n)$.

Theorem 2.4.19 (Qu and Cao [107]). *Let G be an n-vertex connected graph with maximum degree Δ. Then*

$$\xi^{sv}(G) \geq 2n - \Delta + 4(n - \Delta - 1)(\frac{1}{\Delta} + \frac{1}{n-2}),$$

where equality holds iff $G \cong K_\Delta + (K_1 \cup K_{n-\Delta-1})$.

Hua and Yu [82] derived bounds for ξ^{sv} in terms of Wiener index, total-eccentricity and minimum degree.

Theorem 2.4.20 (Hua and Yu [82]). *Consider an n-vertex connected graph G having at least 3 vertices. Then*

$$\xi^{sv}(G) \geq \tau(G),$$

where equality holds iff $G \cong K_n$.

Theorem 2.4.21 (Hua and Yu [82]). *Consider an n-vertex connected graph G having at least 3 vertices and minimum degree δ. Then*

$$\xi^{sv}(G) \leq \frac{2(n-\delta)}{\delta} W(G),$$

where equality holds iff $G \cong K_n$ or $G \cong K_n - \frac{n}{2}e$ for even n.

Bielak and Wolska [12] extended the results of Hua and Yu [82] and give bounds for $\xi^{sv}(G)$. The ξ^{sv} of one pentagonal carbon nanocones was studied in [100].

For any n-vertex tree T with $n \geq 5$, different from path and star, P_n and S_n should be the extremals of all indices which measure the branching in a molecule. We can observe that most of the distance-based indices satisfy this basic requirement to be branching measures. For topological indices defined in terms of distances, the question that which n-vertex trees have their extremals other than S_n and P_n, is still open [65].

2.5 Energy and Estrada index of graphs

Gutman [60] defined the concept of energy of a simple graph for the first time in 1978, whereas Estrada defined the notion of Estrada index in 2000. A huge number of research papers have been published since then, focusing on their mathematical properties as well as their applications. Many variations of these indices have also been introduced, such as Laplacian Estrada index [132,151], Siedel Estrada index [6], Gaussian Estrada index [45], Zagreb energy and Zagreb Estrada index [108], harmonic energy and harmonic Estrada index [87], etc.

Determining the eigenvalues of a graph is a challenging problem. This complication gave the motivation to study the upper and lower bounds for these indices. Attempts have also been made to use computational tools, such as MATLAB, HyperChem [86] and TOPOCLUJ [30], for calculating the eigenvalues of a graph and several spectrum-based indices of graphs.

In the following, we give some important bounds on energy of a graph and then we briefly describe some results obtained by computational techniques/softwares approximating these indices.

Theorem 2.5.1 (McCelland [99]). *If G is a graph of order n and size m, then*

$$\sqrt{2m + n(n-1)\det(A(G))^{\frac{2}{n}}} \leq \mathcal{E}(G) \leq \sqrt{2mn}.$$

A graph G is said to be non-singular if $\det(A(G)) \neq 0$, where $\det(A(G))$ denotes the determinant of $A(G)$. In the following, we give the lower bound of energy of non-singular graphs.

Theorem 2.5.2 (Das et al. [25]). *If G is an n-vertex non-singular graph having m edges, we have $\mathcal{E}(G) \geq \sqrt{2m + n(n-1)} \geq n$.*

Theorem 2.5.3 (Caporossi et al. [17]). *If G is a graph of size m, then $2\sqrt{m} \leq \mathcal{E}(G) \leq 2m$, with equality on the left side iff G is complete bipartite with some isolated vertices and equality on the right side iff G is a matching of m edges with some isolated vertices.*

Theorem 2.5.4 (Gutman [61]). *If G is an n-vertex graph, then $\mathcal{E}(G) \geq 2\sqrt{n-1}$, with equality iff $G \cong K_{1,n-1}$.*

Koolen and Moulton [91] conjectured that for a given $\epsilon > 0$, there exists a graph G of order n such that for almost all $n \geq 1$, $\mathcal{E}(G) \geq (1-\epsilon)\frac{n}{2}(\sqrt{n}+1)$, which was later proved by Nikiforov [105]

Peña et al. [26] gave the following bound for an n-vertex graph having size m.

Theorem 2.5.5 (Peña et al. [26]). *Let G be an n-vertex graph having size m. Then $\mathcal{EE}(G)$ satisfies*

$$\sqrt{n^2+4m} \leq \mathcal{EE}(G) \leq n-1+e^{\sqrt{2m}},$$

where equality holds on both sides iff $G \cong \overline{K}_n$.

Peña et al. [26] conjectured that path and star graphs are minimal and maximal for $\mathcal{EE}$, respectively. This conjecture was proved in 2009 by Deng [27]. In the same paper, the author also proved these bounds to be true for all graphs. Zhang et al. [144] determined the unique tree with maximum $\mathcal{EE}$ among all n-vertex trees with given matching number and also with given diameter. Some more bounds on $\mathcal{EE}$ can be found in [10, 149]. Some upper bounds for the $\mathcal{EE}$ of bipartite graphs are presented in [131]. The authors in [67] used a Monte Carlo approach to approximate the $\mathcal{EE}$ of graphs.

Ashrafi [3] studied the experimental results on energy $\mathcal{E}$ and Estrada index $\mathcal{EE}$ of nanotubes by using software tools such as MATLAB, HyperChem and TOPOCLUJ. Tabar et al. [133] computed the lower bounds on the $\mathcal{EE}$ of molecular graphs of some dendrimers. Similarly, Ashrafii and Sadati [5] and Hayat et al. [76] studied the $\mathcal{E}$ and $\mathcal{EE}$ of one pentagonal nanocones by using computational tools.

Chapter 3

Extremal graphs for total-eccentricity index

In this chapter, we find extremal trees, unicyclic and bicyclic graphs for total-eccentricity index. Moreover, we find extremal conjugated graphs for total-eccentricity index in all of these families.

3.1 Preliminaries and basic results

The basic calculation of the total-eccentricity index can be performed for some special families of graphs as an introductory exercise. For an n-vertex graph G with $n \geq 4$, a few such calculations are performed below.

1. For a k-regular graph G, we have $\tau(G) = \frac{\xi(G)}{k}$,
2. $\tau(K_n) = n$,
3. $\tau(K_{m,n}) = 2(m+n)$, where $m, n \geq 2$,
4. The total-eccentricity index of a star S_n, a cycle C_n and a path P_n is given by

$$\tau(S_n) = 2n - 1, \tag{3.1}$$

$$\tau(C_n) = \begin{cases} \frac{n}{2} & \text{if } n \equiv 0(\text{mod}2) \\ \frac{n-1}{2} & \text{if } n \equiv 1(\text{mod}2), \end{cases}$$

$$\tau(P_n) = \begin{cases} \frac{3n^2}{4} - \frac{n}{2} & \text{if } n \equiv 0(\text{mod}2) \\ \frac{3n^2}{4} - \frac{n}{2} - \frac{1}{4} & \text{if } n \equiv 1(\text{mod}2). \end{cases} \tag{3.2}$$

This chapter is structured as follows: In Section 3.2, we study extremal trees corresponding to the total-eccentricity index. In Section 3.3, we study the extremal unicyclic and bicyclic graphs for total-eccentricity index and Section 3.4 deals with the study of extremal conjugated trees for total-eccentricity index. In Section 3.5, we study the extremal conjugated unicyclic and bicyclic graphs corresponding to the total-eccentricity index.

3.2 Extremal trees for total-eccentricity index

It is known that the star and the path respectively minimizes and maximizes the total-eccentricity index among all trees of a given order [23,129]. We go further and for a given tree T with n vertices, $n \geq 4$, we find a sequence of n-vertex trees $T_1, T_2, \ldots, T_k$ such that

$$\tau(T) < \tau(T_1) < \ldots < \tau(T_k) = \tau(P_n). \tag{3.3}$$

Similarly, for a given tree T with n vertices, $n \geq 4$, we find a sequence of n-vertex trees $T'_1, T'_2, \ldots, T'_l$ such that

$$\tau(T) > \tau(T'_1) > \ldots > \tau(T'_l) = \tau(S_n). \tag{3.4}$$

Consider an n-vertex tree T with vertex set $V(T)$ and edge set $E(T)$. The following inequalities are easy to see:

$$\begin{aligned} &\mathrm{rad}(T) \leq \mathrm{diam}(T) \leq 2\,\mathrm{rad}(T), &(3.5)\\ &\frac{1}{2}\mathrm{diam}(T) \leq \mathrm{rad}(T) \leq e_T(v), \quad \forall\ v \in V(T). \end{aligned}$$

Recall that the radius of a connected graph G is defined as:

$$\mathrm{rad}(G) = \min\{e_G(v) \mid v \in V(G)\}. \tag{3.6}$$

A vertex $v \in V(T)$ is said to be an eccentric vertex of a vertex $u \in V(T)$ if $d_T(u, v) = e_T(u)$. Let $E_T(u)$ denote the set of all eccentric vertices of u in T. For any $w \in E_T(u)$, the shortest (u, w)-path is called an eccentric path for u. It is known that the center of a tree is K_1 if $\mathrm{diam}(T) = 2\mathrm{rad}(T)$ and is K_2 if $\mathrm{diam}(T) = 2\mathrm{rad}(T) - 1$ [88]. Moreover, every diametrical path in a tree T contains $C(T)$ [19]. Clearly every diametrical path in T is an eccentric path for some peripheral vertex v in T. In the next lemma, we prove a result about the eccentric vertices in a tree.

Lemma 3.2.1. *Let T be an n-vertex tree and P be a diametrical (u, v)-path in T. Then for any $x \in V(T)$, either $u \in E_T(x)$ or $v \in E_T(x)$.*

Proof. Let $x \in V(T)$. On contrary, assume that $u \notin E_T(x)$ and $v \notin E_T(x)$. Let $v' \in E_T(x)$. Without loss of generality, assume that $d_T(x, v) \geq d_T(x, u)$. Then

$$d_T(x, v') > d_T(x, v) \geq d_T(x, u). \tag{3.7}$$

Let $u', u'' \in V(P)$ such that $d_T(x, u') = \min\{d_T(x, w) \mid w \in V(P)\}$ and $d_T(v', u'') = \min\{d_T(v', w) \mid w \in V(P)\}$. Then

$$\begin{aligned} d_T(x, v') &= d_T(x, u') + d_T(u', v') &(3.8)\\ d_T(x, v) &= d_T(x, u') + d_T(u', v) &(3.9)\\ d_T(x, u) &= d_T(x, u') + d_T(u', u). \end{aligned}$$

From (3.7)-(3.9), we obtain

$$d_T(u', v') > d_T(u', v). \tag{3.10}$$

Also inequality (3.7) together with equations (3.9) and (3.10) gives

$$d_T(u', v) \geq d_T(u', u). \tag{3.11}$$

We consider following three cases:
Case 1. When P and (x, v')-path have a vertex in common. If u'' lies on (x, v)-path then by using (3.10), we get

$$\begin{aligned} d_T(u, v') &= d_T(u, u') + d_T(u', v') \\ &> d_T(u, u') + d_T(u', v) \\ &= d_T(u, v) = \text{diam}(T). \end{aligned}$$

This contradicts the fact that P is a diametrical path.
Case 2. If u'' lies on (x, u)-path then using (3.10) and (3.11), we obtain

$$\begin{aligned} d_T(v, v') &= d_T(v, u') + d_T(u', v') \\ &> d_T(u, u') + d_T(u', v) \\ &= d_T(u, v) = \text{diam}(T). \end{aligned}$$

This is again a contradiction.

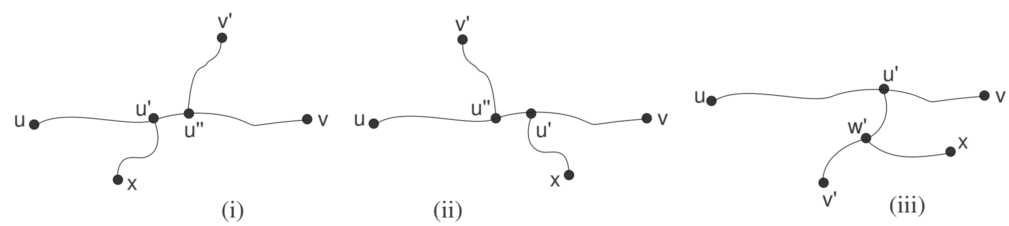

Figure 3.1: The trees corresponding to the cases discussed in Lemma 3.2.1.

Case 3. When P and (x, v')-path have no vertex in common. We denote (u, v')-path by P'. Let $w' \in V(P')$ such that $d_T(x, w') = \min\{d_T(x, w) \mid w \in V(P')\}$. Then

$$d_T(x, v') = d_T(x, w') + d_T(w', v') \tag{3.12}$$

$$d_T(x, v) = d_T(x, w') + d_T(w', v). \tag{3.13}$$

Inequality (3.7) along with equations (3.12) and (3.13) gives

$$d_T(w', v') > d_T(w', v). \tag{3.14}$$

Using (3.14), we obtain

$$\begin{aligned} d_T(u, v') &= d_T(u, w') + d_T(w', v') \\ &> d_T(u, w') + d_T(w', v) \\ &= d_T(u, u') + d_T(u', w') + d_T(w', u') + d_T(u', v) \\ &= d_T(u, v) + 2d_T(u', w') \geq \text{diam}(T), \end{aligned}$$

which is a contradiction. The proof is complete. □

In the next result, we construct a new tree from the given tree with larger total-eccentricity index.

Lemma 3.2.2. *Let $T \ncong P_n$ be an n-vertex tree, $n \geq 4$, and u, v be the end-vertices of a diametrical path in T. Take a pendant vertex x of T distinct from u and v and let y be the unique neighbour of x. Construct a tree $T' \cong \{T - \{xy\}\} \cup \{xu\}$. Then $\tau(T) < \tau(T')$.*

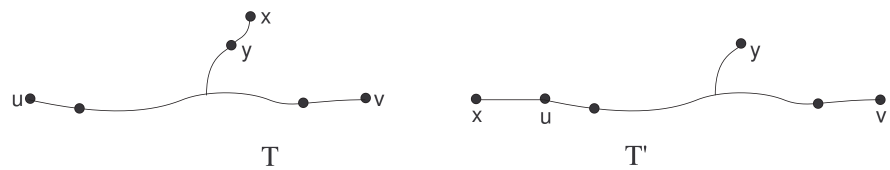

Figure 3.2: The trees T and T' constructed in Lemma 3.2.2.

Proof. We note that (x, v)-path is a diametrical path in T' and

$$e_{T'}(x) = e_T(u) + 1 = \text{diam}(T) + 1 > e_T(x). \tag{3.15}$$

By the construction of T', we have

$$\begin{align} d_{T'}(w, v) &= d_T(w, v) \qquad \forall\ w \in V(T) \setminus \{x\} \tag{3.16}\\ d_{T'}(w, x) &= d_T(w, u) + 1 \qquad \forall\ w \in V(T) \setminus \{x\}. \tag{3.17}\end{align}$$

By Proposition 3.2.1, we have

$$\begin{align} e_T(w) &= \max\{d_T(w, u), d_T(w, v)\} \qquad \forall\ w \in V(T) \tag{3.18}\\ e_{T'}(w) &= \max\{d_{T'}(w, x), d_{T'}(w, v)\} \qquad \forall\ w \in V(T). \tag{3.19}\end{align}$$

Thus for each $w \in V(T) \setminus \{x\}$, equations (3.16)-(3.19) imply

$$\begin{align} e_{T'}(w) &= \max\{d_{T'}(w, x), d_{T'}(w, v)\} = \max\{d_T(w, u) + 1, d_T(w, v)\} \\ &\geq \max\{d_T(w, u), d_T(w, v)\} = e_T(w). \tag{3.20}\end{align}$$

Thus, from inequalities (3.15)-(3.20), we obtain

$$\begin{aligned} \tau(T') &= \sum_{w \in V(T) \setminus \{x\}} e_{T'}(w) + e_{T'}(x) \\ &> \sum_{w \in V(T) \setminus \{x\}} e_T(w) + e_T(x) \\ &= \tau(T). \end{aligned}$$

This completes the proof. $\square$

Now we find the trees with minimal and maximal total-eccentricity index among the class of n-vertex trees. We device an algorithm to reduce a given tree into a path. Let T be an n-vertex tree, $n \geq 4$ and let $u, v \in V(T)$ be the end-vertices of a diametrical path in T. Define

$$A_{u,v} = \{xy \in E(T) \mid d_T(x) = 1, x \in V(T) \setminus \{u, v\}\}. \tag{3.21}$$

Algorithm 1

input:	An n-vertex tree T, $n \geq 4$.
output:	The tree P_n.
Step 0:	Take a diametrical (u, v)-path in T and define $A_{u,v}$ by (3.21).
Step 1:	If $A_{u,v} = \emptyset$ then Stop.
Step 2:	For an $xy \in A_{u,v}$ define $T := \{T - \{xy\}\} \cup \{ux\}$. Set $u := x$ and update $A_{u,v}$ by (3.21); go to Step 1.

Next, we discuss the termination and correctness of Algorithm 1. When the algorithm goes from Step A to Step B, we will use the notation [Step A $\rightarrow$ Step B].

Theorem 3.2.1 (Termination)**.** *The Algorithm 1 terminates after a finite number of iterations.*

Proof. Initially $A_{u,v}$ is defined at Step 0 and modified at Step 2 in each iteration. Modification of $A_{u,v}$ at Step 2 implies that if a pendant edge is removed from $A_{u,v}$, it will not appear again in $A_{u,v}$ in the subsequent iterations of Algorithm 1. Thus [Step 2 $\rightarrow$ Step 1] is executed at most $n - 1$ times. Hence Algorithm 1 terminates after a finite number of iterations. □

Theorem 3.2.2 (Correctness)**.** *If Algorithm 1 terminates then it outputs P_n.*

Proof. We can obviously see that after the execution of Step 2 in any iteration of Algorithm 1, the modified graph T at Step 2 is again an n-vertex tree. Also, by definition of $A_{u,v}$, we see that T has exactly two pendant vertices when $A_{u,v} = \emptyset$. Thus, when Algorithm 1 terminates at Step 1, the tree T has exactly two pendant vertices, that is, $T = P_n$. □

Using Lemma 3.2.2 and Algorithm 1, we prove the following theorem.

Theorem 3.2.3. *Let $n \geq 4$. Then among the n-vertex trees, the path P_n has the maximal total-eccentricity index. Thus for any n-vertex tree T, we have $\tau(T) \leq \tau(P_n)$.*

Proof. Let $T \ncong P_n$ be an n-vertex tree. By Lemma 3.2.2, the total-eccentricity index of the modified tree T strictly increases at Step 2 in each iteration of Algorithm 1. The Algorithm 1 terminates when $T \cong P_n$. This shows that P_n has the maximal total-eccentricity index. □

Corollary 3.2.3. *Let T be a tree on n vertices, then*

$$\tau(T) \leq \frac{3n^2}{4} - \frac{n}{2}, \tag{3.22}$$

where equality holds when T is a path on n vertices and $n \equiv 0(\text{mod}2)$.

Proof. The result follows by using Theorem 3.2.3 and equation (3.2). □

By Lemma 3.2.2, we see that when the Algorithm 1 goes from Step 2 to Step 1, the total-eccentricity index of the modified tree strictly increases. Thus, if the Algorithm 1 terminates after k iterations, it generates a sequence of trees $T_1, T_2, \ldots, T_k$, of same order n satisfying (3.3).

Example 3.2.4. *Consider a tree T of order 9 shown in Figure 3.3. The Algorithm 1 will generate a sequence of trees $T_1, T_2, T_3 \cong P_9$ such that $\tau(T) < \tau(T_1) < \tau(T_2) < \tau(T_3) = \tau(P_9)$. We remark that this sequence is not unique. The modification of the tree at Step 2 depends upon the choice of pendant edge xy.*

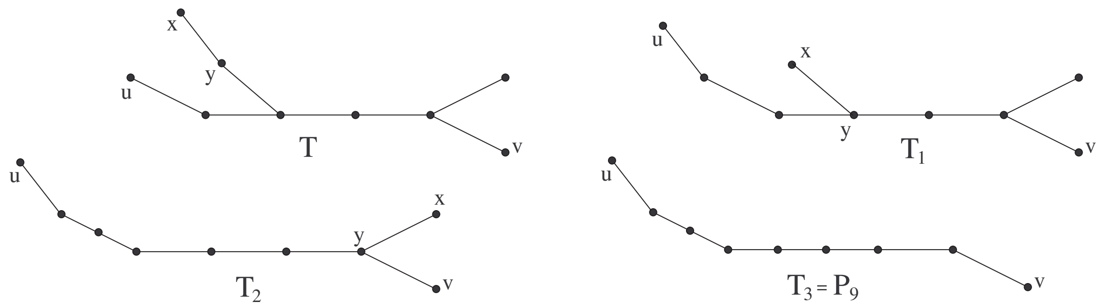

Figure 3.3: Sequence of trees generated by Algorithm 1 at Step 2 in each iteration.

Next we propose an algorithm to reduce a given tree into a star. Let T be an n-vertex tree and $c \in V(T)$ with $e_T(c) = \text{rad}(T)$. We define A_r by

$$A_r = \{xy \in E(T) \mid d_T(x, c) = \text{rad}(T)\}. \tag{3.23}$$

Algorithm 2

input: An n-vertex tree T, $n \geq 4$.
output: The tree S_n.
Step 0: Find rad(T) by (3.6), a vertex $c \in V(T)$ with $e_T(c) = \text{rad}(T)$ and define A_r by (3.23).
Step 1: If rad$(T) = 1$, then Stop.
Step 2: For an edge $xy \in A_r$, define $T := \{T - \{yx\}\} \cup \{cx\}$ and $A_r := A_r \setminus \{xy\}$.
Step 3: If $A_r \neq \emptyset$ then go to Step 2; else define rad(T) by (3.6) and A_r by (3.23); go to Step 1.

Next, we discuss the correctness and termination of the Algorithm 2.

Theorem 3.2.4 (Termination)**.** *The Algorithm 2 terminates after a finite number of iterations.*

Proof. Note that initially rad(T) and A_r are defined at Step 0. The set A_r reduces at Step 2. If [Step 3 → Step 2] is executed then A_r reduces. Thus [Step 3 → Step 2] can be executed for a finite number of times. If $A_r = \emptyset$ at Step 3 then r decreases at Step 3. Thus [Step 3 → Step 1] can be executed for a finite number of times. Therefore the algorithm will terminate after a finite number of iterations. □

Theorem 3.2.5 (Correctness)**.** *If Algorithm 2 terminates then it outputs S_n.*

Proof. When Algorithm 2 terminates at Step 1 then $\mathrm{rad}(T) = 1$ and c remains the central vertex of T, that is, $d_T(c, x) = 1$ for all $x \in V(T) \setminus \{c\}$. This shows that $T \cong S_n$. □

The following theorem gives trees with minimal total-eccentricity index.

Theorem 3.2.6. *Among all n-vertex trees with $n \geq 4$, the star S_n has minimal total-eccentricity index.*

Proof. Let $T \ncong S_n$ be an n-vertex tree, $n \geq 4$ and let c be a central vertex of T. Define A_r by (3.23). We construct a new set of edges not in $E(T)$ by

$$\tilde{A}_r = \{cx \mid x \in V(T) \text{ with } d_T(x, c) = \mathrm{rad}(T)\}$$

and define a tree T' by

$$T' \cong \{T - A_r\} \cup \tilde{A}_r.$$

Then we note that $\mathrm{rad}(T') = \mathrm{rad}(T) - 1$. Thus by the construction of T', we observe that

$$e_{T'}(u) \leq e_T(u) \quad \forall\, u \in V(T). \tag{3.24}$$

Moreover, c is a central vertex of T', that is,

$$e_{T'}(c) = \mathrm{rad}(T) - 1 < e_T(c). \tag{3.25}$$

From (3.24) and (3.25), we obtain

$$\tau(T') < \tau(T).$$

In fact, if T is a tree at Step 1 with $\mathrm{rad}(T) > 1$ in any iteration of Algorithm 2, then T' is a tree at Step 3 when $A_r = \emptyset$. Thus when [Step 3 → Step 1] is executed, the total-eccentricity index strictly decreases. Since Algorithm 2 outputs S_n, we have $\tau(S_n) < \tau(T)$. Thus the assertion holds. □

Corollary 3.2.5. *For an n-vertex tree T, we have*

$$\tau(T) \geq 2n - 1. \tag{3.26}$$

Proof. By Theorem 3.2.6 and equation (3.1), the proof is obvious. □

From the proof of Theorem 3.2.6, we note that when [Step 3 → Step 1] is executed, the total-eccentricity index of the modified tree strictly decreases. Thus, if the Algorithm 2 terminates after l iterations, it generates a sequence of trees $T'_1, T'_2, \ldots, T'_l$, of same order n satisfying (3.4).

Example 3.2.6. *Consider a tree T of order 14 shown in Figure 3.4. The Algorithm 2 will generate a sequence of trees $T'_1, T'_2, T'_3 \cong S_{14}$ such that $\tau(T) > \tau(T'_1) > \tau(T'_2) > \tau(T'_3) = \tau(S_{14})$. We remark that this sequence is not unique. The modification of the tree at Step 2 depends upon the choice of pendant edge xy. The step-wise procedure is explained in Figure 3.4.*

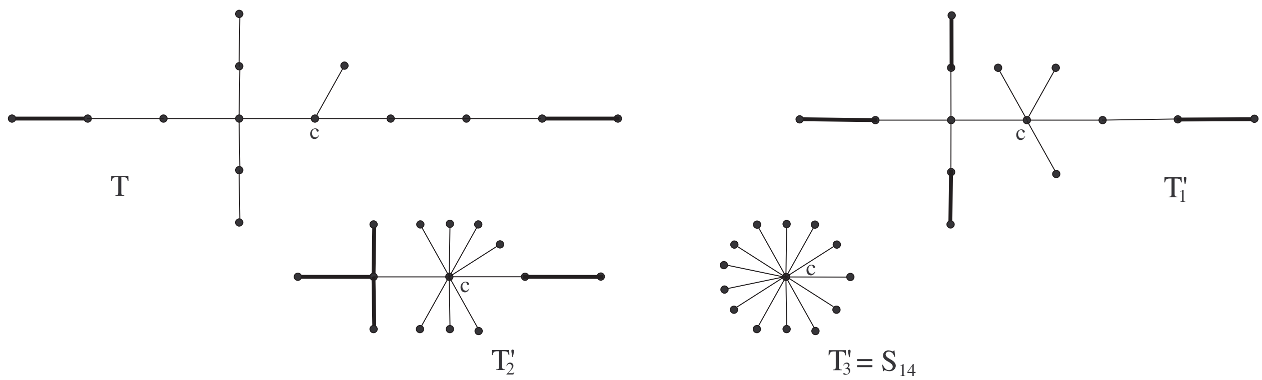

Figure 3.4: Sequence of trees generated by Algorithm 2 when [Step 2 → Step 1] is executed.

3.3 Extremal unicyclic and bicyclic graphs for total-eccentricity index

In this section, we find graphs with minimal and maximal total-eccentricity index among the n-vertex unicyclic and bicyclic graphs. In the next theorem, we find the graph with minimal total-eccentricity index among all unicyclic graphs.

Theorem 3.3.1. *Among all n-vertex unicyclic graphs, $n \geq 4$, the graph U_1 shown in Figure 3.5 has the minimal total-eccentricity index.*

Proof. Let $U \ncong U_1$ be an n-vertex unicyclic graph, $n \geq 4$. Then $e_U(u) \geq 2$ for each $u \in V(U)$. Note that $e_{U_1}(u) \leq 2$ for each $u \in V(U_1)$. Thus

$$\tau(U) \geq \tau(U_1).$$

The proof is complete. □

Corollary 3.3.1. *For any unicyclic graph U, $\tau(U) \geq 2n - 1$.*

Proof. After simple computation we see that $\tau(U_1) = 2n - 1$. Thus the proof is obvious by using Theorem 3.3.1. □

In the next theorem, we find an n-vertex unicyclic graph with maximal total-eccentricity index.

Theorem 3.3.2. *Among all n-vertex unicyclic graphs, $n \geq 4$, the graph U_2 shown in Figure 3.5 has maximal total-eccentricity index.*

Proof. Let $T \ncong P_n$ be an n-vertex tree and $T_1 \cong U_2 - \{v_1v_2\}$. We show that $\tau(T) \leq \tau(T_1)$. There exists a pendant vertex $u_1 \in V(T)$ such that $e_T(u) = e_{T-u_1}(u)$ for all $u \in V(T) \setminus \{u_1\}$. Then from Theorem 3.2.3, we obtain

$$\tau(T - u_1) \leq \tau(T_1 - v_1). \tag{3.27}$$

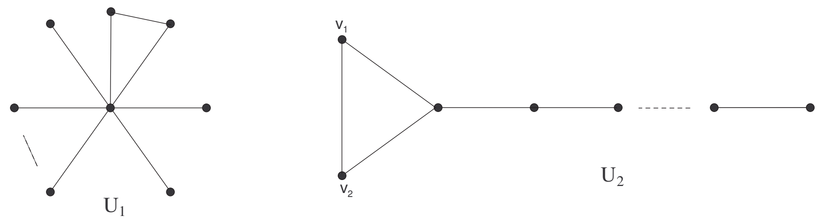

Figure 3.5: Extremal unicyclic graphs U_1 and U_2 for total-eccentricity index.

Note that $e_{T_1-v_1}(u) = e_{T_1}(u)$ for each $u \in V(T_1) \setminus \{v_1\}$ and $e_{T_1}(v_1) = n-2$. Thus

$$\tau(T_1) = \tau(T_1 - v_1) + n - 2. \tag{3.28}$$

Also, $e_{T-u_1}(u) = e_T(u)$ for each $u \in V(T) \setminus \{u_1\}$ and $e_T(u_1) \leq n-2$. Thus

$$\tau(T) \leq \tau(T - u_1) + n - 2. \tag{3.29}$$

From (3.27)-(3.29), we obtain

$$\tau(T) \leq \tau(T_1).$$

Also observe that $\tau(T_1) = \tau(U_2)$. Thus $\tau(T) \leq \tau(U_2)$. Now, if we join any two non-adjacent vertices in T, it gives us a unicyclic graph U and $\tau(U) \leq \tau(T)$. Thus, $\tau(U) \leq \tau(U_2)$. This completes the proof. □

Corollary 3.3.2. *For any unicyclic graph U, we have $\tau(U) \leq \frac{n(n-1)}{2} - 1$.*

Proof. After simple computation, we see that $\tau(U_2) = \frac{n(n-1)}{2} - 1$. Thus the proof is obvious by using Theorem 3.5.2. □

Now we find the extremal bicyclic graphs for total-eccentricity index. The following remark can be obtained by simple computation.

Remark 1. *Let B_1, B_1', B_2 and B_2' be n-vertex bicyclic graphs shown in Figure 3.6. Then the total-eccentricity index of these graphs is given by*

1. $\tau(B_1) = \tau(B_1') = 2n - 1.$
2. $\tau(B_2) = \begin{cases} \frac{3}{4}n^2 - \frac{3}{2}n - 2 & \text{when } n \text{ is even} \\ \frac{3}{4}n^2 - \frac{3}{2}n - \frac{9}{4} & \text{when } n \text{ is odd.} \end{cases}$
3. $\tau(B_2') = \begin{cases} \frac{3}{4}n^2 - n - 2 & \text{when } n \text{ is even} \\ \frac{3}{4}n^2 - n - \frac{7}{4} & \text{when } n \text{ is odd.} \end{cases}$

Remark 2. *Let G be a connected graph and C_k be a cycle of length k in G. Then each diametrical path in G contains at most $\lfloor \frac{k}{2} \rfloor + 1$ vertices of C_k and at most $\lfloor \frac{k}{2} \rfloor$ edges of C_k.*

Theorem 3.3.3. *Among all n-vertex bicyclic graphs, $n \geq 5$, the graph B_1 shown in Figure 3.6 has minimal total-eccentricity index.*

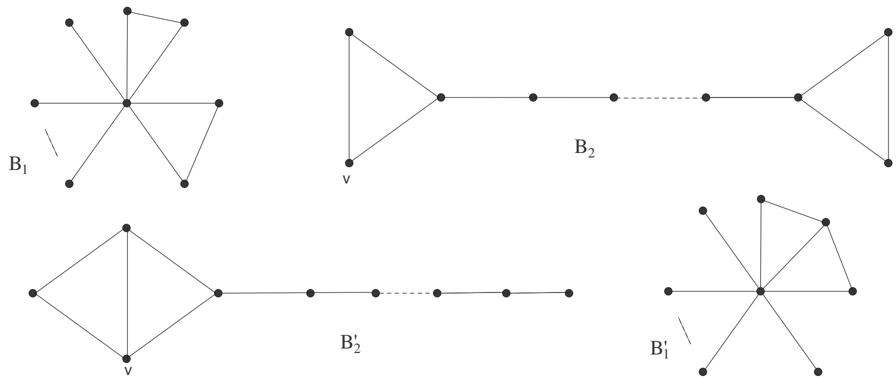

Figure 3.6: Bicyclic graphs B_1, B_1', B_2 and B_2'.

Proof. Consider a bicyclic graph $B \ncong B_1$. Then $e_B(v) \geq 2$ for all $v \in V(B)$. Since, $e_{B_1}(v) \leq 2$ for all $v \in V(B_1)$. Thus, $\tau(B_1) \leq \tau(B)$. □

Corollary 3.3.3. *For any bicyclic graph B, we have $\tau(B) \geq 2n - 1$.*

Proof. By Remark 1 and Theorem 3.3.3, the proof is obvious. □

Let $\mathcal{B}_1$ denotes the class of those n-vertex bicyclic graphs which have exactly two cycles, $n \geq 5$. Then the maximal graph corresponding to total-eccentricity index in $\mathcal{B}_1$ is obtained in the next result.

Lemma 3.3.4. *Among all n-vertex bicyclic graphs in $\mathcal{B}_1$, $n \geq 5$, the graph B_2 shown in Figure 3.6 has the maximal total-eccentricity index.*

Proof. First note that $B_2 - v \cong U_2$ and $\tau(B_2) = \tau(U_2) + n - 3$, where U_2 is the $n-1$ vertex unicyclic graph shown in Figure 3.5. Let $B \in \mathcal{B}_1$ be any n-vertex bicyclic graph. Then there exist two disjoint edges $e_1, e_2 \in E(B)$ such that $B - \{e_1, e_2\}$ is a tree and $B - \{e_1, e_2\}$ has at least four pendant vertices. Let $T \cong B - \{e_1, e_2\}$. Then

$$e_T(v) \leq n - 3, \quad \forall\, v \in V(T). \tag{3.30}$$

Obviously $\tau(B) \leq \tau(T)$. Since $T \ncong P_n$, using Lemma 3.2.1 there exists a pendant vertex $u_1 \in V(T)$ such that

$$e_T(u) = e_{T-u_1}(u), \quad \forall\, u \in V(T) \setminus \{u_1\}. \tag{3.31}$$

Note that $T - u_1 \ncong P_{n-1}$. Then as shown in the proof of Theorem 3.5.2 that

$$\tau(T - u_1) \leq \tau(U_2). \tag{3.32}$$

From (3.30) and (3.31), we obtain

$$\tau(T) \leq \tau(T - u_1) + n - 3. \tag{3.33}$$

From (3.32) and (3.33), we have

$$\tau(B) \leq \tau(T - u_1) + n - 3 \leq \tau(U_2) + n - 3 = \tau(B_2).$$

The proof is complete. □

Let $\mathcal{B}_2$ denotes the class of all n-vertex bicyclic graphs which have exactly three cycles, $n \geq 5$. Then we have the following result.

Lemma 3.3.5. *Among all n-vertex bicyclic graphs in $\mathcal{B}_2$, $n \geq 5$, the graph B_2' shown in Figure 3.6 has the maximal total-eccentricity index.*

Proof. Let $B_2' \in \mathcal{B}_2$ be the graph shown in Figure 3.6. Note that $B_2' - v \cong P_{n-1}$ and

$$\tau(B_2') = \tau(P_{n-1}) + n - 3. \tag{3.34}$$

We show that, B_2' has maximal total-eccentricity index in $\mathcal{B}_2$. Let $B \in \mathcal{B}_2$ with cycles C_{k_1}, C_{k_2} and C_{k_3}. Without loss of generality, assume that $k_1 \leq k_2 \leq k_3$. Then $3 \leq k_1, k_2 \leq n-1$ and $4 \leq k_3 \leq n$. Since B is not a path, it holds that $\text{diam}(B) \leq n-2$.

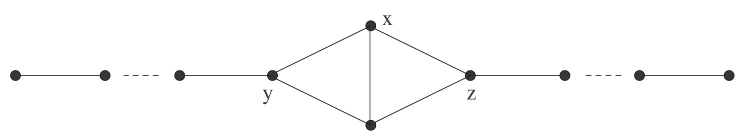

Figure 3.7: A bicyclic graph $B \in \mathcal{B}_2$. Here at most y or z are of degree 2.

Case 1. When $\text{diam}(B) = n-2$. Let P be a diametrical path in B. By Remark 2, P contains at most $\lfloor \frac{k}{2} \rfloor + 1$ vertices of C_{k_3}. With similar arguments, we have $k_1 = k_2 = 3$. Since length of P is $n-2$, there is exactly one vertex, say x, of C_{k_3} which does not belong to $V(P)$. Then x is a common vertex in C_{k_1}, C_{k_2} and C_{k_3} and $e_B(x) \leq n-3$. The graph in this case is shown in Figure 3.7. We see that $B - x \cong P_{n-1}$ and

$$\begin{aligned} \tau(B) &= \tau(P_{n-1}) + e_B(x) \\ &\leq \tau(P_{n-1}) + (n-1) \\ &= \tau(B_2'). \end{aligned}$$

Case 2. When $\text{diam}(B) \leq n-3$. Then there exist two edges $e_1, e_2 \in E(B)$ such that $T \cong B - \{e_1, e_2\}$ is a tree and

$$e_T(v) \leq n-3 \quad \forall\, v \in V(T).$$

Following Lemma 3.5.3, we can show that $\tau(B) \leq \tau(B_2')$. This completes the proof. □

From Lemma 3.5.3 and Lemma 3.3.5, we have the following result.

Theorem 3.3.4. *Among all n-vertex bicyclic graphs, $n \geq 5$, the graph B_2' shown in Figure 3.6 has the maximal total-eccentricity index.*

Proof. Since $\tau(B_2) < \tau(B_2')$, the assertion follows from Lemmas 3.5.3 and 3.3.5. □

Corollary 3.3.6. *For any bicyclic graph B, we have $\tau(B) \leq \frac{3}{4}n^2 - n - 2$.*

Proof. By using Remark 1 and Lemmas 3.5.3 and 3.3.5, the proof is obvious. □

3.4 Extremal conjugated trees for total-eccentricity index

Consider a conjugated n-vertex tree T with perfect a matching M, where $n \geq 2$. It can be observed that $|M| = \frac{n}{2}$. We define some families of trees which will be used in the later discussion. A subdivided star $S_{n,2}$, of order $2n-1$ is obtained by subdividing every edge in S_n once. A double star $DS_{k,n-k}$, where $k \geq 2$ and $n-k \geq 2$, of order n is obtained by joining the centers of the stars S_k and S_{n-k} by an edge. The graphs $S_{n,2}$ and $DS_{k,n-k}$ are shown in Figure 3.8.

The following results will be required to find extremal conjugated trees for total-eccentricity index. We construct a tree S_* by deleting a pendant vertex from $S_{n,2}$ as shown in Figure 3.8. We will see that S_* is the unique conjugated tree of order $2(n-1)$ with $\frac{2(n-1)}{2}$ pendant vertices.

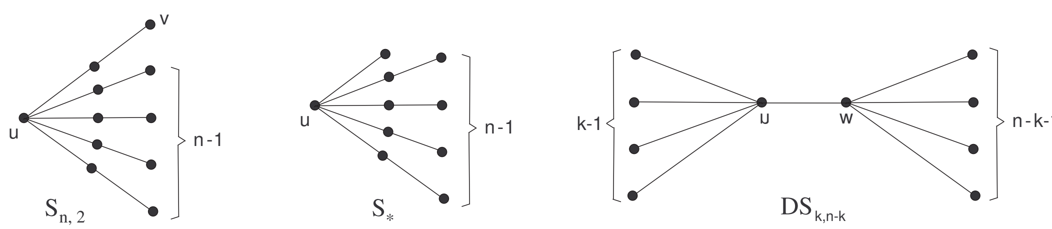

Figure 3.8: The subdivided star $S_{n,2}$, the tree $S_* \cong S_{n,2} - v$ and a double star $DS_{k,n-k}$.

Lemma 3.4.1. *Let T be an n-vertex tree with $n \geq 4$. When $\mathrm{diam}(T) = 3$ then $T \cong DS_{k,n-k}$, where $2 \leq k \leq n-2$.*

Proof. When $\mathrm{diam}(T) = 3$, we consider a diametrical path $v_1v_2v_3v_4$. Since $\mathrm{diam}(T) = 3$, the remaining $n-4$ vertices are adjacent to v_2 or v_3. Thus $T \cong DS_{k,n-k}$ for $2 \leq k \leq n-2$. □

Remark 3. *The total-eccentricity index of $S_{n,2}$, S_* and $DS_{k,n-k}$ is given by*

$$\tau(S_{n,2}) = \frac{7n}{2} - \frac{3}{2}, \quad \tau(S_*) = \frac{7n}{2} - 2 \quad \text{and} \quad \tau(DS_{k,n-k}) = 3n - 2.$$

Remark 4. *An n-vertex conjugated tree, $n \geq 4$, can have at most $\frac{n}{2}$ pendant vertices. If T is an n-vertex conjugated tree with exactly $\frac{n}{2}$ pendant vertices then $T \cong S_*$, where S_* is shown in Figure 3.8.*

Let T be an n-vertex conjugated tree, $n \geq 4$, with a perfect matching M and let c be a vertex in $V(T)$ with $e_T(c) = \mathrm{rad}(T)$. Let $w \in V(T)$ such that $d_T(c,w) = \mathrm{rad}(T)$. Then there exist $u, v \in V(T)$ such that uvw is a path of length 2 with $d_T(w) = 1$ and $vw \in M$. We denote the set of all such paths of length 2 in T by B_r and define it as follows.

$$B_r = \{uv \mid uvw \text{ is a path in } T \text{ with } d_T(c,w) = \mathrm{rad}(T)\}. \tag{3.35}$$

Now we proceed to find the conjugated trees with minimal total-eccentricity index. We first device an algorithm to construct the tree S_* from a given n-vertex tree T, $n \geq 4$.

Algorithm 3

input:	An n-vertex conjugated tree T, $n \geq 4$.
output:	The tree S_*.
Step 0:	Find rad(T) by (3.6), a vertex $c \in V(T)$ with $e_T(c) = \text{rad}(T)$ and define B_r by (3.35).
Step 1:	If rad(T) = 2, then Stop.
Step 2:	For an edge $uv \in B_r$, define $T := \{T - \{uv\}\} \cup \{cv\}$ and $B_r := B_r \setminus \{uv\}$.
Step 3:	If $B_r \neq \emptyset$ then go to Step 2; else define rad(T) by (3.6) and B_r by (3.35); go to Step 1.

Now we discuss the correctness and termination of Algorithm 3.

Theorem 3.4.1 (Termination)**.** *The Algorithm 3 terminates after a finite number of iterations.*

Proof. The proof follows from Theorem 3.2.4. □

Theorem 3.4.2 (Correctness)**.** *If the Algorithm 3 terminates then it outputs S_*.*

Proof. Let T be an n-vertex conjugated tree, $n \geq 4$, with a perfect matching M. Let $c \in V(T)$ such that $e_T(c) = \text{rad}(T)$. Define B_r by (3.35) and let $uv \in B_r$. Then there exists $w \in V(T)$ such that $d_T(w) = 1$ and $vw \in M$. Since T is conjugated, we have $d_T(v) = 2$ and $uv \notin M$. Therefore $\{T - \{uv\}\} \cup \{cv\}$ is also a conjugated tree with a perfect matching M. This shows that after the execution of Step 2 in any iteration of Algorithm 3, the modified graph at Step 2 is again an n-vertex conjugated tree. Thus, when Algorithm 3 terminates at Step 1, it outputs an n-vertex conjugated tree. We finally show that when the algorithm terminates at Step 1, then $T \cong S_*$.

By the modifications of the tree at Step 2, the vertex c remains the central vertex of the modified tree when [Step 3 → Step 1] is executed. If Algorithm 3 terminates at Step 1 then $\text{rad}(T) = 2$ and $e_T(c) = 2$. This shows that $d_T(c, x) \leq 2$ for each $x \in V(T)$ at Step 1. Since T is also a conjugated tree at Step 1, there is exactly one pendant vertex adjacent to c. This shows that $T \cong S_*$. □

Theorem 3.4.3. *Among all n-vertex conjugated trees, $n \geq 4$, the graph S_* shown in Figure 3.8 has the minimal total-eccentricity index.*

Proof. Let $T \ncong S_*$ be an n-vertex conjugated tree, $n \geq 4$, and let c be a central vertex of T. Define B_r by (3.35). We construct a new set of edges not in $E(T)$ by

$$\tilde{B}_r = \{cv \mid uv \in B_r, v, w \in V(T)\}$$

and define a new conjugated tree T' by

$$T' \cong \{T - B_r\} \cup \tilde{B}_r.$$

Then we note that rad(T') is $r - 1$ or $r - 2$. By the construction of T', we observe that

$$e_{T'}(x) \leq e_T(x) \quad \forall\, x \in V(T). \tag{3.36}$$

Moreover, since c is a central vertex of T', we have

$$e_{T'}(c) \leq \text{rad}(T) - 1 < e_T(c). \tag{3.37}$$

From (3.36) and (3.37), we obtain

$$\tau(T') < \tau(T).$$

In fact, if T is conjugated tree at Step 1 with $\text{rad}(T) > 2$ in any iteration of Algorithm 3, then T' is a conjugated tree at Step 3 when $B_r = \emptyset$. Thus when [Step 3 → Step 1] is executed, the total-eccentricity index strictly decreases. Since Algorithm 3 outputs S_*, we have $\tau(S_*) < \tau(T)$. □

Corollary 3.4.2. *Let T be an n-vertex conjugated tree, then*

$$\tau(T) \leq \frac{7n}{2} - 2, \tag{3.38}$$

where equality holds when $T \cong S_*$.

Proof. The result follows by using Remark 3 and Theorem 3.4.3. □

Among the class of all n-vertex conjugated trees, the maximal conjugated tree corresponding to the total-eccentricity index in presented in the next theorem.

Theorem 3.4.4. *Among all n-vertex conjugated trees, the path P_n has the maximal total-eccentricity index.*

Proof. The proof is obvious from Theorem 3.2.3. □

3.5 Extremal conjugated unicyclic and bicyclic graphs for total-eccentricity index

The extremal trees, unicyclic and bicyclic graphs, and extremal conjugated trees corresponding to total-eccentricity index were computed in the previous chapter. In this chapter, we extend these results to the computation of extremal conjugated unicyclic and bicyclic graphs corresponding to total-eccentricity index.

Recall that a vertex w is called an eccentric vertex of a vertex v in G if $d_G(v, w) = e_G(v)$. The set of all eccentric vertices of v in a graph G is denoted by $E_G(v)$. In the following, we give a known result on location of center in a connected graph from [74] and some results on extremal graphs corresponding to total-eccentricity proved in Section 3.3.

Theorem 3.5.1 (Harary and Norman [74])**.** *The center of a connected graph G is contained in a block of G.*

The only possible blocks in a unicyclic graph are K_1, K_2 or a cycle C_k. Thus the following corollary gives the center of an n-vertex conjugated unicyclic graph $\overline{U}$.

Corollary 3.5.1. *If $\overline{U}$ is an n-vertex conjugated unicyclic graph with a unique cycle C_k, then $C(\overline{U}) = K_1$ or K_2, or $C(\overline{U}) \subseteq C_k$*

The following are some results from Section 3.3 on the extremal unicyclic and bicyclic graphs for total-eccentricity index.

Theorem 3.5.2 (Farooq et al. [98])**.** *Among all n-vertex unicyclic graphs, $n \geq 4$, the graph U_2 shown in Figure 3.5 has maximal total-eccentricity index.*

Theorem 3.5.3 (Farooq et al. [98])**.** *Among all n-vertex bicyclic graphs, $n \geq 5$, the graph B_2 shown in Figure 3.6 has the maximal total-eccentricity index.*

Let $\{v_1, v_2, \ldots, v_n\}$ be the vertices of a path P_n. Let U_2 be a unicyclic graph obtained from P_n by joining v_1 and v_3 by an edge. Similarly, let B_2 be a bicyclic graph obtained from P_n by joining v_1 with two vertices v_3 and v_4. Note that when $n \equiv 0 \pmod 2$, the graphs U_2 and B_2 are conjugated and are denoted by $\overline{U}_2$ and $\overline{B}_2$, respectively. For $n \equiv 0 \pmod 2$, let S_n^* be an n-vertex conjugated tree obtained by identifying one vertex each from $\frac{n-2}{2}$ copies of P_3 and deleting a single pendent vertex. Let v be the unique central vertex of S_n^*. Let $\overline{U}_1$ be a conjugated unicyclic graph obtained from S_n^* by adding an edge between v and any vertex not adjacent to v. In a similar fashion, let $\overline{B}_1$ be a conjugated bicyclic graph obtained from S_n^* by adding two edges between v and any two vertices not adjacent to v (see Figure 3.9). One can easily compute the following:

$$\begin{aligned} \tau(\overline{U}_1) &= \tfrac{7}{2}n - 3, \quad \tau(\overline{U}_2) = \tfrac{3n^2}{4} - n - \tfrac{3}{4}, \\ \tau(\overline{B}_1) &= \tfrac{7}{2}n - 4, \quad \tau(\overline{B}_2) = \tfrac{3}{4}n^2 - n - 2. \end{aligned} \tag{3.39}$$

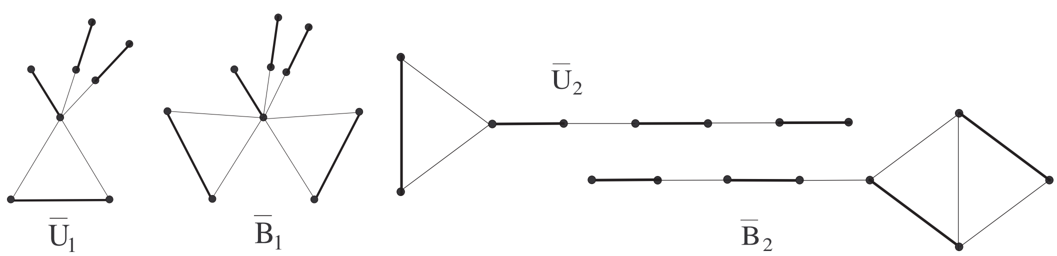

Figure 3.9: The 8-vertex conjugated unicyclic and bicyclic graphs $\overline{U}_1$, $\overline{U}_2$, $\overline{B}_1$ and $\overline{B}_2$.

Using Theorem 3.5.1 and Corollary 3.5.1, we prove the following result.

Remark 5. *When $n = 4$, the graph shown in Figure 3.10(a) has the smallest total-eccentricity index among all 4-vertex conjugated unicyclic graphs. When $n = 6$, the graphs shown in Figure 3.10(b) and Figure 3.10(c) have smallest total-eccentricity index among 6-vertex conjugated unicyclic graphs. When $n = 8$, the graph shown in Figure 3.10(d) has smallest total-eccentricity index among 8-vertex conjugated unicyclic graphs.*

Theorem 3.5.4. *Let $n \equiv 0 \pmod 2$ and $n \geq 10$. Then among all n-vertex conjugatedl unicyclic graphs, the graph $\overline{U}_1$ shown in Figure 3.9 has the minimal total-eccentricity index.*

Proof. Let $\overline{U}_1$ be the n-vertex conjugated unicyclic graph shown in Figure 3.9. Let $\overline{U}$ be an arbitrary n-vertex conjugated unicyclic graph with a unique cycle C_k. We show that

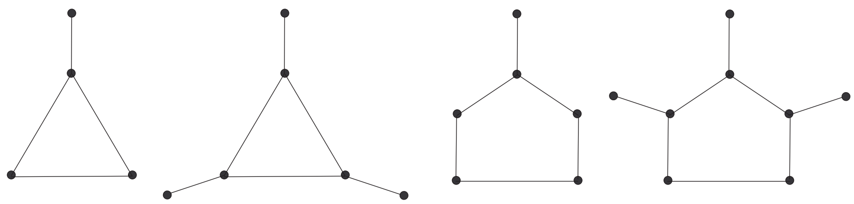

Figure 3.10: The n-vertex conjugated unicyclic graphs with minimal total-eccentricity index when $n = 4, 6, 8$.

$\tau(\overline{U}) \geq \tau(\overline{U_1})$. Let n_i denote the number of vertices with eccentricity i in $\overline{U}$. If $k \geq 8$ or $\text{rad}(\overline{U}) \geq 4$ then

$$\tau(\overline{U}) \geq 4n > \frac{7n}{2} - 3 = \tau(\overline{U}_1).$$

In the rest of the proof, we assume that $k \in \{3, 4, 5, 6, 7\}$ and $\text{rad}(\overline{U}) \in \{2, 3\}$. Let $k \in \{6, 7\}$. If x is a vertex of $\overline{U}$ such that x is not on C_k, then $e_{\overline{U}}(x) \geq 4$. Also, it is easily seen that there are at most five vertices on C_k with eccentricity 3. Thus

$$\tau(\overline{U}) \geq 3(5) + 4(n-5) = 4n - 5 > \frac{7n}{2} - 3 = \tau(\overline{U}_1). \tag{3.40}$$

We complete the proof by considering the following cases.

Case 1. When $\text{rad}(\overline{U}) = 3$ and $k \in \{3, 4, 5\}$. By Corollary 3.5.1, $C(\overline{U}) = K_1$ or $C(\overline{U}) = K_2$ or $C(\overline{U}) \subseteq C_k$. This shows that $\overline{U}$ has at most five vertices with eccentricity 3. Thus the inequality (3.40) holds in this case.

Case 2. When $\text{rad}(\overline{U}) = 2$ and $k \in \{4, 5\}$. Then $\text{diam}(\overline{U}) \leq 2\text{rad}(\overline{U}) \leq 4$ and there will be exactly one vertex in $C(\overline{U})$. That is, $n_2 = 1$. Let v be the vertex with $e_{\overline{U}}(v) = 2$. Then $v \in V(C_k)$. Considering several possibilities for longest possible paths (of length 2) starting from v and that $\overline{U}$ is conjugated, one can see that $\overline{U}$ is isomorphic to one of the graphs shown in Figure 3.11. Moreover, observe that $n_4 \geq \frac{n}{2} - 1$..

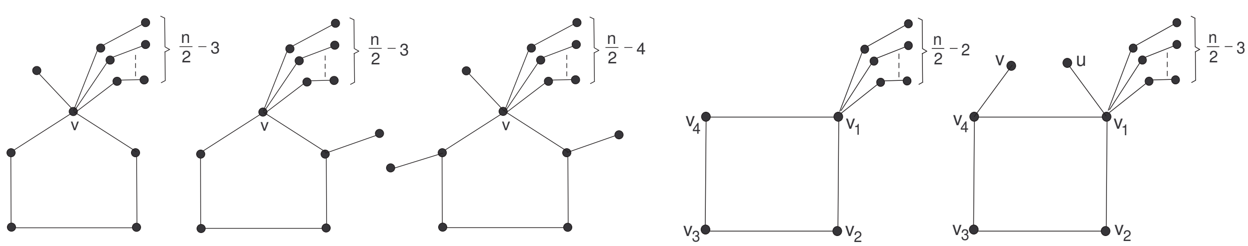

Figure 3.11: The n-vertex conjugated unicyclic graphs discussed in Case 2.

Since $n_2 + n_3 + n_4 = n$ and $n_2 = 1$, we can write

$$\begin{aligned}
\tau(\overline{U}) &= 2n_2 + 3n_3 + 4n_4 \\
&= 2 + 3(n_3 + n_4) + n_4 \\
&= 3n - 1 + n_4 \\
&\geq 3n - 1 + \frac{n}{2} - 1 = \frac{7n}{2} - 2 > \tau(\overline{U}_1).
\end{aligned}$$

Case 3. When $\text{rad}(\overline{U}) = 2$ and $k = 3$. Then $n_2 = 1$ (see Figure 3.12). Let v be the unique central vertex of $\overline{U}$. Then either v is a vertex of C_3 or v is adjacent to a vertex of C_3. When $v \in V(C_3)$, then $\overline{U}$ is isomorphic to one of the graphs shown in Figure 3.12(a), 3.12(b) or 3.12(c). In this case, all vertices with eccentricity 4 are pendent. This gives $n_4 \geq \frac{n}{2} - 2$. Therefore

$$\begin{aligned} \tau(\overline{U}) &= 2(1) + 3(n_3 + n_4) + n_4 \\ &\geq 3n - 1 + \frac{n}{2} - 2 \\ &= \frac{7n}{2} - 3 = \tau(\overline{U}_1). \end{aligned}$$

Similarly, if the central vertex v is not on C_3, then $\overline{U}$ is isomorphic to one of the graphs shown in Figure 3.12(d) or 3.12(e). Note that $n_4 \geq \frac{n}{2}$. Thus $\tau(\overline{U}) \geq 2(1)+3(n-1)+\frac{n}{2} = \frac{7n}{2}-1 > \tau(\overline{U}_1)$.

Combining all the cases, we see that $\overline{U}_1$ is the minimal graph for total-eccentricity index. This completes the proof. □

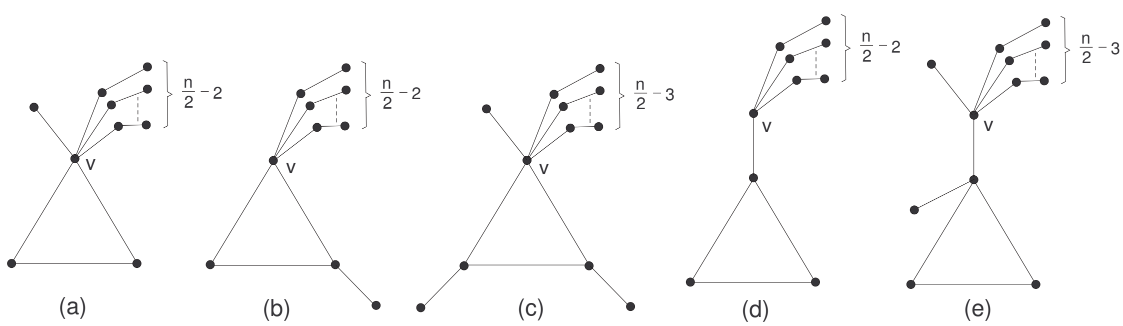

Figure 3.12: The n-vertex conjugated unicyclic graphs discussed in Case 3.

The following theorem gives the maximal conjugated unicyclic graphs for total-eccentricity index.

Theorem 3.5.5. *Let $n \equiv 0 \pmod 2$. Then the n-vertex conjugated unicyclic graph corresponding to the maximal total-eccentricity index is the graph $\overline{U}_2$ shown in Figure 3.9.*

Proof. Note that the class of all n-vertex conjugated unicyclic graphs forms a subclass of the class of all n-vertex unicyclic graphs. From Theorem 3.5.2 we see that among all n-vertex unicyclic graphs, the graph U_2 (see Figure 3.5) has the largest total-eccentricity index. Since U_2 admits a a perfect matching when $n \equiv 0(\text{mod}2)$, the result follows. □

Corollary 3.5.2. *For an n-vertex conjugated unicyclic graph $\overline{U}$, we have $\frac{7n}{2} - 3 \leq \tau(\overline{U}) \leq \frac{3n^2}{4} - n - \frac{3}{4}$.*

Proof. Using Theorem 3.5.4, Theorem 3.5.5 and equation (3.39), we obtain the required result. □

The next theorem gives the minimal conjugated bicyclic graphs for total-eccentricity index.

Remark 6. *Let $n = 4$. Then among all 4-vertex conjugated bicyclic graphs, one can easily see that the graph shown in Figure 3.13(a) has the minimal total-eccentricity index. Similarly, when $n = 6$ and 8, then the graphs respectively shown in Figure 3.13(b) and Figure 3.13(c) have the minimal total-eccentricity index among all 6-vertex and 8-vertex conjugated bicyclic graphs.*

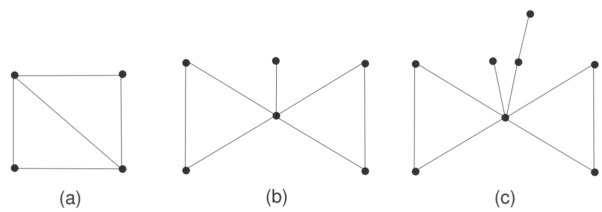

Figure 3.13: The n-vertex conjugated bicyclic graphs with minimal total-eccentricity index when $n = 4, 6$ and 8.

Theorem 3.5.6. *Let $n \equiv 0 \pmod 2$ and $n \geq 10$. Then among the n-vertex conjugated bicyclic graphs, the graph $\overline{B}_1$ shown in Figure 3.9 has the minimal total-eccentricity index.*

Proof. Let $\overline{B}_1$ be the n-vertex conjugated bicyclic graph shown in Figure 3.9. Let $\overline{B}$ be an arbitrary n-vertex conjugated bicyclic graph and $\overline{B} \ncong \overline{B}_1$. Let $C(\overline{B})$ denote the center of $\overline{B}$ and n_i denote the number of vertices with eccentricity i. The proof is divided into two cases depending upon the number of cycles in $\overline{B}$.

Case 1. When $\overline{B}$ contains two edge-disjoint cycles C_{k_1} and C_{k_2} of lengths k_1 and k_2, respectively. Without loss of generality, assume that $k_1 \leq k_2$. If $\text{rad}(\overline{B}) \geq 4$ or $k_2 \geq 8$, then

$$\tau(\overline{B}) \geq 4n > \frac{7n}{2} - 4 = \tau(\overline{B}_1).$$

Thus, we assume that $k_2 \in \{3, 4, 5, 6, 7\}$ and $\text{rad}(\overline{B}) \in \{2, 3\}$. If $k_2 \in \{6, 7\}$, then for any vertex $x \notin V(C_{k_2})$, $e_{\overline{B}}(x) \geq 4$. Moreover, as $k_2 \leq 7$, the number of vertices with eccentricity 3 are at most 7. Thus

$$\tau(\overline{B}) \geq 3(7) + 4(n-7) = 4n - 7 > \frac{7n}{2} - 4 = \tau(\overline{B}_1). \tag{3.41}$$

We consider the following three subcases.

(a) Let $\text{rad}(\overline{B}) = 3$ and $k_2 \in \{3, 4, 5\}$. By Theorem 3.5.1, we have $|V(C(\overline{B}))| \leq 7$. Thus $\tau(\overline{B})$ satisfies equation (3.41).

(b) Let $\text{rad}(\overline{B}) = 2$ and $k_2 \in \{4, 5\}$. Take $v \in V(C(\overline{B}))$. We observe that the center $C(\overline{B})$ is contained in C_{k_2} and $n_2 = 1$. Assume v to be the unique central vertex of $\overline{B}$. Then for several possible choices for possible pendent vertices in the conjugated graph $\overline{B}$, one can observe that $\overline{B}$ is one of the graphs shown in Figure 3.14. Moreover $n_4 \geq \frac{n}{2} - 2$. Then $\tau(\overline{B}) \geq 2n_2 + 3n_3 + 4n_4 = 2n_2 + 3(n_3 + n_4) + n_4 \geq 2(1) + 3(n-1) + \frac{n}{2} - 2 = \frac{7n}{2} - 3 > \tau(\overline{B}_1)$.

(c) When $\text{rad}(\overline{B}) = 2$ and $k_1 = k_2 = 3$. If $C(\overline{B}) \subseteq C_{k_2}$, then $C(\overline{B}) = K_1$, otherwise $n \leq 8$ which is not true. Similarly, if $C(\overline{B}) \nsubseteq C_{k_2}$, then $C(\overline{B}) = K_2$ or K_1. Since $n_2 \ngeq 2$, we have $n_2 = 1$. Let c be the unique central vertex. Then $\overline{B}$ is isomorphic to one of the

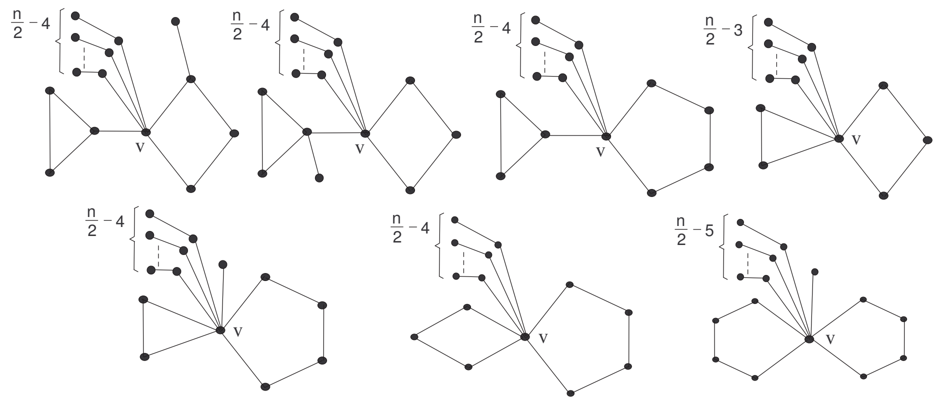

Figure 3.14: The n-vertex conjugated bicyclic graphs discussed in Case 1-(b).

graphs shown in Figure 3.15. When c is not a vertex of C_{k_1} or C_{k_2}, then $n_4 \geq \frac{n}{2} + 1$ and $\tau(\overline{B}) \geq 2(1) + 3(n-1) + \frac{n}{2} + 1 = \frac{7n}{2} > \tau(\overline{B}_1)$. If c is a vertex of C_{k_1} or C_{k_2}, then $n_4 \geq \frac{n}{2} - 3$. Thus $\tau(\overline{B}) \geq 2(1) + 3(n-1) + \frac{n}{2} - 3 = \frac{7n}{2} - 4 = \tau(\overline{B}_1)$.

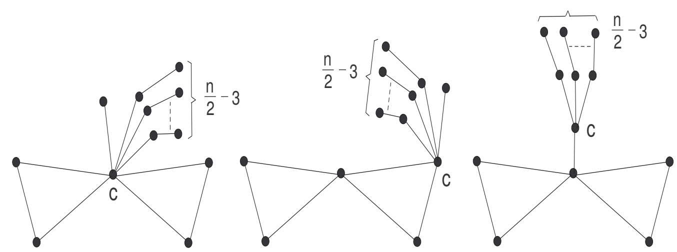

Figure 3.15: The n-vertex conjugated bicyclic graphs studied in Case 1-(c).

Case 2. When cycles of $\overline{B}$ share some edges. Then there are cycles C_{k_1}, C_{k_2} and C_{k_3} in $\overline{B}$ of lengths k_1, k_2 and k_3, respectively. Without loss of generality, assume that $k_1 \leq k_2 \leq k_3$. Then $k_1, k_2 \geq 3$ and $k_3 \geq 4$. Let Q be the subgraph of $\overline{B}$ induced by the vertices of C_{k_1}, C_{k_2} and C_{k_3}. Clearly, Q contains the cycle C_{k_3}. Assume that $V(C_{k_3}) = \{v_1, v_2, \ldots, v_{k_3}\}$. Then $\overline{B}$ is minimal with respect to total-eccentricity index if Q can be obtained from the cycle C_{k_3} by adding the edge $v_1 v_{\lfloor \frac{k_3}{2} \rfloor + 1}$ or $v_1 v_{\lfloor \frac{k_3}{2} \rfloor + 2}$.

When $k_3 \geq 13$, then $e_{\overline{B}}(w) \geq 4$ for all $w \in V(\overline{B})$. This gives us $\tau(\overline{B}) \geq 4n > \tau(\overline{B}_1)$. Assume that $\text{rad}(\overline{B}) \leq 3$ and $k_3 \leq 12$. We consider the following two subcases:

(a) When $k_3 \in \{9, 10, 11, 12\}$. Then $\text{rad}(\overline{B}) = 3$. There exists a vertex c with degree 3 in Q such that $c \in C(\overline{B})$ and c has at most $\frac{n-10}{2} + 1$ neighbours not in Q. Clearly, all of these vertices will have eccentricity 4. Then $\frac{n}{2} - 5$ such vertices can have unique pendent vertices with eccentricity 5. Moreover, there will be at least one vertex with eccentricity 5 in Q, otherwise $\text{rad}(\overline{B}) \neq 3$. Thus $n_5 \geq \frac{n}{2} - 4$. Moreover, at most 3 vertices in Q can have eccentricity 3. This gives $1 \leq n_3 \leq 3$. When $k_3 = 9$, such a graph $\overline{B}$ is shown in Figure 3.16(a). The vertex $v \in V(Q)$ such that $e_{\overline{B}}(v) = 5$ is also shown in the figure. Using the facts that $n = n_3 + n_4 + n_5$

and $n_4 + n_5 = n - n_3 \geq n - 3$. We get

$$\begin{aligned}\tau(\overline{B}) &= 3n_3 + 4n_4 + 5n_5 \\ &= 3n_3 + 4(n_4 + n_5) + n_5 \\ &\geq 3(1) + 4(n-3) + \frac{n}{2} - 4 \\ &= \frac{9n}{2} - 13 \geq \tau(\overline{B}_1).\end{aligned}$$

(b) When $k_3 \in \{4, 5, 6, 7, 8\}$. We first assume that $\text{rad}(\overline{B}) = 3$. Then by Theorem 3.5.1, we have $1 \leq n_3 \leq 8$. Thus $\tau(\overline{B}) \geq 3(8) + 4(n-8) = 4n - 8 \geq \tau(\overline{B}_1)$. On the other hand, when $\text{rad}(\overline{B}) = 2$. Then $n_2 = 1$. When $C(\overline{B}) \nsubseteq Q$, then the minimal graph $\overline{B}$ is isomorphic to the graph shown in Figure 3.16(b). Clearly, $n_4 \geq \frac{n}{2}$. Thus $\tau(\overline{B}) = 2n_2 + 3(n_3 + n_4) + n_4 \geq 2(1) + 3(n-1) + \frac{n}{2} = \frac{7n}{2} - 1 > \tau(\overline{B}_1)$. When $C(\overline{B}) \subseteq Q$, then $\overline{B}$ is isomorphic to one of the graphs shown in Figures 3.16(c)−3.16(h). It can be seen that $n_4 \geq \frac{n}{2} - 2$. Thus we can write $\tau(\overline{B}) = 2n_2 + 3(n_3 + n_4) + n_4 \geq 2(1) + 3(n-1) + \frac{n}{2} - 2 = \frac{7n}{2} - 3 = \tau(\overline{B}_1)$.

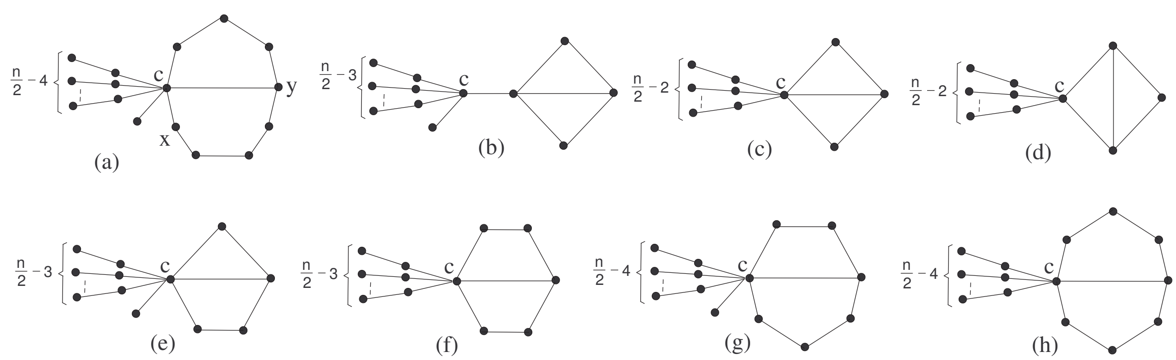

Figure 3.16: The conjugated bicyclic graphs studied in Case 2. The vertices c, x and y represent central vertices.

Combining the results of Case 1 and Case 2, we see that among all conjugated bicyclic graphs, $\overline{B}_1$ has the minimal total-eccentricity index. The proof is complete. □

Theorem 3.5.7. *Let $n \equiv 0 \pmod 2$. Then among the n-vertex conjugated bicyclic graphs, the graph $\overline{B}_2$ shown in Figure 3.9 has the maximal total-eccentricity index.*

Proof. For $n \equiv 0(\text{mod}2)$, the proof can be derived from the proof of Theorem 3.5.3. □

Corollary 3.5.3. *For any conjugated bicyclic graph $\overline{B}$, we have $\frac{7n}{2} - 4 \leq \tau(\overline{B}) \leq \frac{3n^2}{4} - n - 2$.*

Proof. The result follows by using Theorem 3.5.6, Theorem 3.5.7 and equation (3.41). □

3.6 Summary of the results

In this chapter, we studied the maximal and minimal graphs with respect to total-eccentricity index among trees, unicyclic and bicyclic graphs. We also studied the extremal conjugated trees corresponding to total-eccentricity index. Moreover, we extended the results of Farooq et al. [98] and studied the extremal conjugated unicyclic and bicyclic graphs for total-eccentricity index.

Chapter 4

Product graphs and some distance-based topological indices

In this chapter, we compute the "adjacent-eccentric distance sum index" $\xi^{sv}(G)$ and "eccentric-adjacency index" $\xi^{ad}(G)$ of the join and corona product of any finite number of graphs. These indices were defined respectively in Equations (2.9) and (2.10).

4.1 Preliminaries

First, for the sake of simplicity, we need to define some new indices which are modified forms of previously defined topological indices and they will be used later in this chapter to reduce some mathematical expressions. We define the inverse degree-distance $DD^{-1}(G)$, the inverse connective-eccentricity index $\xi_{ce}^{-1}(G)$ and the inverse total-eccentricity index $\tau^{-1}(G)$ of a graph G as:

$$DD^{-1}(G) = \sum_{u \in V(G)} \frac{D_G(u)}{d_G(u)}, \quad \xi_{ce}^{-1}(G) = \sum_{u \in V(G)} \frac{e_G(u)}{d_G(u)}, \quad \tau^{-1}(G) = \sum_{u \in V(G)} \frac{1}{e_G(u)}.$$

Now we give some notions about directed and mixed graphs which will be used in the rest of this chapter. In Section 4.2, we compute ξ^{sv} of join and corona products of graphs and Section 4.3 deals with the calculation of ξ^{ad} of the product graphs under consideration. In the last section, we give a brief conclusion and discussion on the results.

A directed graph $\overrightarrow{G}$ is a graph with vertex set $V(G)$ and the set of directed edges (or arcs) denoted as $E(\overrightarrow{G})$, where $(u,v) \in E(\overrightarrow{G})$ is an arc in $\overrightarrow{G}$ with initial vertex u and terminal vertex v, and $(u,v) \neq (v,u)$. For a vertex $v \in V(\overrightarrow{G})$, we define the notion $d_{\overrightarrow{G}}(v)$ of degree of v in $\overrightarrow{G}$ as:

$$d_{\overrightarrow{G}}(v) = \text{Number of directed edges terminating at } v. \tag{4.1}$$

A directed path in $\overrightarrow{G}$ is a path such that all of its edges have the same direction. The distance $d_{\overrightarrow{G}}(u,v)$ between two vertices $u,v \in V(\overrightarrow{G})$ is defined as the length of a shortest directed path between u and v. The underlying graph G of a directed graph $\overrightarrow{G}$ can be obtained by ignoring the directions of its edges. A mixed graph is a graph containing both directed and undirected edges. A mixed graph $\overleftrightarrow{G}$ can be considered as a directed graph $\overrightarrow{G}$ if we replace every undirected edge in $\overleftrightarrow{G}$ by two directed edges with opposite directions.

Before we proceed, let us compute the adjacent-eccentric distance sum of some special families of graphs.

Example 4.1.1. *For some special families of graphs on at least four vertices, the adjacent-eccentric distance sum index is given as follows.*

1. $\xi^{sv}(K_n) = n$.
2. $\xi^{sv}(K_{m,n}) = 2(m+n) + \frac{4m(m-1)}{n} + \frac{4n(n-1)}{m}$.
3. $\xi^{sv}(S_n) = 4n^2 - 10n + 7$.
4. $\xi^{sv}(P_n) = \begin{cases} n^3 + n(n-1)^2 - \frac{n}{2}(13n-37) - 22 & \text{when } n \text{ is even} \\ \frac{(n-1)^2(25n^2+130n+9)}{192} & \text{when } n \text{ is odd.} \end{cases}$

4.2 Adjacent eccentric-distance sum of join and corona product of graphs

Let G_1 and G_2 be two graphs with order n_1 and n_2, respectively, and let $n = n_1 + n_2$. A vertex $u \in V(G)$ is said to be well-connected if u is adjacent to all other vertices in G. Let $N(G_1)$ and $N(G_2)$ respectively denote the sets of all well-connected vertices of G_1 and G_2 and let $|N(G_1)| = m_1$ and $|N(G_2)| = m_2$. Then the adjacent-eccentric distance sum of the join of two graphs is obtained in the following theorem.

Theorem 4.2.1. *For any two connected graphs G_1 and G_2, the adjacent-eccentric distance sum of $G_1 + G_2$ is given by*

$$\xi^{sv}(G_1+G_2) = 3(m_1+m_2) - 2n + 4(n-1)\alpha(G),$$

where $\alpha(G) = \sum_{i=1}^{2} \sum_{u \in V(G_i) - N(G_i)} \frac{1}{d_{G_i}(u)+n-n_i}$.

Proof. Let $G = G_1 + G_2$. Then for any $u \in V(G)$, the degree and eccentricity of u in G is given by

$$d_G(u) = d_{G_i}(u) + n - n_i, \text{ when } u \in V(G_i) \text{ and } i \in \{1,2\}. \quad (4.2)$$

$$e_G(u) = \begin{cases} 1 & \text{when } u \in N(G_i) \\ 2 & \text{otherwise.} \end{cases} \quad (4.3)$$

Using (4.2) and (4.3), we get

$$\begin{aligned}
\xi^{sv}(G) &= \sum_{u\in V(G)} \frac{e_G(u)D_G(u)}{d_G(u)} \\
&= \sum_{u\in V(G)}\sum_{v\in V(G)} \frac{e_G(u)d_G(u,v)}{d_G(u)} \\
&= \sum_{i=1}^{2}\Bigg[\sum_{u\in N(G_i)}\sum_{v\in V(G)\setminus\{u\}} \frac{1\times 1}{d_{G_i}(u)+n-n_i} + \sum_{u\in V(G_i)\setminus N(G_i)}\sum_{v\in N_{G_i}(u)\cup\cup_{i\neq j=1}^{2}V(G_j)} \frac{2\times 1}{d_{G_i}(u)+n-n_i} \\
&\quad + \sum_{u\in V(G_i)\setminus N(G_i)}\sum_{v\in V(G_i)\setminus\{N_{G_i}(u)\cup\{u\}\}} \frac{2\times 2}{d_{G_i}(u)+n-n_i}\Bigg] \\
&= \sum_{i=1}^{2}\left[\frac{m_i(n_1+n_2-1)}{n_i-1+n-n_i} + 2\sum_{u\in V(G_i)\setminus N(G_i)} \frac{d_{G_i}(u)+n-n_i}{d_{G_i}(u)+n-n_i} + 4\sum_{u\in V(G_i)\setminus N(G_i)} \frac{n_i-d_{G_i}(u)-1}{d_{G_i}(u)+n-n_i}\right]
\end{aligned}$$

$$\begin{aligned}
&= \sum_{i=1}^{2}\left[\frac{m_i(n-1)}{n-1} + 2(n_i-m_i) - 4(n_i-m_i) + 4\sum_{u\in V(G_i)\setminus N(G_i)} \frac{n-1}{d_{G_i}(u)+n-n_i}\right] \\
&= 3(m_1+m_2) - 2n + 4(n-1)\sum_{i=1}^{2}\sum_{u\in V(G_i)\setminus N(G_i)} \frac{1}{d_{G_i}(u)+n-n_i} \\
&= 3(m_1+m_2) - 2n + 4(n-1)\alpha(G), \quad \square
\end{aligned}$$

where $\alpha(G) = \sum\limits_{i=1}^{2}\sum\limits_{u\in V(G_i)-N(G_i)} \frac{1}{d_{G_i}(u)+n-n_i}$.

Corollary 4.2.1. *Let $G = G_1 + G_2 + \ldots + G_k$ be the join of k connected graphs. Then the adjacent-eccentric distance sum of G is given by*

$$\xi^{sv}(G) = 3\sum_{i=1}^{k} m_i - 2n + 4(n-1)\alpha(G),$$

where $\alpha(G) = \sum\limits_{i=1}^{k}\sum\limits_{u\in V(G_i)\setminus N(G_i)} \frac{1}{d_{G_i}(u)+n-n_i}$.

Proof. The proof is analogous to the proof of Theorem 3.21. $\square$

Let G be an n-vertex graph with $V(G) = \{v_i \mid 1 \le i \le n\}$. For $t \ge 1$, let W be a set of vertices $\{w_i^j \mid 1 \le i \le n,\ 1 \le j \le t\}$ and let $\overleftrightarrow{G}(t)$ be a mixed graph obtained from G such that $V(\overleftrightarrow{G}(t)) = V(G) \cup W$ and $E(\overleftrightarrow{G}(t)) = E(G) \cup \{(v_i, w_i) \mid 1 \le i \le n\}$. Analogously, we define $\overleftrightarrow{G}(0) = G$. Let $\overrightarrow{G}(t)$ be the directed graph obtained from $\overleftrightarrow{G}(t)$ by replacing every undirected edge by two directed edges with opposite directions. Then we have $d_G(v) + t = d_{\overrightarrow{G}(t)}(v)$ and $e_G(v) = e_{\overrightarrow{G}(t)}(v)$ for all $v \in V(G)$.

Example 4.2.2. *Let G be a graph as shown in Figure 4.1-(a). The mixed graph $\overleftrightarrow{G}(2)$ obtained from G is shown in Figure 4.1-(b). The directed graph $\overrightarrow{G}(2)$ is obtained from $\overleftrightarrow{G}(2)$ by replacing every undirected edge by two directed edges with opposite directions. Note that $d_G(v) + 2 = d_{\overrightarrow{G}(2)}(v)$ and $e_G(v) = e_{\overrightarrow{G}(2)}(v)$ for all $v \in V(G)$.*

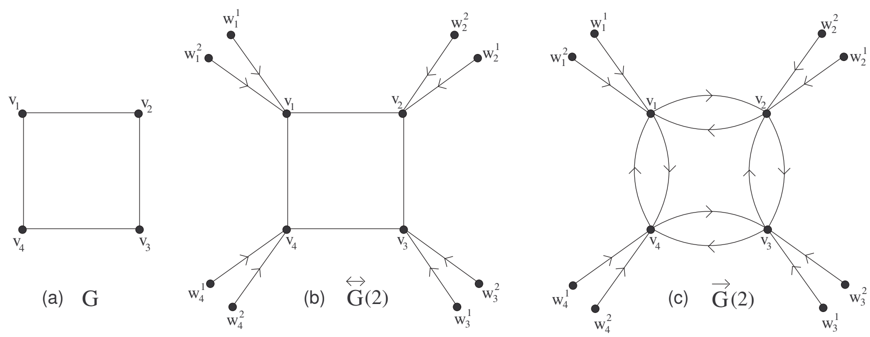

Figure 4.1: A simple graph G is shown in (a), a mixed graph (b) obtained form (a) and the corresponding directed graph (c).

Let G_1 and G_2 be two graphs of order n_1 and n_2, respectively. Let $G'_1 = \overrightarrow{G_1}(n_2)$ and $G'_2 = \overrightarrow{G_2}(1)$. Then the adjacent-eccentric distance sum of the corona product of G_1 and G_2 is given by the following theorem.

Theorem 4.2.2. *For any two connected graphs G_1 and G_2, the adjacent-eccentric distance sum of the corona product of G_1 and G_2 is given by*

$$\begin{aligned}\xi^{sv}(G_1 \odot G_2) &= (n_2+1)\xi^{sv}(G'_1) + n_1 n_2 \xi^{-1}_{ce}(G'_1) + (n_2+1)d^{-1}(G'_1) + (n_1 n_2) r(G'_1) \\ &\quad + (n_2+1)\xi^{ds}(G_1) r(G'_2) + 2(n_2+1)W(G_1) r(G'_2) - n_2 \tau(G_1) \\ &\quad - 2n_1 n_2 + (2n_1 n_2 + n_1 - 1)\tau(G_1) r(G'_2) + 2n_1(2n_1 n_2 + n_1 - 1) r(G'_2).\end{aligned}$$

Proof. Let $G = G_1 \odot G_2$, where G_1 and G_2 are two graphs of order n_1 and n_2, respectively. Then for any $u \in V(G)$, the degree and eccentricity of u in G is given by

$$d_G(u) = \begin{cases} d_{G_1}(u) + n_2 & \text{when } u \in V(G_1) \\ d_{G_2}(u) + 1 & \text{when } u \in V(G_2^i). \end{cases} \tag{4.4}$$

$$e_G(u) = \begin{cases} e_{G_1}(u) + 1 & \text{when } u \in V(G_1) \\ e_{G_1}(x_i) + 2 & \text{when } u \in V(G_2^i). \end{cases} \tag{4.5}$$

$$D_G(u) = \begin{cases} (n_2+1)D_{G_1}(u) + n_1 n_2 & \text{when } u \in V(G_1) \\ (n_2+1)D_{G_1}(x_i) + 2n_1 n_2 - d_{G_2}(u) + n_1 - 2 & \text{when } u \in V(G_2^i). \end{cases} \tag{4.6}$$

Let $G_1' = \overrightarrow{G_1}(n_2)$ and $G_2' = \overrightarrow{G_2}(1)$. Using (4.4), (4.5) and (4.6), we obtain

$$\begin{aligned}
\xi^{sv}(G) &= \sum_{u\in V(G)} \frac{e_G(u)D_G(u)}{d_G(u)} \\
&= \sum_{u\in V(G_1)} \frac{e_G(u)D_G(u)}{d_G(u)} + \sum_{u\in V(G_2^i)} \frac{e_G(u)D_G(u)}{d_G(u)} \\
&= \sum_{u\in V(G_1)} \frac{(e_{G_1}(u)+1)\big[(n_2+1)D_{G_1}(u)+n_1n_2\big]}{d_{G_1}(u)+n_2} \\
&\quad +\sum_{i=1}^{n_1}\sum_{u\in V(G_2^i)} \frac{(e_{G_1}(x_i)+2)\big[(n_2+1)D_{G_1}(x_i)+2n_1n_2-d_{G_2}(u)+n_1-2\big]}{d_{G_2}(u)+1} \\
&= \sum_{u\in V(G_1)} \frac{(n_2+1)e_{G_1}(u)D_{G_1}(u)}{d_{G_1}(u)+n_2} + \sum_{u\in V(G_1)} \frac{n_1n_2e_{G_1}(u)}{d_{G_1}(u)+n_2} + \sum_{u\in V(G_1)} \frac{(n_2+1)D_{G_1}(u)}{d_{G_1}(u)+n_2} \\
&\quad + \sum_{u\in V(G_1)} \frac{n_1n_2}{d_{G_1}(u)+n_2} + \sum_{i=1}^{n_1}\Bigg[\sum_{u\in V(G_2^i)} \frac{(n_2+1)e_{G_1}(x_i)D_{G_1}(x_i)}{d_{G_2}(u)+1} + \sum_{u\in V(G_2^i)} \frac{2(n_2+1)D_{G_1}(x_i)}{d_{G_2}(u)+1} \\
&\quad - \sum_{u\in V(G_2^i)} \frac{(d_{G_2}(u)+1)e_{G_1}(x_i)}{d_{G_2}(u)+1} - \sum_{u\in V(G_2^i)} \frac{2(d_{G_2}(u)+1)}{d_{G_2}(u)+1} + \sum_{u\in V(G_2^i)} \frac{(2n_1n_2+n_1-1)e_{G_1}(x_i)}{d_{G_2}(u)+1} \\
&\quad + \sum_{u\in V(G_2^i)} \frac{2(2n_1n_2+n_1-1)}{d_{G_2}(u)+1}\Bigg] \\
&= (n_2+1)\xi^{sv}(G_1') + n_1n_2\xi_{ce}^{-1}(G_1') + (n_2+1)d^{-1}(G_1') + (n_1n_2)r(G_1') + (n_2+1)\xi^{ds}(G_1)r(G_2') \\
&\quad +2(n_2+1)W(G_1)r(G_2') - n_2\tau(G_1) - 2n_1n_2 + (2n_1n_2+n_1-1)\tau(G_1)r(G_2') \\
&\quad +2n_1(2n_1n_2+n_1-1)r(G_2'). \quad \square
\end{aligned}$$

Now we compute the corona product of k graphs defined as $G = G_1 \odot G_2 \odot \ldots \odot G_k$, where G_1 is a graph with $V(G_1) = \{x_1, x_2, \ldots, x_{n_1}\}$ and $G_t = K_1$ for $2 \le t \le k$. Let V_j^i be a class of vertices in $V(G)$ defined as

$$V_j^i = \{w \in V(G) \mid d(x_i, w) = j\}, \qquad 1 \le j \le k-1 \text{ and } 1 \le i \le n_1 \tag{4.7}$$

such that the edge set of (x_i, w)-path in G does not intersect with $E(G_1)$, for $1 \le i \le n_1$. Clearly $V(G) = V(G_1) \cup \big\{ \cup_{i=1}^{n_1} \cup_{j=1}^{k-1} V_j^i \big\}$. Let us represent each vertex $v \in V_j^i$ uniquely by $v = v(\alpha_0, \alpha_1, \cdots, \alpha_s)$, where $\alpha_0 < \alpha_1 < \cdots < \alpha_s$ and $1 \le i \le n_1$, $1 \le j \le k-1$, $1 \le s \le k$. The corona product $G = G_1 \odot G_2 \odot G_3 \odot G_4$, where $G_1 = C_4$ and $G_2 = G_3 = G_4 = K_1$ is shown in Figure 4.2. The labels of vertices for one branch of G and the vertex classes V_j^i's for $i = 2$ and $1 \le j \le 3$ can also be viewed in the same figure. We assume that $\alpha_0 = 1$ and $\alpha_{s+1} = 0$. In the following, we present the expressions for the degree and eccentricity of a

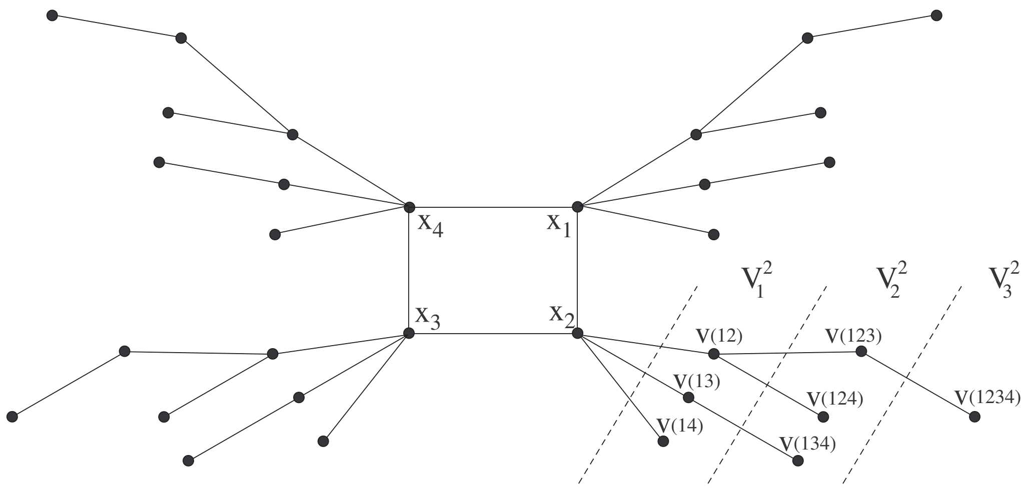

Figure 4.2: The corona product G of four graphs G_1, G_2, G_3 and G_4, where $G_1 = C_4$ and G_2, G_3, G_4 are K_1. For simplicity, the vertices for only one branch of G are labelled. Moreover, the vertex classes V_j^i's are mentioned for $i = 2$ and $1 \leq j \leq 3$.

vertex in G .

$$d_G(v) = \begin{cases} d_{G_1}(v) + k - 1 & v \in V(G_1) \\ \\ k - \alpha_j + 1 & v \in V_j^i, \end{cases} \tag{4.8}$$

$$e_G(v) = \begin{cases} e_{G_1}(v) + k - 1 & v \in V(G_1) \\ \\ e_{G_1}(x_i) + j + k - 1 & v \in V_j^i, \end{cases} \tag{4.9}$$

where $1 \leq i \leq n_1$ and $1 \leq j \leq k - 1$.

Now we derive the expressions for the sum of all distances in G starting from $v \in V_j^i$, for some $i \in \{1,2,\ldots,n_1\}$ and $j \in \{1,2,\ldots,k-1\}$. When $v \in V_j^i$ then

$$\begin{aligned}
D_G(v) &= D(v(\alpha_0,\alpha_1,\cdots,\alpha_s))\\
&= \sum_{w\in V_j^i\cup\{x_i\}} d_G(v,w) + \sum_{w\in G_1\backslash\{x_i\}} d_G(v,w) + \sum_{w\in V_j^r,\ r\neq i} d_G(v,w)\\
&= \sum_{l=1}^{s} l + \sum_{t=0}^{s}\sum_{l=1}^{k-\alpha_t}(s-t+l)\left[\binom{k-\alpha_t}{l} - \binom{k-\alpha_{t+1}}{l-1}\right] + \sum_{t=1,\ t\neq i}^{n_1}\{s+d_{G_1}(x_i,x_t)\}\\
&\quad + \sum_{t=1,\ t\neq i}^{n_1}\left\{s(2^{k-1}-1) + d_{G_1}(x_i,x_t)(2^{k-1}-1) + \sum_{l=1}^{k-1} l\binom{k-1}{l}\right\}\\
&= \frac{s(s+1)}{2} + \sum_{t=0}^{s}\sum_{l=1}^{k-\alpha_t}(s-t+l)\left[\binom{k-\alpha_t}{l} - \binom{k-\alpha_{t+1}}{l-1}\right]\\
&\quad + \sum_{t=1,\ t\neq i}^{n_1}\left\{2^{k-1}s + 2^{k-1}d_{G_1}(x_i,x_t) + \sum_{l=1}^{k-1} l\binom{k-1}{l}\right\}\\
&= \frac{s(s+1)}{2} + \sum_{t=0}^{s}\{t-s+2^{k-\alpha_t}(s-t)+2^{k-\alpha_t-1}(k-\alpha_t)\} - \sum_{t=0}^{s}\sum_{l=1}^{k-\alpha_t}(s-t\\
&\quad +l)\binom{k-\alpha_{t+1}}{l-1} + s(n_1-1)2^{k-1} + 2^{k-1}D_{G_1}(x_i) + (k-1)(n_1-1)2^{k-2}\\
&= \frac{2s(s+1)}{2} - s(s+1) + s(n_1-1)2^{k-1} + (k-1)(n_1-1)2^{k-2} + 2^{k-1}D_{G_1}(x_i)\\
&\quad + \sum_{t=0}^{s} 2^{k-\alpha_t-1}(2s-2t+k-\alpha_t) - \sum_{t=0}^{s}\sum_{l=1}^{k-\alpha_t}(s-t+l)\binom{k-\alpha_{t+1}}{l-1}\\
&= 2^{k-2}(n_1-1)(k+2s-1) + 2^{k-1}D_{G_1}(x_i)\\
&\quad + \sum_{t=0}^{s} 2^{k-\alpha_t-1}(2s-2t+k-\alpha_t) - \sum_{t=0}^{s}\sum_{l=1}^{k-\alpha_t}(s-t+l)\binom{k-\alpha_{t+1}}{l-1}. \qquad (4.10)
\end{aligned}$$

When $v = x_i \in G_1$ (that is, $s=0$) for $1 \leq i \leq n_1$, we have

$$\begin{aligned}
D_G(v) &= D_G(x_i) = \sum_{w\in V_j^i} d_G(v,w) + \sum_{w\in G_1\backslash\{x_i\}} d_G(v,w) + \sum_{w\in V_j^r,\ r\neq i} d_G(v,w)\\
&= \sum_{l=1}^{k-1} l\binom{k-1}{l} + \sum_{t=1,\ t\neq i}^{n_1} d_{G_1}(x_i,x_t) + \sum_{t=1,\ t\neq i}^{n_1} d_{G_1}(x_i,x_t)(2^{k-1}-1)\\
&\quad + \sum_{t=1,\ t\neq i}^{n_1}\sum_{l=1}^{k-1} l\binom{k-1}{l}\\
&= (k-1)2^{k-2} + D_{G_1}(x_i) + (2^{k-1}-1)D_{G_1}(x_i) + (n_1-1)(k-1)2^{k-2}\\
&= n_1(k-1)2^{k-2} + 2^{k-1}D_{G_1}(x_i). \qquad (4.11)
\end{aligned}$$

In the next theorem, we find the adjacent-eccentric distance sum of the corona product of k graphs.

Theorem 4.2.3. *Let $G = G_1 \odot G_2 \odot \ldots \odot G_k$ be the corona product of k number of connected graphs such that $G_t = K_1$ for $2 \le t \le k$. Then the adjacent-eccentric distance sum of G is given by equation* (4.16)*.*

Proof. Let $G = G_1 \odot G_2 \odot \ldots \odot G_k$ and $V(G) = \{x_1, x_2, \ldots, x_{n_1}\}$. Let $G_t = K_1$ for $2 \le t \le k$. Moreover, let $n = n_1 + k - 1$. The vertex class V_j^i in G is defined by (4.7) for $1 \le j \le k-1$ and $2 \le i \le n_1$. Then under these conditions, the degree, eccentricity and sum of distances for any $v \in V(G)$ are defined respectively in (4.8), (5.2) and (4.10)-(4.11). Now we compute the adjacent-eccentric distance sum of G as follows.

$$\begin{aligned}
\xi^{sv}(G) &= \sum_{u \in V(G)} \frac{e_G(u) D_G(u)}{d_G(u)} \\
&= \sum_{u \in V(G_1)} \frac{e_G(u) D_G(u)}{d_G(u)} + \sum_{\substack{u \in V_j^i,\ 2 \le i \le n_1 \\ 1 \le j \le k-1}} \frac{e_G(u) D_G(u)}{d_G(u)} \\
&= \sum_{u \in V(G_1)} \frac{(e_{G_1}(u) + k - 1) D_G(u)}{d_{G_1}(u) + k - 1} + \sum_{\substack{u \in V_j^i,\ 2 \le i \le n_1 \\ 1 \le j \le k-1}} \frac{(e_{G_1}(x_i) + j + k - 1) D_G(u)}{k - \alpha_j + 1} \\
&= A + B, \qquad (4.12)
\end{aligned}$$

where A and B are given by

$$A = \sum_{u \in V(G_1)} \frac{(e_{G_1}(u) + k - 1)(n_1(k-1)2^{k-2} + 2^{k-1} D_{G_1}(u))}{d_{G_1}(u) + k - 1}. \qquad (4.13)$$

$$\begin{aligned}
B &= \sum_{\substack{u \in V_j^i,\ 2 \le i \le n_1 \\ 1 \le j \le k-1}} \frac{(e_{G_1}(x_i) + j + k - 1)\Big(2^{k-2}(n_1 - 1)(k + 2s - 1) + 2^{k-1} D_{G_1}(x_i)\Big)}{k - \alpha_j + 1} \\
&+ \sum_{\substack{u \in V_j^i,\ 2 \le i \le n_1 \\ 1 \le j \le k-1}} \frac{(e_{G_1}(x_i) + j + k - 1) \sum_{t=0}^{s} 2^{k - \alpha_t - 1}(2s - 2t + k - \alpha_t)}{k - \alpha_j + 1} \\
&- \sum_{\substack{u \in V_j^i,\ 2 \le i \le n_1 \\ 1 \le j \le k-1}} \frac{(e_{G_1}(x_i) + j + k - 1) \sum_{t=0}^{s} \sum_{l=1}^{k - \alpha_t} (s - t + l) \binom{k - \alpha_{t+1}}{l - 1}}{k - \alpha_j + 1}. \qquad (4.14)
\end{aligned}$$

Let $G_1' = \overrightarrow{G_1}(k-1)$ then expression (4.13) can be rewritten as

$$\begin{aligned}
A &= 2^{k-2} n(k-1) \xi_{ce}^{-1}(G_1') + 2^{k-1} \xi^{sv}(G_1') + 2^{k-2}(k-1)^2 n_1 r(G_1') \\
&\quad + 2^{k-1}(k-1) d^{-1}(G_1'). \qquad (4.15)
\end{aligned}$$

By substituting (4.15) in (4.12), we get

$$\begin{aligned}
\xi^{sv}(G) &= 2^{k-2} n(k-1) \xi_{ce}^{-1}(G_1') + 2^{k-1} \xi^{sv}(G_1') + 2^{k-2}(k-1)^2 n_1 r(G_1') \\
&\quad + 2^{k-1}(k-1) d^{-1}(G_1') + B. \quad \square \qquad (4.16)
\end{aligned}$$

4.3 Eccentric-adjacency index of join and corona product of graphs

First, we compute the eccentric-adjacency index of some special families of graphs.

Example 4.3.1. *For some special families of graphs on at least four vertices, the eccentric-adjacency index is given as follows.*

1. $\xi^{ad}(K_n) = n(n-1)^2$.
2. $\xi^{ad}(K_{m,n}) = \frac{mn(m+n)}{2}$.
3. $\xi^{ad}(S_n) = \frac{(n-1)^2}{2} + n - 1$.
4. $\xi^{ad}(P_n) = \begin{cases} \frac{4}{n-1} + \frac{6}{n-2} + 8\sum_{i=3}^{\frac{n}{2}} \frac{1}{n-i} & \text{when } n \text{ is even} \\ \frac{12}{n-1} + \frac{6}{n-2} + 8\sum_{i=3}^{\frac{n-1}{2}} \frac{1}{n-i} & \text{when } n \text{ is odd.} \end{cases}$

Throughout this section we denote the order, size and the number of well-connected vertices of the graph G_i respectively by n_i, e_i and m_i, $1 \leq i \leq k$. Moreover, let $n = n_1 + n_2 + \ldots + n_k$ and $e = e_1 + e_2 + \ldots + e_k$. In the following theorem, we compute the eccentric-adjacency index for the join of two graphs.

Theorem 4.3.1. *Let G_1 and G_2 are two connected graphs. Then the eccentric-adjacency index of the join of G_1 and G_2 is given by*

$$\begin{aligned}\xi^{ad}(G_1 + G_2) &= (m_1 + m_2)(2e_1 + 2e_2 + 2n_1n_2 - n_1 - n_2 + 1) + \frac{1}{2}\big\{M_1(G_1) + M_1(G_2) \\ &\quad + m_1(2n_1 + n_2 - n_1^2 - 2n_1n_2 - 2e_2 - 1) + m_2(2n_2 + n_1 - n_2^2 - 2n_1n_2 - 2e_1 \\ &\quad - 1) + n_1^2n_2 + n_2^2n_1 + 4(e_1n_2 + e_2n_1)\big\},\end{aligned}$$

where n_i, e_i and m_i respectively denote the order, size and the number of well-connected vertices of G_i, $i \in \{1, 2\}$.

Proof. Let $G = G_1 + G_2$. Let $N(G_i)$ contains all well-connected vertices of G_i and let e_i and m_i respectively denote the size and the number of well-connected vertices of G_i, $i \in \{1, 2\}$. Then for any vertex $u \in V(G_i)$, $i \in \{1, 2\}$, the degree and eccentricity of u can be defined as

$$d_G(u) = d_{G_i}(u) + n - n_i \quad \text{and} \quad e_G(u) = \begin{cases} 1 & u \in N(G_i) \\ 2 & \text{otherwise.} \end{cases} \tag{4.17}$$

Then the eccentric-adjacency index of G is calculated as follows.

$$\begin{aligned}
\xi^{ad}(G) &= \xi^{ad}(G_1+G_2)\\
&= \sum_{u\in V(G)} \frac{S_G(u)}{e_G(u)}\\
&= \sum_{u\in N(G_1)} S_G(u) + \sum_{u\in N(G_2)} S_G(u) + \frac{1}{2}\sum_{u\in V(G_1)\setminus N(G_1)} S_G(u) + \frac{1}{2}\sum_{u\in V(G_2)\setminus N(G_2)} S_G(u)\\
&= \sum_{u\in N(G_1)}\sum_{v\in N_G(u)} d_G(v) + \sum_{u\in N(G_2)}\sum_{v\in N_G(u)} d_G(v)\\
&\quad \frac{1}{2}\sum_{u\in V(G_1)\setminus N(G_1)}\sum_{v\in N_G(u)} d_G(v) + \frac{1}{2}\sum_{u\in V(G_2)\setminus N(G_2)}\sum_{v\in N_G(u)} d_G(v)
\end{aligned}$$

$$\begin{aligned}
&= m_1\{2e_1-n_1+1+(n_1-1)n_2+2e_2+n_1n_2\}+m_2\{2e_2-n_1+1+(n_2-1)n_1\\
&\quad +2e_1+n_1n_2\}+\frac{1}{2}\sum_{u\in V(G_1)\setminus N(G_1)}\big(d^2_{G_1}(u)+n_2d_{G_1}(u)+2e_2+n_2n_1\big)\\
&\quad +\frac{1}{2}\sum_{u\in V(G_2)\setminus N(G_2)}\big(d^2_{G_2}(u)+n_1d_{G_2}(u)+2e_1+n_2n_1\big)\\
&= (m_1+m_2)(2e_1+2e_2+2n_1n_2-n_1-n_2+1)\\
&\quad +\frac{1}{2}\big\{M_1(G_1)+M_1(G_2)-m_1(n_1-1)^2+n_2(2e_1-m_1(n_1-1))+(n_1-m_1)\big(2e_2\\
&\quad +n_2n_1\big)-m_2(n_2-1)^2+n_1(2e_2-m_2(n_2-1))+(n_2-m_2)\big(2e_1+n_2n_1\big)\big\}
\end{aligned}$$

$$\begin{aligned}
&= (m_1+m_2)(2e_1+2e_2+2n_1n_2-n_1-n_2+1)\\
&\quad +\frac{1}{2}\big\{M_1(G_1)+M_1(G_2)+m_1(2n_1+n_2-n_1^2-2n_1n_2-2e_2-1)\\
&\quad +m_2(2n_2+n_1-n_2^2-2n_1n_2-2e_1-1)+n_1^2n_2+n_2^2n_1+4(e_1n_2+e_2n_1)\big\}. \qquad \square
\end{aligned}$$

Now we find the eccentric-adjacency index of the join of k graphs.

Corollary 4.3.2. *The eccentric-adjacency index of the join of connected graphs $G_1, G_2, \ldots, G_k$ is given by*

$$\begin{aligned}
\xi^{ad}(G_1+G_2+\cdots+G_k) &= \sum_{i=1}^{k} m_i\big\{2e-n+2nn_i-2n_i^2+1\big\}+\frac{1}{2}\sum_{i=1}^{k}\big\{M_1(G_i)-m_i(n_i-1)^2\\
&\quad +(n-n_i)(2e_i-m_i(n_i-1))+(n_i-m_i)\big(2(e-e_i)+(n-n_i)n_i\big)\big\},
\end{aligned}$$

where n_i, e_i and m_i respectively denote the order, size and the number of well-connected vertices of G_i, $i\in\{1,2,\ldots,k\}$. Moreover $n=\sum_{i=1}^{k} n_i$ and $e=\sum_{i=1}^{k} e_i$.

Proof. Using the expression (4.17) for $i \in \{1, 2, \ldots, k\}$, we get

$$\begin{aligned}
\xi^{ad}(G) &= \xi^{ad}(G_1 + \ldots + G_k) \\
&= \sum_{i=1}^{k} \sum_{u \in V(G_i)} \frac{S_G(u)}{e_G(u)} \\
&= \sum_{i=1}^{k} \Big\{ \sum_{u \in N(G_i)} S_G(u) + \frac{1}{2} \sum_{u \in V(G_i) \setminus N(G_i)} S_G(u) \Big\} \\
&= \sum_{i=1}^{k} m_i \{2e_i - n_i + 1 + (n_i - 1)(n - n_i) + 2(e - e_i) + \sum_{\substack{j=1 \\ j \neq i}}^{k} n_j(n - n_j)\} \\
&\quad \frac{1}{2} \sum_{i=1}^{k} \Big\{ \sum_{u \in V(G_i) \setminus N(G_i)} \sum_{v \in N_{G_i}(u)} (d_{G_i}(v) + n - n_i) + \sum_{u \in V(G_i) \setminus N(G_i)} \sum_{\substack{j=1 \\ j \neq i}}^{k} \sum_{v \in V(G_j)} (d_{G_j}(v) \\
&\quad + n - n_j) \Big\} \\
&= \sum_{i=1}^{k} m_i \{2e_i - n_i + 1 + (n_i - 1)(n - n_i) + 2(e - e_i) + (n - n_i)n_i\} \\
&\quad \frac{1}{2} \sum_{i=1}^{k} \Big\{ \sum_{u \in V(G_i) \setminus N(G_i)} \big(d^2_{G_i}(u) + (n - n_i)d_{G_i}(u)\big) + \sum_{u \in V(G_i) \setminus N(G_i)} \sum_{\substack{j=1 \\ j \neq i}}^{k} \big(2e_j + n_j(n \\
&\quad - n_j)\big) \Big\} \\
&= \sum_{i=1}^{k} m_i \{2e - n + 2nn_i - 2n_i^2 + 1\} + \frac{1}{2} \sum_{i=1}^{k} \{M_1(G_i) - m_i(n_i - 1)^2 \\
&\quad + (n - n_i)(2e_i - m_i(n_i - 1)) + (n_i - m_i)\big(2(e - e_i) + (n - n_i)n_i\big)\}. \quad \square
\end{aligned}$$

Now we define some notions to obtain and simplify the results of eccentricity-adjacency index of corona products of graphs. Let G be an n-vertex graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$. Let W be a collection of n directed (w_i^0, w_i^t)-paths on $t+1$ vertices, $1 \leq i \leq n$. We obtain the mixed graph $\overleftrightarrow{G_p}(t)$ by identifying w_i^0 with v_i for $1 \leq i \leq n$. Let $\overrightarrow{G_p}(t)$ be the directed graph obtained from $\overleftrightarrow{G_p}(t)$ by replacing every undirected edge by two directed edges with opposite directions. Then by equation (4.1) we have $d_G(v) = d_{\overrightarrow{G_p}(t)}(v)$ and $e_G(v) + t = e_{\overrightarrow{G_p}(t)}(v)$ for all $v \in V(G)$. These notions can be understood by the following example.

Example 4.3.3. *Let G_1 be a graph as shown in Figure 4.3-(a). The mixed graph $\overleftrightarrow{G}_{1,p}(2)$ obtained from G_1 is shown in Figure 4.3-(b). The directed graph $\overrightarrow{G}_{1,p}(2)$ is obtained from the mixed graph $\overleftrightarrow{G}_{1,p}(2)$ by replacing every undirected edge by two directed edges with opposite directions. Then $d_G(v) = d_{\overrightarrow{G}_{1,p}(2)}(v)$ and $e_G(v) + 2 = e_{\overrightarrow{G}_{1,p}(2)}(v)$ for all $v \in V(G)$.*

Let $G_1' = \overrightarrow{G}_{1,p}(1)$ and $G_1'' = \overrightarrow{G}_{1,p}(2)$ and let m_i is the number of well-connected vertices

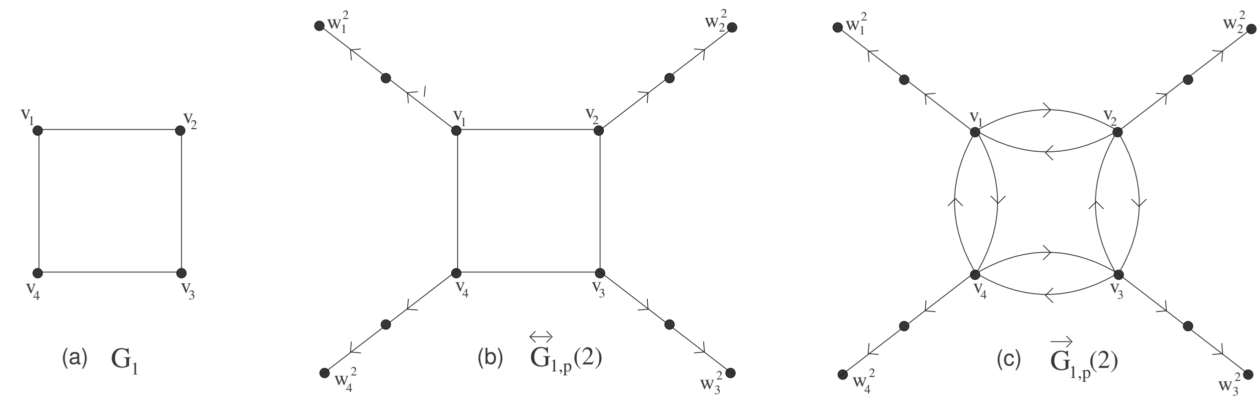

Figure 4.3: A simple graph G_1 is shown in (a), a mixed graph (b) obtained form G_1 and the corresponding directed graph shown in (c).

in G_i, $i \in \{1,2\}$. Similarly, let $G_2' = \overrightarrow{G}_{2,p}(1)$ and $G_2'' = \overrightarrow{G}_{2,p}(2)$. In the next theorem, we find the eccentric-adjacency index of the corona product of two graphs.

Theorem 4.3.2. *Let G_1 and G_2 are two connected graphs. Then the eccentric-adjacency index of the corona product of G_1 and G_2 is given by*

$$\begin{aligned}\xi^{ad}(G_1 \odot G_2) &= \xi^{ad}(G_1') + n_2\xi^{ce}(G_1') + n_2\xi^{ce}(G_1'') + (2e_2 + n_2)\tau^{-1}(G_1') + \big(n_2^2 + 2e_2 \\ &\quad + M_1(G_2)\big)\tau^{-1}(G_1''),\end{aligned}$$

where n_i and e_i respectively denote the order and size of the graph G_i, $i \in \{1,2\}$.

Proof. Let $G = G_1 \odot G_2$ and let $V(G_1) = \{x_1, x_2, \ldots, v_{n_1}\}$. Then for any vertex $u \in V(G)$, the degree and eccentricity of u in G is given by

$$d_G(u) = \begin{cases} d_{G_1}(u) + n_2 & \text{when } u \in V(G_1) \\ d_{G_2}(u) + 1 & \text{when } u \in V(G_2^i). \end{cases} \tag{4.18}$$

$$e_G(u) = \begin{cases} e_{G_1}(u) + 1 & \text{when } u \in V(G_1) \\ e_{G_1}(x_i) + 2 & \text{when } u \in V(G_2^i). \end{cases} \tag{4.19}$$

Then the eccentric-adjacency index of G is given by

$$\begin{aligned}\xi^{ad}(G_1 \odot G_2) &= \sum_{u \in V(G)} \frac{S_G(u)}{e_G(u)} \\ &= \sum_{u \in V(G_1)} \frac{S_G(u)}{e_G(u)} + \sum_{\substack{u \in V(G_2^i) \\ 1 \le i \le n_1}} \frac{S_G(u)}{e_G(u)} \\ &= \sum_{u \in V(G_1)} \sum_{v \in N_G(u)} \frac{d_G(v)}{e_G(u)} + \sum_{\substack{u \in V(G_2^i) \\ 1 \le i \le n_1}} \sum_{v \in N_G(u)} \frac{d_G(v)}{e_G(u)}\end{aligned}$$

$$= \sum_{u\in V(G_1)} \left(\frac{1}{e_G(u)} \sum_{v\in N_{G_1}(u)} d_G(v) + \frac{1}{e_G(u)} \sum_{\substack{v\in N_{G_2^i}(u)\\ 1\le i\le n_1}} d_G(v) \right) + \sum_{\substack{u\in V(G_2^i)\\ 1\le i\le n_1}} \left(\frac{1}{e_G(u)} \sum_{v\in N_{G_1}(u)} d_G(v) \right.$$

$$\left. + \frac{1}{e_G(u)} \sum_{\substack{v\in N_{G_2^j}(u)\\ 1\le j\le n_1}} d_G(v) \right)$$

$$= \sum_{u\in V(G_1)} \left(\frac{S_{G_1}(u) + n_2 d_{G_1}(u)}{e_G(u)} + \frac{2e_2 + n_2}{e_G(u)} \right) + \sum_{i=1}^{n_1} \sum_{u\in V(G_2^i)} \left(\frac{d_{G_1}(x_i) + n_2}{e_G(u)} \right.$$

$$\left. + \frac{S_{G_2}(u) + d_{G_2}(u)}{e_G(u)} \right)$$

$$= \sum_{u\in V(G_1)} \frac{S_{G_1}(u)}{e_{G_1}(u)+1} + \sum_{u\in V(G_1)} \frac{n_2 d_{G_1}(u)}{e_{G_1}(u)+1} + \sum_{u\in V(G_1)} \frac{2e_2+n_2}{e_{G_1}(u)+1} + \sum_{i=1}^{n_1} \sum_{u\in V(G_2^i)} \frac{d_{G_1}(x_i)}{e_{G_1}(x_i)+2}$$

$$+ \sum_{i=1}^{n_1} \sum_{u\in V(G_2^i)} \frac{n_2}{e_{G_1}(x_i)+2} + \sum_{i=1}^{n_1} \sum_{u\in V(G_2^i)} \frac{S_{G_2}(u)}{e_{G_1}(x_i)+2} + \sum_{i=1}^{n_1} \sum_{u\in V(G_2^i)} \frac{d_{G_2}(u)}{e_{G_1}(x_i)+2}$$

$$= \xi^{ad}(G_1') + n_2\xi^{ce}(G_1') + (2e_2+n_2)\tau^{-1}(G_1') + n_2\xi^{ce}(G_1'') + n_2^2\tau^{-1}(G_1'') + \tau^{-1}(G_1'')M_1(G_2)$$
$$+ 2e_2\tau^{-1}(G_1'')$$

$$= \xi^{ad}(G_1') + n_2\xi^{ce}(G_1') + n_2\xi^{ce}(G_1'') + (2e_2+n_2)\tau^{-1}(G_1') + \big(n_2^2 + 2e_2 + M_1(G_2)\big)\tau^{-1}(G_1''). \quad \square$$

In the next theorem, we find the eccentric-adjacency index of the corona product of k graphs by assuming $G_1' = \overrightarrow{G}_{1,p}(k-1)$, $G_1'' = \overrightarrow{G}_{1,p}(k)$ and $G_1''' = \overrightarrow{G}_{1,p}(j+k-1)$.

Theorem 4.3.3. *Let $G = G_1 \odot G_2 \odot \cdots \odot G_k$ be the corona product of k number connected graphs. Then the eccentric-adjacency index of G is given by* (4.23).

Proof. Let $G = G_1 \odot \ldots \odot G_k$, $n = n_1 + n_2 + \ldots + n_k$ and $m = m_1 + m_2 + \ldots + m_k$. We represent the ratios of sum of degrees of neighbours of a vertex and its eccentricity, for vertices in G_1, V_1^i and V_j^i for $2 \le j \le k-1$, $1 \le i \le n_1$ separately.

First we write the ratios of $S_G(v)$ and $e_G(v)$ for some $v \in V(G_1)$ as

$$\sum_{v\in G_1} \frac{S_G(v)}{e_G(v)} = \sum_{i=1}^{n_1} \frac{S_G(x_i)}{e_G(x_i)}$$

$$= \sum_{i=1}^{n_1} \left\{ \frac{S_{G_1}(x_i) + \sum_{t=2}^{k} \left(2m_t + n_t + n_t \sum_{s=t+1}^{k} n_s \right)}{e_{G_1}(x_i) + k - 1} \right.$$

$$\left. + \sum_{i=1}^{n_1} \frac{d_{G_1}(x_i) \sum_{t=2}^{k} \left(2m_t + n_t + n_t \sum_{s=t+1}^{k} n_s \right)}{e_{G_1}(x_i) + k - 1} \right\}$$

$$
\begin{aligned}
&= \sum_{i=1}^{n_1} \frac{S_{G_1}(x_i)}{e_{G_1}(x_i)+k-1} + \sum_{t=2}^{k}(2m_t+n_t+n_t\sum_{s=t+1}^{k} n_s)\sum_{i=1}^{n_1}\frac{1+d_{G_1}(x_i)}{e_{G_1}(x_i)+k-1}\\
&= \xi^{ad}(G_1') + \sum_{t=2}^{k}\big(2m_t+n_t+n_t\sum_{s=t+1}^{k} n_s\big)\big(\tau^{-1}(G_1')+C^{\xi}(G_1')\big)\\
&= \xi^{ad}(G_1') + \big(2m+n-2m_1-n_1+(n-n_1)\sum_{t=2}^{k}\sum_{s=t+1}^{k} n_s\big)\big(\tau^{-1}(G_1')\\
&\quad +C^{\xi}(G_1')\big).
\end{aligned} \tag{4.20}
$$

Now we write the ratios of $S_G(v)$ and $e_G(v)$ for some $v \in V(V_1^i)$ and $1 \le i \le n_1$ as follows.

$$
\begin{aligned}
\sum_{\substack{v\in V_1^i\\ 1\le i\le n_1}} \frac{S_G(v)}{e_G(v)} &= \sum_{i=1}^{n_1}\sum_{l=2}^{k}\sum_{v\in G_l}\Big\{\frac{S_{G_l}(v)+d_{G_l}(v)+\sum_{t=l+1}^{k}(2m_t+n_t+d_{G_l}(v)n_t)+\sum_{t=2}^{k} n_t}{e_{G_1}(x_i)+k}\\
&\quad + \frac{\sum_{t=l+1}^{k-1}\sum_{s=t+1}^{k} n_t n_s}{e_{G_1}(x_i)+k}\Big\} + \sum_{i=1}^{n_1}\sum_{l=2}^{k}\sum_{v\in G_l}\frac{d_{G_1}(x_i)}{e_{G_1}(x_i)+k}\\
&= \sum_{l=2}^{k}\Big\{M_1(G_l)+2m_l+\sum_{t=l+1}^{k}(2m_t n_l+n_t n_l+2m_l n_t)+n_l\sum_{t=2}^{k} n_t\Big\}\sum_{i=1}^{n_1}\frac{1}{e_{G_1}(x_i)+k}\\
&\quad + \sum_{l=2}^{k}\Big\{n_l\sum_{t=l+1}^{k-1}\sum_{s=t+1}^{k} n_t n_s\Big\}\sum_{i=1}^{n_1}\frac{1}{e_{G_1}(x_i)+k} + \sum_{l=2}^{k}\sum_{v\in G_l}\sum_{i=1}^{n_1}\frac{d_{G_1}(x_i)}{e_{G_1}(x_i)+k}\\
&= \tau^{-1}(G_1'')\sum_{l=2}^{k}\sum_{t=l+1}^{k}(2m_t n_l+n_t n_l+2m_l n_t) + \sum_{l=2}^{k}\Big\{n_l\sum_{t=l+1}^{k-1}\sum_{s=t+1}^{k} n_t n_s\Big\}\tau^{-1}(G_1'')\\
&\quad +\tau^{-1}(G_1'')\sum_{l=2}^{k} M_1(G_l) + (n-n_1)C^{\xi}(G_1'') + (2m-2m_1+(n-n_1)^2)\tau^{-1}(G_1'').
\end{aligned} \tag{4.21}
$$

Similarly, for some $v \in V_j^i$, where $2 \le j \le k-1$ and $1 \le i \le n_1$, we have

$$
\begin{aligned}
\sum_{\substack{v\in V_j^i\\ 1\le j\le k-1\\ 1\le i\le n_1}} \frac{S_G(v)}{e_G(v)} &= \sum_{l=j+1}^{k}\sum_{v\in G_l}\Big[\sum_{\substack{s_t\in\{2,3,\ldots,l-1\}\\ s_1<s_2<\ldots<s_{j-1}}}\prod_{t=1}^{j-1} n_{s_t}\Big\{S_{G_l}(v)+d_{G_l}(v)+d_{G_l}(v)\sum_{t=l+1}^{k} n_t\\
&\quad + \sum_{t=l+1}^{k}(2m_t+n_t)+\sum_{t=l+1}^{k-1}\sum_{s=t+1}^{k} n_t n_s + 1\Big\}\Big]\sum_{i=1}^{n_1}\frac{1}{e_{G_1}(x_i)+j+k-1}\\
&\quad +2n_l\sum_{\substack{s_t\in\{2,3,\ldots,l-1\}\\ s_1<s_2<\ldots<s_{j-1}}}\Big[\Big(\prod_{t=1}^{j-2} n_{s_t}\Big)m_{s_{j-1}}\Big]\sum_{i=1}^{n_1}\frac{1}{e_{G_1}(x_i)+j+k-1}
\end{aligned}
$$

$$= \sum_{l=j+1}^{k}\Bigg[\sum_{\substack{s_t\in\{2,3,\ldots,l-1\}\\ s_1<s_2<\ldots<s_{j-1}}}\prod_{t=1}^{j-1} n_{s_t}\Bigg\{M_1(G_l)+2m_l+2m_l\sum_{t=l+1}^{k} n_t+n_l\sum_{t=l+1}^{k}(2m_t+n_t)$$

$$+n_l\sum_{t=l+1}^{k-1}\sum_{s=t+1}^{k} n_t n_s+n_l\Bigg\}\Bigg]\tau^{-1}(G_1''')+2n_l\sum_{\substack{s_t\in\{2,3,\ldots,l-1\}\\ s_1<s_2<\ldots<s_{j-1}}}\Bigg[\Bigg(\prod_{t=1}^{j-2} n_{s_t}\Bigg)m_{s_{j-1}}\Bigg]\tau^{-1}(G_1'''). \quad (4.22)$$

By using equation (5.2) and equations (4.20)-(4.22), we get

$$\begin{aligned}\xi^{ad}(G) &= \sum_{v\in V(G)}\frac{S_G(v)}{e_G(v)}\\ &= \sum_{v\in V(G_1)}\frac{S_G(v)}{e_G(v)}+\sum_{\substack{v\in V_1^i\\ 1\le i\le n_1}}\frac{S_G(v)}{e_G(v)}+\sum_{\substack{v\in V_j^i\\ 2\le j\le k-1\\ 1\le i\le n_1}}\frac{S_G(v)}{e_G(v)}\end{aligned}$$

$$= \xi^{ad}(G_1')+\Big(2m+n-2m_1-n_1+(n-n_1)\sum_{l=2}^{k}\sum_{t=l+1}^{k} n_t\Big)\big(\tau^{-1}(G_1')+C^{\xi}(G_1')\big)$$

$$+\tau^{-1}(G_1'')\sum_{l=2}^{k}\sum_{t=l+1}^{k}(2m_t n_l+n_t n_l+2m_l n_t)+\sum_{l=2}^{k}\Bigg\{n_l\sum_{t=l+1}^{k-1}\sum_{s=t+1}^{k} n_t n_s\Bigg\}\tau^{-1}(G_1'')$$

$$+\tau^{-1}(G_1'')\sum_{l=2}^{k} M_1(G_l)+(n-n_1)C^{\xi}(G_1'')+(2m-2m_1+(n-n_1)^2)\tau^{-1}(G_1'')$$

$$+\sum_{l=j+1}^{k}\Bigg[\sum_{\substack{s_t\in\{2,3,\ldots,l-1\}\\ s_1<s_2<\ldots<s_{j-1}}}\prod_{t=1}^{j-1} n_{s_t}\Bigg\{M_1(G_l)+2m_l+\sum_{t=l+1}^{k}(2m_t n_l+n_t n_l+2m_l n_t)$$

$$+n_l\sum_{t=l+1}^{k-1}\sum_{s=t+1}^{k} n_t n_s+n_l\Bigg\}\Bigg]\tau^{-1}(G_1''')+2n_l\sum_{\substack{s_t\in\{2,3,\ldots,l-1\}\\ s_1<s_2<\ldots<s_{j-1}}}\Bigg[\Bigg(\prod_{t=1}^{j-2} n_{s_t}\Bigg)m_{s_{j-1}}\Bigg]\tau^{-1}(G_1'''). \quad (4.23)$$

□

4.4 Summary of the results and discussion

In this chapter, we computed adjacent-eccentric distance sum index $\xi^{sv}(G)$ and eccentric-adjacency index $\xi^{ad}(G)$ for a graph G which can be the join or corona product of any number, say k, of connected graphs ($k \geq 2$). We can use the results given in the previous sections to obtain $\xi^{sv}(G)$ and $\xi^{ad}(G)$ of some special families of graphs obtained by join or corona products of graphs. For instance, the wheel graph W_n and fan graph f_n of order n are respectively defined as $W_n = K_1 + C_{n-1}$ and $f_n = K_1 + P_{n-1}$. The wheel graph W_9 and fan graph f_6 is shown in Figure 4.4.

Using Theorem 3.21, we have $\alpha(W_n) = \sum_{u \in V(C_{n-1})} \frac{1}{d_{C_{n-1}}(u)+1} = \frac{n-1}{3}$. Substituting this in the expression of $\xi^{sv}(W_n)$, we get

$$\begin{aligned} \xi^{sv}(W_n) = \xi^{sv}(K_1 + C_{n-1}) &= 3(1+0) - 2n + 4(n-1)\alpha(G) \\ &= 3 - 2n + 4(n-1)\frac{n-1}{3} \\ &= 3 - 2n + \frac{4(n-1)^2}{3}. \end{aligned}$$

Similarly, for the graph f_n we have $\alpha(f_n) = \sum_{u \in V(P_{n-1})} \frac{1}{d_{P_{n-1}}(u)+1} = 1 + \frac{n-3}{3}$. So we can compute $\xi^{sv}(f_n)$ as follows.

$$\begin{aligned} \xi^{sv}(f_n) = \xi^{sv}(K_1 + P_{n-1}) &= 3(1+0) - 2n + 4(n-1)\alpha(G) \\ &= 3 - 2n + 4(n-1)\frac{n}{3}. \end{aligned}$$

Using Theorem 4.3.1, we can obtain $\xi^{ad}(W_n)$ as

$$\begin{aligned} \xi^{ad}(W_n) = \xi^{ad}(K_1 + C_{n-1}) &= (2(n-1) + 2(n-1) - 1 - (n-1) + 1) + \frac{1}{2}\{4(n-1) \\ &\quad +(2 + n - 1 - 1 - 2(n-1) - 2(n-1) - 1) + n - 1 \\ &\quad +(n-1)^2 + 4(n-1)\} \\ &= \frac{1}{2}\{12(n-1) + (n-1)^2\}, \end{aligned}$$

and for the fan graph f_n, we get the expression for ξ^{ad} as follows.

$$\begin{aligned} \xi^{ad}(f_n) = \xi^{ad}(K_1 + P_{n-1}) &= (2(n-2) + 2(n-1) - 1 - (n-1) + 1) + \frac{1}{2}\{0 + 2 + 4(n-3) \\ &\quad +(2 + (n-1) - 1 - 2(n-1) - 2(n-2) - 1) + (n-1) \\ &\quad +(n-1)^2 + 4(n-2)\} \\ &= 3n - 5 + \frac{1}{2}\{6n - 14 + (n-1)^2\}. \end{aligned}$$

We can use Theorem 4.3.1 to compute ξ^{ad} of necklace-type graphs defined as $N(P_n, P_2) = P_n \odot P_2$. The graph $N(P_7, P_2)$ is shown in Figure 4.4.

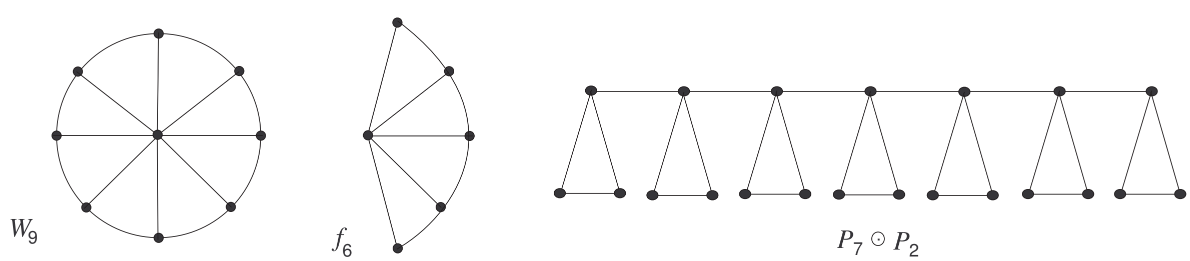

Figure 4.4: A wheel graph W_7, fan graph f_4 and a necklace-type graph $N = P_7 \odot P_2$.

By Theorem 4.3.2, the adjacent-eccentricity index $\xi^{ad}(P_n \odot P_2)$ of the necklace-type graph is given by

$$\begin{aligned}\xi^{ad}(N) = \xi^{ad}(P_{n_1} \odot P_2) &= \xi^{ad}(P'_n) + 2\xi^{ce}(P'_n) + 2\xi^{ce}(P''_n) + (2+2)\tau^{-1}(P'_n) \\ &\quad +(4+2+2)\tau^{-1}(P''_n) \\ &= \xi^{ad}(P'_n) + 2\xi^{ce}(P'_n) + 2\xi^{ce}(P''_n) + 4\tau^{-1}(P'_n) + 8\tau^{-1}(P''_n)\end{aligned}$$

Using this formula, $\xi^{ad}(P_7 \odot P_2)$ can be calculated as follows.

$$\begin{aligned}\xi^{ad}(P_7 \odot P_2) &= \xi^{ad}(P'_7) + 2\xi^{ce}(P'_7) + 2\xi^{ce}(P''_7) + 4\tau^{-1}(P'_7) + 8\tau^{-1}(P''_7) \\ &= 4.17 + 2(2.25) + 2(1.89) + 4(1.27) + 8(1.07) \\ &= 26.09.\end{aligned}$$

The direct calculation shows that $\xi^{ad}(P_7 \odot P_2) = 26.08$, which is quite satisfactory.

The main vault in the computation of the indices $\xi^{sv}(G)$ and $\xi^{ad}(G)$ is the unavailability of closed analytical expressions for the inverse degree $r(G)$ and inverse total-eccentricity $\tau^{-1}(G)$ of a graph G. We invite the reader to investigate these inverse indices which would be an interesting and challenging mathematical exercise!

Chapter 5

Distance-based indices of some graph families

In this chapter, we consider some infinite families of 3-fence graphs namely ladder, circular ladder and Möbius ladders. We compute the eccentricity-based topological indices of these graphs and their line graphs. Also, we study the relation between the indices of these graphs with their line graphs. Furthermore, we construct a square grid from the ladder graph and study the eccentricity-based topological indices for this grid graph and its line graph.

5.1 Some 3-fence graphs and their eccentric-connectivity indices

A ladder graph with n cycles of length 4 is denoted as $L[n]$ and is shown in Fig. 1. The order and size of $L[n]$ is $2n+2$ and $3n+1$, respectively. The circular ladder, denoted by $CL[n]$, with $n \geq 2$, is obtained from the ladder $L[n]$ by joining the vertices u_n with u_1 and v_n with v_1 by edges (see Fig. 1). The order and size of $CL[n]$ are $2n+2$ and $3n+3$, respectively. A Mobius ladder or a Mobius strip $ML[n]$ is obtained from a circular ladder $CL[n]$ by twisting it a single time. Thus the order and size of a Mobius ladder $ML[n]$ is the same as the order and size of a circular ladder $CL[n]$.

In this section, we compute the eccentric-connectivity index of the graphs $L[n]$, $CL[n]$ and $ML[n]$. For each of these graphs, we form a group of vertices which have same degree and eccentricity and take one representative from this group. In the Tables 1-3, we present these representative vertices for each graph alongwith their degrees, eccentricities and frequency of occurrence.

In the following theorem, we calculate the eccentric connectivity index of the ladder graph $L[n]$.

Theorem 5.1.1. *The eccentric-connectivity index of $L[n]$ is given by*

$$\xi(L[n]) = \begin{cases} 12nt - 6t^2 - n + 18t + 2 & n \text{ is even} \\ 12nt - 6t^2 - 4n + 18t - 4 & n \text{ is odd,} \end{cases}$$

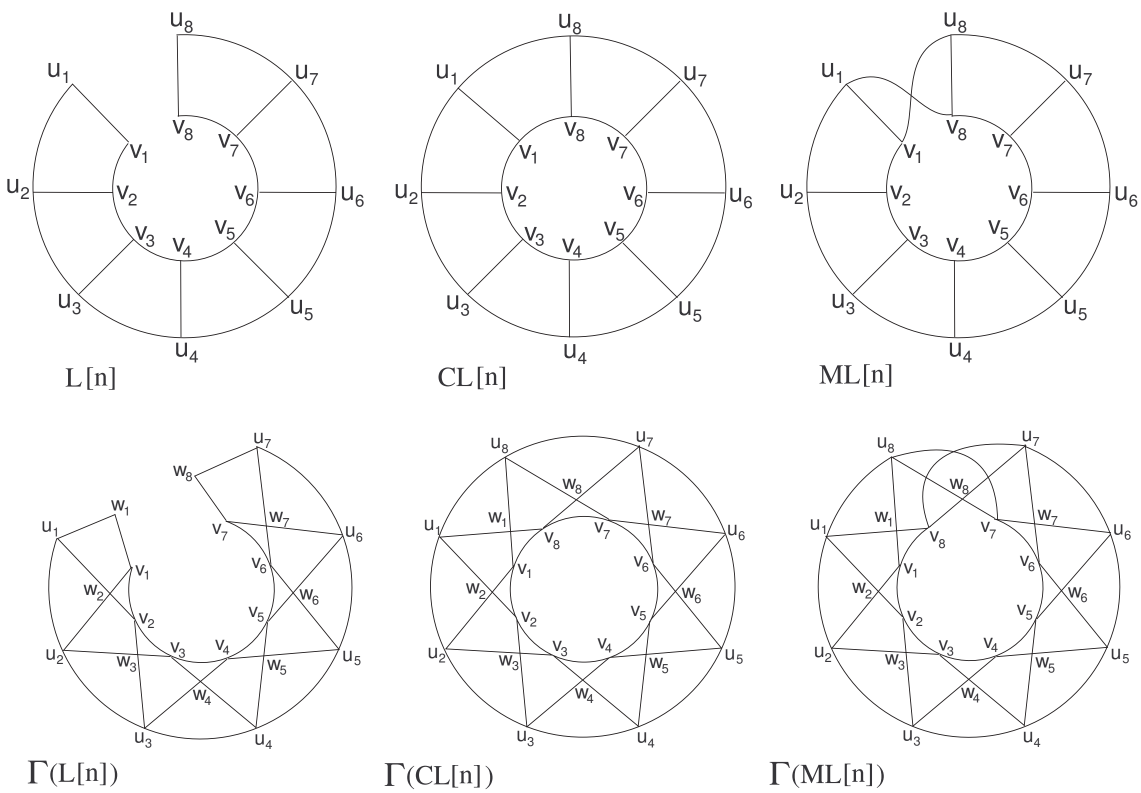

Figure 5.1: Some 3-fence graphs (for $n = 7$) and their corresponding line graphs.

Representative vertices	**Degree**	**Eccentricity**	**Frequency**
u_1	2	$n+1$	4
u_i $(2 \leq i \leq \lceil \frac{n}{2} \rceil$, n is odd)	3	$n-i+2$	4
u_i $(2 \leq i < \frac{n+2}{2}$, n is even)	3	$n-i+2$	4
$u_{\frac{n+2}{2}}$ (when n is even)	3	$\frac{n+2}{2}$	2

Table 5.1: The vertices of $L[n]$ are presented along with their frequencies with respect to degrees and eccentricities.

Representative Vertex	**Degree**	**Eccentricity**	**Frequency**
u	3	$\lceil \frac{n}{2} \rceil + 1$	$2n+2$

Table 5.2: The vertices of $CL[n]$ are presented along with their frequencies with respect to degrees and eccentricities.

Representative Vertices	**Degree**	**Eccentricity**	**Frequency**
u	3	$\lceil \frac{n}{2} \rceil$	$2n+2$

Table 5.3: The vertices of $ML[n]$ are presented along with their frequencies with respect to degrees and eccentricities.

where $t = \lceil \frac{n}{2} \rceil$.

Proof. The vertices of the graph $L[n]$ are labelled by u_i and v_i for $1 \leq i \leq n$ as shown in Figure 5.1. In Table 5.1, the representatives from these vertices are presented along with their degrees and eccentricities. If n is even then by using Table 5.1, we get

$$\begin{aligned}\xi(L[n]) &= \sum_{u \in V(D_1[n])} d(u)\varepsilon(u) \\ &= (2 \times 4)(n+1) + \frac{1}{2}(3 \times 2)(n+2) + \sum_{i=2}^{t}(3 \times 4)(n-i+2) \\ &= 12nt - 6t^2 - n + 18t + 2.\end{aligned}$$

When n is odd then by using Table 5.1, we get

$$\begin{aligned}\xi(L[n]) &= (2 \times 4)(n+1) + \sum_{i=2}^{t}(3 \times 4)(n-i+2) \\ &= 12nt - 6t^2 - 4n + 18t - 4.\end{aligned}$$

This completes the proof. □

Similarly, the next two results can easily be proved by using Table 5.2 and Table 5.3, respectively.

Theorem 5.1.2. *The eccentric-connectivity index of the circular ladder $CL[n]$ is given by*

$$\xi(CL[n]) = 6(n+1)(t+1),$$

where $t = \lceil \frac{n}{2} \rceil$.

Theorem 5.1.3. *The eccentric-connectivity index of the Mobius ladder $ML[n]$ is given by*

$$\xi(ML[n]) = 6t(n+1),$$

where $t = \lceil \frac{n}{2} \rceil$.

The next three results provide the total-eccentricity index of the graphs $L[n]$, $CL[n]$, $ML[n]$ and can easily be derived from Tables 5.1-5.3.

Corollary 5.1.1. *The total-eccentricity index of the ladder $L[n]$ is given by*

$$\zeta(L[n]) = \begin{cases} 4nt - 2t^2 + n + 6t + 2 & n \text{ is even} \\ 4nt - 2t^2 + 6t & n \text{ is odd,} \end{cases}$$

where $t = \lceil \frac{n}{2} \rceil$.

Corollary 5.1.2. *The total-eccentricity index of the circular ladder $CL[n]$ is given by*

$$\zeta(CL[n]) = 2(n+1)(t+1),$$

where $t = \lceil \frac{n}{2} \rceil$.

Representative Vertices	Degree	Eccentricity	Frequency
u_1	3	n	4
u_i ($2 \leq i \leq \frac{n}{2}$, n is even)	4	$n-i+1$	4
u_i ($2 \leq i < \lceil \frac{n}{2} \rceil$, n is odd)	4	$n-i+1$	4
$u_{\lceil \frac{n}{2} \rceil}$ (when n is odd)	4	$\frac{n+1}{2}$	2
w_1	2	$n+1$	2
w_i ($2 \leq i \leq \frac{n}{2}$, n is even)	4	$n-i+2$	2
w_i ($2 \leq i < \lceil \frac{n}{2} \rceil$, n is odd)	4	$n-i+2$	2
$w_{\frac{n}{2}+1}$ (when n is even)	4	$\frac{n+2}{2}$	1
$w_{\lceil \frac{n}{2} \rceil}$ (when n is odd)	4	$\frac{n+3}{2}$	2

Table 5.4: The vertices of $\Gamma(L[n])$ are presented along with their frequencies with respect to degrees and eccentricities.

Representative Vertices	Degree	Eccentricity	Frequency
u	4	$\lceil \frac{n}{2} \rceil + 1$	$2n+2$
w	4	$\lceil \frac{n}{2} \rceil + 1$	$n+1$

Table 5.5: The vertices of $\Gamma(CL[n])$ are presented along with their frequencies with respect to degrees and eccentricities.

Representative Vertices	Degree	Eccentricity	Frequency
u	4	$\lfloor \frac{n}{2} \rfloor + 1$	$2n+2$
w	4	$\lfloor \frac{n}{2} \rfloor + 2$	$n+1$

Table 5.6: The vertices of $\Gamma(ML[n])$ are presented along with their frequencies with respect to degrees and eccentricities.

Corollary 5.1.3. *The total-eccentricity index of the Mobius ladder $ML[n]$ is given by*

$$\zeta(ML[n]) = 2t(n+1),$$

where $t = \lceil \frac{n}{2} \rceil$.

Now, we calculate $\xi(G)$ and $\zeta(G)$ of the line graphs of the graphs $L[n]$, $CL[n]$ and $ML[n]$. Again, for each of these graphs, we take representatives from their vertices which have the same degree and eccentricity. In Tables 5.4-5.6, we present these representative vertices for each graph alongwith their degrees, eccentricities and frequency of occurrence.

Theorem 5.1.4. *The eccentric-connectivity index of $\Gamma(L[n])$ is given by*

$$\xi(\Gamma(L[n])) = \begin{cases} 24nt - 12t^2 - 6n + 20t & n \text{ is even} \\ 24nt - 12t^2 - 24n + 44t - 20 & n \text{ is odd,} \end{cases}$$

where $t = \lceil \frac{n}{2} \rceil$.

Proof. The vertices of the graph $\Gamma(L[n])$ are labelled by u_i, v_i and w_j for $1 \leq i \leq n$ and $1 \leq j \leq n$ as shown in Figure 6.1. In Table 5.4, the representatives from these vertices are presented along with their degrees and eccentricities. We first consider the case when n is even. Using Table 5.4, the eccentric-connectivity index is calculated as follows.

$$\begin{aligned}\xi(\Gamma(L[n])) &= \sum_{u\in V(D_1[n])} d(u)\varepsilon(u)\\ &= (3\times 4)n + \sum_{i=2}^{t}(4\times 4)(n-i+1) + (2\times 2)(n+1) + \sum_{i=2}^{t}(4\times 2)(n-i+2)\\ &\quad +4(n+2)\frac{1}{2}\\ &= 24nt - 12t^2 - 6n + 20t.\end{aligned}$$

Next, we consider the case when n is odd. Using Table 5.4, the the eccentric-connectivity index is calculated as follows.

$$\begin{aligned}\xi(\Gamma(L[n])) &= (3\times 4)n + \sum_{i=2}^{t-1}(4\times 4)(n-i+1) + (4\times 2)(n+1)\frac{1}{2} + (2\times 2)(n+1)\\ &\quad + \sum_{i=2}^{t-1}(4\times 2)(n-i+2) + (4\times 2)(n+3)\frac{1}{2}\\ &= 24nt - 12t^2 - 24n + 44t - 20.\end{aligned}$$

This completes the proof. □

Similarly, the next two theorems can be followed by using Tables 5.5-5.6.

Theorem 5.1.5. *The eccentric-connectivity index of $\Gamma(CL[n])$is given by*

$$\xi(\Gamma(CL[n])) = 12nt + 12n + 12t + 12,$$

where $t = \lceil \frac{n}{2} \rceil$.

Theorem 5.1.6. *The eccentric-connectivity index of $\Gamma(ML[n])$ is given by*

$$\xi(\Gamma(ML[n])) = 12nt + 16n + 12t + 16,$$

where $t = \lceil \frac{n}{2} \rceil$.

The next three results provide the total-eccentricity index of the line graphs of the graphs $L[n]$, $CL[n]$ and $ML[n]$, and can be shown easily from Tables 5.4-5.6.

Corollary 5.1.4. *The total-eccentricity index of $\Gamma(L[n])$ is given by*

$$\zeta(\Gamma(L[n])) = \begin{cases} -3t^2 + 6nt + 5t - \frac{n}{2} + 1 & n \text{ is even} \\ -3t^2 + 6nt + 11t - 4n - 4 & n \text{ is odd,} \end{cases}$$

where $t = \lceil \frac{n}{2} \rceil$.

Corollary 5.1.5. *The total-eccentricity index of $\Gamma(CL[n])$ is given by*

$$\zeta(\Gamma(CL[n])) = 3nt + 3n + 3t + 3,$$

where $t = \lceil \frac{n}{2} \rceil$.

Corollary 5.1.6. *The total-eccentricity index of* $\Gamma(ML[n])$ *is given by*

$$\zeta(\Gamma(ML[n])) = 3nt + 4n + 3t + 4,$$

where $t = \lceil \frac{n}{2} \rceil$.

The following two theorems reveal interesting relationship between the eccentricity-based topological indices of 3-fence graphs and their line graphs.

Theorem 5.1.7. *Let* $t = \lceil \frac{n}{2} \rceil$. *Then* $\xi(G)$ *and* $\zeta(G)$ *of the graph* $L[n]$ *and its line graph are related as follows.*

$$\begin{aligned} \frac{1}{2}\xi(\Gamma(L[n])) - \xi((L[n])) &= \begin{cases} -2n - 8t - 2, & n \text{ is even} \\ -8n + 4t - 6 & n \text{ is odd,} \end{cases} \\ \zeta(\Gamma(L[n])) - \frac{3}{2}\zeta(L[n]) &= \begin{cases} -n - 4t - 2 & n \text{ is even} \\ -4n + 2t - 4 & n \text{ is odd.} \end{cases} \end{aligned}$$

Theorem 5.1.8. *Let* $t = \lceil \frac{n}{2} \rceil$ *and* $t' = \lfloor \frac{n}{2} \rfloor$. *The eccentric-connectivity index and the total-eccentricity index of the graphs* $CL[n]$ *and* $ML[n]$ *and their line graphs are related by the following expressions.*

$$\begin{aligned} \xi(\Gamma(CL[n])) - 2\xi(CL[n]) &= 0, \\ \zeta(\Gamma(CL[n])) - \frac{3}{2}\zeta(CL[n]) &= 0, \\ \zeta(\Gamma(ML[n])) - \frac{3}{2}\zeta(ML[n]) &= 2n + 2, \end{aligned}$$

$$\frac{1}{2}\xi(\Gamma(ML[n])) - \xi(ML[n]) = \begin{cases} 8(n+1) & n \text{ is even} \\ 6n(t' - t) + 6(t' - t) + 8(n+1) & n \text{ is odd.} \end{cases}$$

5.2 Eccentricities of the grid graph and its line graph

In this section we construct a grid graph from the ladder graph $L[n]$ and then we construct its line graph and study their eccentricity-based topological indices.

A grid graph or a C_4-grid (see Figure 5.2) can be obtained from a ladder graph $L[n]$ by repeated subdivision of its geometrically parallel edges $u_i v_i \in E(L[n])$ and by joining the newly added vertices (say u'_i) with each other by the edges $u'_i u'_{i+1}$ for $1 \leq i \leq n$. Repeating this process $m - 1$ times, we denote the resultant graph by $L[n, m]$. Applying the same operation of subdivision to the circular ladder $CL[n]$, the resultant graph is called a C_4-nanotube. The eccentricities of the C_4-nanotubes were studied in [32]. Next, we compute $\xi(G)$ when $G \cong L[n, m]$ which can be considered as the 2-dimensional lattice of a C_4-nanotube. We study $\xi(G)$ and $\zeta(G)$ of the grid graphs $L[n, m]$ and their line graphs $\Gamma(L[n, m])$.

Theorem 5.2.1. *Let* $m, n \in \mathbb{N}$ *and* $s = \lfloor \frac{n+2}{2} \rfloor$, $t = \lfloor \frac{m+2}{2} \rfloor$. *The eccentric-connectivity index of the graph* $L[n, m]$ *is computed in the following three cases.*

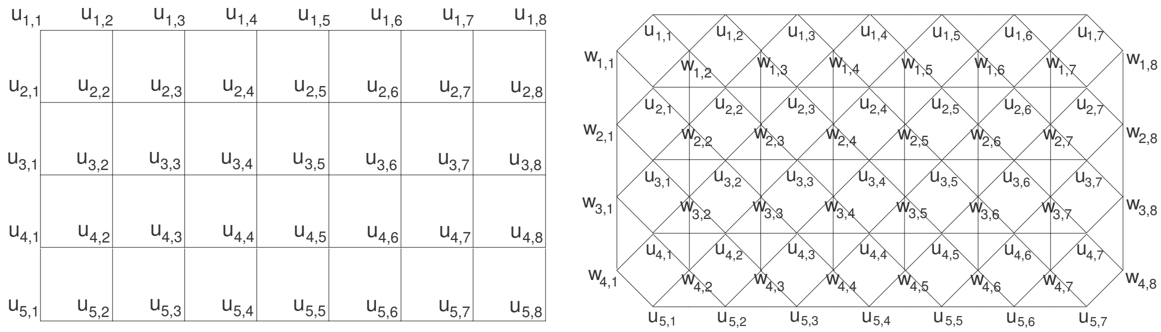

Figure 5.2: The graph of a square grid $L[n, m]$ (left) and its line graph $\Gamma(L[n, m])$ (right), for $n = 7$ and $m = 4$.

(**a**) *If both m and n are odd then*

$$\begin{aligned}\xi(L[n,m]) &= 20m + 20n + 12ns + 12mt + (16t-4)\sum_{i=2}^{s}|m+1-i| \\ &\quad +(16s-4)\sum_{j=2}^{t}|n+1-j|.\end{aligned}$$

(**b**) *If n is even and m is odd, we have*

$$\begin{aligned}\xi(L[n,m]) &= 20m + 14n + 12sn + 12mt + (16s-16)|n-t+1| + (16t-10)|m-s \\ &\quad +1| + (16s-4)\sum_{j=2}^{t}|n+1-j| + (16t-4)\sum_{i=2}^{s-1}|m+1-i|.\end{aligned}$$

(**c**) *If both n and m are even then we have*

$$\begin{aligned}\xi(L[n,m]) &= 14m + 14n + 12tm + 12sn + (16t-10)|m+1-s| + (16s-10)|n+1 \\ &\quad -t| + (16t-4)\sum_{i=2}^{s-1}|m+1-i| + (16s-4)\sum_{j=2}^{t-1}|n+1-j|.\end{aligned}$$

The case when m is even and n is odd can be obtained from ***(b)*** *by rotating the graph $L[n, m]$ by $90°$, that is, by switching n and m.*

Proof. The graph $L[n, m]$ is a rectangular grid with horizontal length n and vertical length m. For any two vertices $u_{i,j}, u_{k,l} \in V(L[n, m])$, the distance is defined by $d(u_{i,j}, u_{k,l}) = |i-k| + |j-l|$. To find the eccentricities of these vertices, we divide this grid into 4 quadrants and two axis lines with centre at $(\frac{n}{2}, \frac{m}{2})$ as shown in Figure 5.3.
The degrees of the vertices $u_{i,j} \in V(L[n, m])$ are as follows.

$$d(u_{i,j}) = \begin{cases} 2 & i \in \{1, m+1\} \text{ and } j \in \{1, n+1\} \\ 3 & i \in \{1, m+1\} \text{ and } 2 \leq j \leq n \text{ or } 2 \leq i \leq m \text{ and } j \in \{1, n+1\} \\ 4 & 2 \leq i \leq m \text{ and } 2 \leq j \leq n. \end{cases} \qquad (5.1)$$

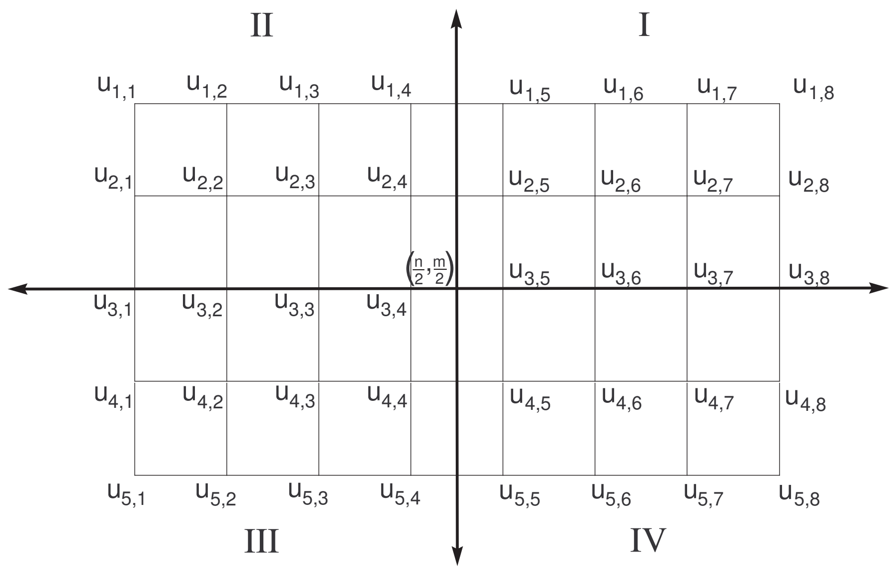

Figure 5.3: The grid graph for $n = 7$ and $m = 4$ is divided into 4 quadrants with center at $(\frac{7}{2}, \frac{4}{2})$.

By the symmetry of the graph $L[n, m]$ we can see that the eccentricities and degrees of the vertices from one quadrant are enough for the computation of eccentric-connectivity index of the graph $L[n, m]$. Let $s = \lfloor \frac{n+2}{2} \rfloor$ and $t = \lfloor \frac{m+2}{2} \rfloor$, then the vertices $u_{i,j}$ are in the first quadrant when $1 \leq i \leq t$ and $1 \leq j \leq s$. The eccentricities of the vertices $u_{i,j}$, $1 \leq i \leq t,\ 1 \leq j \leq s$ are given by

$$e(u_{i,j}) = d(u_{i,j}, u_{m+1,n+1}). \tag{5.2}$$

We have the following three cases.

Case 1. When both n and m are odd. In this case, no vertex $u_{i,j}$, $1 \leq i \leq t,\ 1 \leq j \leq s$ lies on the axis lines. The degrees and eccentricities of these vertices from equations (5.1) and (5.2), respectively, are presented in Table 5.7.

Representative Vertices	**Degree**	**Eccentricity**	**Frequency**
$u_{1,1}$	2	$\lvert m+1-1\rvert + \lvert n+1-1\rvert$	4
$u_{i,1}$ $(2 \leq i \leq t)$	3	$\lvert m+1-i\rvert + \lvert n+1-1\rvert$	4
$u_{1,j}$ $(2 \leq j \leq s)$	3	$\lvert m+1-1\rvert + \lvert n+1-j\rvert$	4
$u_{i,j}$ $(2 \leq i \leq t,\ 2 \leq j \leq s)$	4	$\lvert m+1-i\rvert + \lvert n+1-j\rvert$	4

Table 5.7: The vertices of $L[n, m]$ along with their frequencies of occurrence with respect to degrees and eccentricities.

Using equation (2.8) and Table 5.7, we get the following equation.

$$\begin{aligned}
\xi(L[n,m]) &= 2\times 4(m+n)+3\times 4\sum_{i=1}^{s}(|m+1-i|+n)+3\times 4\sum_{j=1}^{t}(m+|n+1-j|)+\\
&\quad 4\times 4\sum_{i=2}^{s}\sum_{j=2}^{t}(|m+1-i|+|n+1-j|)\\
&= 20m+20n+12ns+12mt+(16t-4)\sum_{i=2}^{s}|m+1-i|+(16s-4)\sum_{j=2}^{t}|n\\
&\quad +1-j|.
\end{aligned}$$

Case 2. When n is even and m is odd. The eccentricities and degrees of the vertices $u_{i,j}$ in this case are the same as in Case **1**. The frequency of the vertices $u_{i,s}$ for $1 \le i \le t$ lie on the axis line, thus taking frequency of these vertices 2, we get the following.

$$\begin{aligned}
\xi(L[n,m]) &= 2\times 4(m+n)+3\times 4\sum_{i=1}^{s-1}(|m+1-i|+n)+3\times 2(|m+1-s|+n)\\
&\quad +3\times 4\sum_{j=1}^{t}(m+|n+1-j|)+4\times 4\sum_{i=2}^{s}\sum_{j=2}^{t}(|m+1-i|+|n+1-j|)\\
&= 20m+14n+12sn+12mt+(16s-16)|n-t+1|+(16t-10)|m-s+1|\\
&\quad +(16s-4)\sum_{j=2}^{t}|n+1-j|+(16t-4)\sum_{i=2}^{s-1}|m+1-i|.
\end{aligned}$$

Case 3. When both m and n are even. The eccentricities and degrees of the vertices $u_{i,j}$ in this case are again same as given in Case **1**. The vertices $u_{t,j}$ for $1 \le j \le s$ and the vertices $u_{i,s}$ for $1 \le i \le t$ lie on the axis lines. Thus taking the frequency of these vertices 2, we get

$$\begin{aligned}
\xi(L[n,m]) &= 2\times 4(m+n)+3\times 4\sum_{i=1}^{s-1}(|m+1-i|+n)+3\times 2(|m+1-s|+n)\\
&\quad +3\times 4\sum_{j=1}^{t-1}(m+|n+1-j|)+3\times 2(m+|n+1-t|)\\
&\quad +4\times 4\sum_{i=2}^{s}\sum_{j=2}^{t}(|m+1-i|+|n+1-j|)\\
&= 14m+14n+12tm+12sn+(16t-10)|m+1-s|+(16s-10)|n+1-t|\\
&\quad +(16t-4)\sum_{i=2}^{s-1}|m+1-i|+(16s-4)\sum_{j=2}^{t-1}|n+1-j|.
\end{aligned}$$

In the next theorem, we calculate the eccentric-connectivity index of the line graph of the graph $L[n,m]$.

Theorem 5.2.2. *For $t = \lceil \frac{m}{2} \rceil$, $s = \lceil \frac{n}{2} \rceil$, the eccentric-connectivity index of the line graph $\Gamma(L[n,m])$ is given by* (**a**) *For $n, m \geq 2$ and m even, we have*

$$\begin{aligned}\xi(\Gamma(L[n,m])) &= 12n^2t - 12nt^2 - 24s^2t + 9m^2 + 18t^2 + 24mnt + 24nst + 18mn \\ &\quad -36mt - 54nt + 12st - 5m - 2n - 2s + 30t - 4.\end{aligned}$$

(**b**) *For $n, m \geq 2$ and m odd, we have*

$$\begin{aligned}\xi(\Gamma(L[n,m])) &= 12n^2t - 12nt^2 - 24s^2t + 9m^2 - 3n^2 + 6s^2 + 18t^2 + 24mnt + 24nst \\ &\quad +12mn - 36mt - 6ns - 48nt + 12st + 7m + 13n - 2s + 18t - 16.\end{aligned}$$

Proof. The eccentricities of vertices of the line graph $\Gamma(L[n,m])$ are as follows. When $1 \leq i \leq t$, the eccentricities of the vertices $u_{i,j}$ are as follows.

$$\varepsilon(u_{i,j}) = \begin{cases} n+m-j-i+1 & 1 \leq j \leq s \\ m+j-i & s+1 \leq j \leq n. \end{cases}$$

Also, $\varepsilon(u_{i+1,j}) = \varepsilon(u_{i,j}) - 1$ and $\varepsilon(u_{i,j}) = \varepsilon(u_{m-i+2,j})$ for $1 \leq i \leq t$ and $1 \leq j \leq n$.

When $1 \leq i \leq \lfloor \frac{m}{2} \rfloor - 1$, the eccentricities of the vertices $w_{i,j}$ are as follows.

$$\varepsilon(w_{i,j}) = \begin{cases} n+m-j-i+1 & 1 \leq j \leq s \\ m+j-i-1 & s+1 \leq j \leq n+1. \end{cases}$$

Also, $\varepsilon(w_{i+1,j}) = \varepsilon(w_{i,j}) - 1$ and $\varepsilon(w_{i,j}) = \varepsilon(w_{n-i+1,j})$ for $1 \leq i \leq t$ and $1 \leq j \leq n+1$. It is easy to see that the degrees of the vertices $u_{i,j}$ and $w_{i,j}$ are as follows.

$$d(u_{i,j}) = \begin{cases} 3 & i = 1, m+1 \text{ and } j = 1, n \\ 4 & i = 1, m+1 \text{ and } 2 \leq j \leq n-1 \\ 5 & 2 \leq i \leq m \text{ and } j = 1, n \\ 6 & 2 \leq i \leq m \text{ and } 2 \leq j \leq n-1, \end{cases}$$

$$d(w_{i,j}) = \begin{cases} 3 & i = 1, m \text{ and } j = 1, n+1 \\ 4 & 2 \leq i \leq m-1 \text{ and } j = 1, n+1 \\ 5 & i = 1, m \text{ and } 2 \leq j \leq n \\ 6 & 2 \leq i \leq m-1 \text{ and } 2 \leq j \leq n-1. \end{cases}$$

Case 1. When m is even. Using equation (2.8) and the eccentricities and degrees of the vertices $u_{i,j}$ $(1 \leq i \leq m+1,\ 1 \leq j \leq n)$ and $w_{i,j}$ $(1 \leq i \leq m,\ 1 \leq j \leq n+1)$, we get

$$\begin{aligned}
\xi(\Gamma(L[n,m])) &= 3 \times 4(n+m-1) + \sum_{j=2}^{s} 4 \times 2(n+m-j) + \sum_{j=s+1}^{n-1} 4 \times 2(m+j-1) \\
&\quad + \sum_{i=2}^{m} 5 \times 2(n+m-i) + \sum_{i=2}^{t} \Bigg(\sum_{j=2}^{s} 6 \times 2(n+m-i-j+1) + \sum_{j=s+1}^{n-1} 6 \times 2(m \\
&\quad -i+j) \Bigg) + \sum_{j=2}^{s} 6(n+(1/2)m-1-j+1) + \sum_{j=s+1}^{n-1} 6(t-1+j) + 3 \times 4(n \\
&\quad +m-1) + \sum_{i=2}^{m-1} 4 \times 2(n+m-i) + \sum_{j=2}^{s} 5 \times 2(n+m-j) + \sum_{j=s+1}^{n} 5 \times 2(m \\
&\quad +j-2) + \sum_{i=2}^{t} \Bigg(\sum_{j=2}^{s} 6 \times 2(n+m-i-j+1) + \sum_{j=s+1}^{n} 6 \times 2(m-i+j-1) \Bigg) \\
&= 12n^2t - 12nt^2 - 24s^2t + 9m^2 + 18t^2 + 24mnt + 24nst + 18mn - 36mt - 54nt \\
&\quad +12st - 5m - 2n - 2s + 30t - 4.
\end{aligned}$$

Case 2. When m is odd. Using equation (2.8) and the eccentricities and degrees of the vertices $u_{i,j}$ $(1 \leq i \leq m+1,\ 1 \leq j \leq n)$ and $w_{i,j}$ $(1 \leq i \leq m,\ 1 \leq j \leq n+1)$, we get

$$\begin{aligned}
\xi(\Gamma(L[n,m])) &= 3 \times 4(n+m-1) + \sum_{j=2}^{s} 4 \times 2(n+m-j) + \sum_{j=s+1}^{n-1} 4 \times 2(m+j-1) \\
&\quad + \sum_{i=2}^{m} 5 \times 2(n+m-i) + \sum_{i=2}^{t} \Bigg(\sum_{j=2}^{s} 6 \times 2(n+m-i-j+1) + \sum_{j=s+1}^{n-1} 6 \times \\
&\quad 2(m-i+j) \Bigg) + 3 \times 4(n+m-1) + \sum_{i=2}^{m-1} 4 \times 2(n+m-i) + \sum_{j=2}^{s} 5 \times \\
&\quad 2(n+m-j) + \sum_{j=s+1}^{n} 5 \times 2(m+j-2) + \sum_{i=2}^{t} \Bigg(\sum_{j=2}^{s} 6 \times 2(n+m-i \\
&\quad -j+1) + \sum_{j=s+1}^{n} 6 \times 2(m-i+j-1) \Bigg) \\
&= 12n^2t - 12nt^2 - 24s^2t + 9m^2 - 3n^2 + 6s^2 + 18t^2 + 24mnt + 24nst + 12mn \\
&\quad -36mt - 6ns - 48nt + 12st + 7m + 13n - 2s + 18t - 16.
\end{aligned}$$

In the next two results we obtain the τ for $\Gamma(L[n,m])$. These results can be obtained by ignoring the vertex degrees in the computation of the eccentric-connectivity index of $\Gamma(L[n,m])$.

Corollary 5.2.1. *For $n, m \geq 2$, m even and $t = \frac{m}{2}$, $s = \lceil \frac{n}{2} \rceil$, the total-eccentricity index of* *the line graph* $\Gamma(L[n,m])$ *is given by*

$$\begin{aligned}\zeta(\Gamma(L[n,m])) &= 3t^2 - s^2 + 2n^2t + \frac{n^2}{2} - 4s^2t - 2nt^2 + 2m^2 + 4mnt + 4nst + 5mn \\ &\quad + ns - 9nt + 2st - 6mt - \frac{n}{2} + 5t - 2.\end{aligned}$$

Corollary 5.2.2. *For* $n, m \geq 2$, m *odd and* $t = \lceil \frac{m}{2} \rceil$, $s = \lceil \frac{n}{2} \rceil$, *the total-eccentricity index of the line graph* $\Gamma(L[n,m])$ *is given by*

$$\begin{aligned}\zeta(\Gamma(L[n,m])) &= 2n^2t - 2nt^2 - 4s^2t + 2m^2 + 3t^2 + 4nst + 4mnt + 4mn - 6mt - 8nt + 2st \\ &\quad + 2m + 2n + 3t - 4.\end{aligned}$$

5.3 Summary of the results

In this chapter, we considered some 3-fence graphs namely ladder, circular ladder and Möbius ladder and computed their eccentric-connectivity and total-eccentricity indices. We computed the line graphs of these graphs and investigated the eccentricity-based indices of these graphs. Moreover, the study has been carried out on relation between the indices of these graphs and their line graphs. Furthermore, we studied the eccentricities of the grid graph $L[m,n]$ which can be considered as the 2-dimensional lattice of a C_4-nanotube and its line graph $\Gamma(L[m,n])$.

Chapter 6

Some spectrum-based indices of molecular graphs

In this chapter, we use computational tools to approximate the values of energy $\mathcal{E}$ and Estrada index $\mathcal{EE}$ of the molecular graphs of nanocones with growth stage n, denoted by $CNC_k[n]$. We also investigate the approximate values of $\mathcal{E}$ and index of the 2-dimensional lattice of $TUC_4C_8(R)[m,n]$ nanotubes by using computational and statistical tools. The graphs $CNC_k[n]$ and $TUC_4C_8[m,n]$ are defined in the next section.

6.1 Some molecular graphs of nanotubes and nanocones

Graphite in its natural form has carbon nanocones on its surface. These nanocones have been been observed since 1968 [56]. The height of these nanocones varies from 1 micrometer to 40 and their bases are attached to graphite. The walls of these nanocones are mostly curved. The laboratory made nanocones are generally more regular than these naturally occurring nanocones.

Due to potential applications in industry, carbon nanostructures have attracted considerable attention [83]. Recently, it has been proposed that carbon nanocones also have applications in energy as well as in molecular gas storage devices [1, 143, 146]. The molecular graph of $CNC_k[n]$ nanocones has a conical structure with a cycle of length k at its core and n layers of hexagons placed at the conical surface around its center (see Fig. 6.1).

There are several characterizations with respect to the structure of carbon nanotubes. For example, the thickness of a nanotube, its length and number of layers, moreover the types of walls with respect to the nature of rings which cove them. Carbon nanotubes and many times much stronger in constitution and construction and much lighter in weight than steel, and have remarkable applications in electronics and nanotechnology. Consider 2-dimensional lattice of a $TUC_4C_8(R)[m,n]$ nanotube. It is composed of n layers ($n \geq 1$), where each layer contains $m+1$ cycles of length 4 and each cycle of length 4 is in the form of a rhombus (see Figure 6.2).

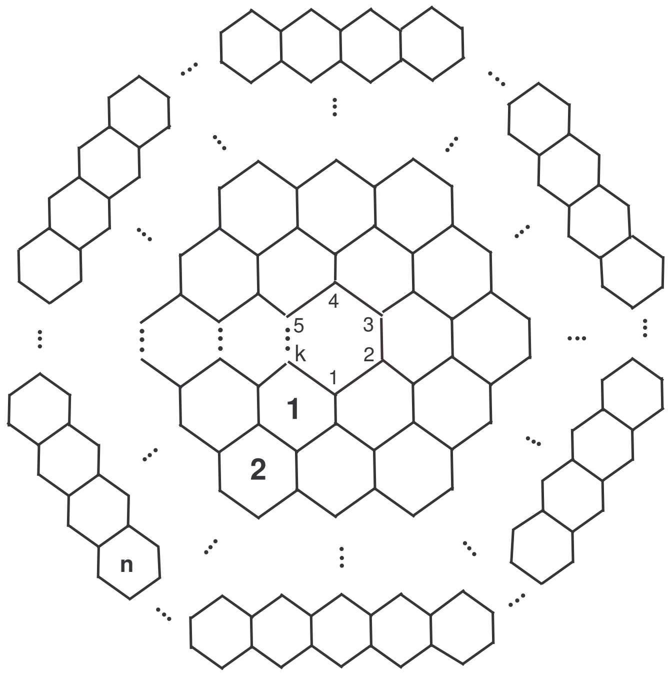

Figure 6.1: The graph of $CNC_k[n]$ nanocone.

Two consecutive layers are joined by adding edges between the corresponding vertices of the cycles of length 4. Two such layers give us a period of this nanotube, where there are m octagons in each period. We can obtain a next period by adding another layer to the bottom of this nanotube.

Ashrafi and Sadati [5] suggested a curve to estimate the $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_5[n]$. Next, we find estimated values of $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_k[n]$ nanocones for $k \geq 3$ by suggesting general curves. These curves give much better approximations of$\mathcal{E}$ and $\mathcal{EE}$ for $CNC_5[n]$ as compared to the curves suggested by Ashrafi and Sadati [5].

6.2 Calculation of $\mathcal{E}$ and $\mathcal{EE}$ for $CNC_k[n]$ nanocones (for $k = 3, 4, 5$)

The molecules of $CNC_3[n]$ are drawn in HyperChem [86] for $1 \leq n \leq 11$. There is a software tool named TopoCluj [30] which is used to obtain the adjacency matrix of our graphs. Then $\mathcal{E}$ and $\mathcal{EE}$ are calculated using MATLAB. The obtained data is shown in Table 6.1.

By using "cftoolbox" of MATLAB, a power curve of the form $an^b + c$ is fitted to the data shown in Table 6.1. A polynomial can approximate a smooth curve with small error and the curves with exponential increase are better fitted with power or exponential functions. Our calculations show that the behaviour of $\mathcal{E}$ and $\mathcal{EE}$ of nanocones is exponential. Thus the $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_3[n]$ can be estimated by the following curves:

$$\mathcal{E}(CNC_3[n]) \cong 7.68n^{1.854} + 11.75, \quad (6.1)$$

$$\mathcal{EE}(CNC_3[n]) \cong 15.62n^{1.861} + 23.44. \quad (6.2)$$

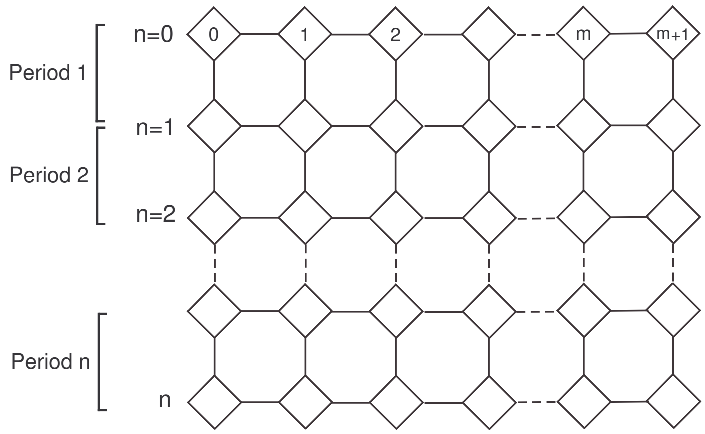

Figure 6.2: The graph of $TUC_4C_8(R)[m,n]$ nanotube.

n	Energy	Estrada index
1	17.285918460265211	34.902282086936083
2	39.927994243587236	80.963645191149396
3	71.958281219523982	146.6524905652332
4	113.3970122940882	231.9695783788370
5	164.2574898928459	336.9149088724020
6	224.5486057576022	461.4884820459496
7	294.2762041727111	605.6902978994802
8	373.4440212903026	769.5203564329929
9	462.0544073288664	952.9786576464878
10	560.1088533736765	1156.065201539966
11	667.6083318445358	1378.779988113426

Table 6.1: Exact values of $\mathcal{E}$ and $\mathcal{EE}$ for $CNC_3[n]$ nanocones, where $n \in \{1, 2, \ldots, 11\}$, obtained by (2.11) and (2.12).

Next, we calculate $\mathcal{E}(CNC_4[n])$ and $\mathcal{EE}(CNC_4[n])$ by following the same procedure as we followed before. The curves given by equations (6.3) and (6.4), estimating the $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_4[n]$, are obtained from the data presented in Table 6.2.

$$\mathcal{E}(CNC_4[n]) \cong 10.24n^{1.854} + 15.13, \tag{6.3}$$
$$\mathcal{EE}(CNC_4[n]) \cong 20.83n^{1.861} + 29.57. \tag{6.4}$$

Ashrafi and Sadati [5] conjectured that the $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_5[n]$ nanocones can be estimated by the equations

$$\mathcal{E}(CNC_5[n]) = 28.7372(1.2)^{n-1}, \tag{6.5}$$

$$\mathcal{EE}(CNC_5[n]) = 55.5639(1.2)^{n-1}. \tag{6.6}$$

The exact values of $\mathcal{E}$ and $\mathcal{EE}$ calculated by using equations (2.11) and (2.12) are given in Table 6.3. Our calculations suggest that the $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_5[n]$ nanocones can be estimated

n	Energy	Estrada index
1	22.655237944642849	44.851875023929438
2	52.477341729732132	106.2661197003211
3	95.499127855630348	193.8512465676944
4	150.5722714744230	307.6073636524728
5	218.5422165873519	447.5344709772261
6	298.8399203726523	613.6325685419566
7	391.8867276200732	805.9016563466638
8	497.4022714706196	1024.341734391347
9	615.5823182586247	1268.952802676007
10	746.3056582427638	1539.734861200645
11	889.6498190605680	1836.687909965259

Table 6.2: Exact values of $\mathcal{E}$ and $\mathcal{EE}$ for $CNC_4[n]$ nanocones, where $n \in \{1, 2, \ldots, 11\}$, obtained by (2.11) and (2.12).

by the exponential curves given by

$$\mathcal{E}(CNC_5[n]) \cong 12.8n^{1.854} + 19.49, \quad (6.7)$$
$$\mathcal{EE}(CNC_5[n]) \cong 26.04n^{1.861} + 36.46. \quad (6.8)$$

One can easily check that the equations (6.7) and (6.8) give higher accuracy as compared to equations (6.5) and (6.6). For example, for $n = 11$ the equations (6.5) and (6.6) give

$$\mathcal{E}(CNC_5[11]) = 177.9331679, \quad \mathcal{EE}(CNC_5[11]) = 344.0370234.$$

However, equations (6.7) and (6.8) give

$$\mathcal{E}(CNC_5[11]) = 1110.809733, \quad \mathcal{EE}(CNC_5[11]) = 2294.193967,$$

which is much closer to the exact values of $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_5[11]$.

6.3 Calculation of $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_k[n]$ nanocones (for $k \geq 3$)

One can observe that the equations (6.1), (6.3) and (6.7) are of the form an^b+c. Here $b = 1.854$ and the coefficients a and c increase linearly. We estimate the coefficients a and c, for $k \geq 3$, as follows.

$$a = 2.56(k-2) + 5.12, \quad c = 3.87(k-2) + 7.717.$$

Similarly, the equations (6.2), (6.4) and (6.8), are of the form $an^b + c$. Here $b = 1.861$ and the coefficients a and c respectively increase linearly and quadratically. We estimate the coefficients a and c, for $k \geq 3$ as follows.

$$a = 5.21(k-2) + 10.41, \quad c = 4.585(k-2)^{1.225} + 18.85.$$

n	Energy	Estrada index
1	28.737240867972083	55.563929323677989
2	66.430609112555430	132.3316121087914
3	119.8435927566387	241.8130206666559
4	188.8925953205016	384.0081670226269
5	273.6709036427948	558.9170511785687
6	374.1500925987631	766.5396731344816
7	490.3666383558780	1006.876032890366
8	622.3109849474412	1279.926130446221
9	769.9959809125679	1585.689965802046
10	933.4195515448562	1924.167538957842
11	1112.585456091773	2295.358849913610

Table 6.3: The exact values of $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_5[n]$ nanocones, $1 \leq n \leq 11$, calculated by using equations (2.11) and (2.12).

We suggest general curves to estimate the $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_k[n]$ nanocones ($k \geq 3$ and $n \geq 1$) by

$$\mathcal{E}(CNC_k[n]) = (2.56(k-2)+5.12)n^{1.854} + 3.87(k-2) + 7.717, \quad (6.9)$$

$$\mathcal{EE}(CNC_k[n]) = (5.21(k-2)+10.41)n^{1.861} + 4.585(k-2)^{1.225} + 18.85. \quad (6.10)$$

6.4 Analysis of the results on nanocones

Since the molecular graphs have usually large order, it becomes very hard to obtain and handle their data. In such cases, the computational and statistical methods provide very useful tools. These tools reduce the time and effort that is required to perform a certain task. In this context, we have estimation tools to obtain the desired quantities by extrapolation. We have derived the approximation curves given by equations (6.9) and (6.10) for the $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_k[n]$ nanocones.
Some estimated values of $\mathcal{E}(CNC_k[n])$ and $\mathcal{EE}(CNC_k[n])$ calculated from equations (6.9) and (6.10), respectively, are compared with the corresponding exact values in Table 6.4.

For $k \in \{3, 4, \ldots, 10\}$ the curves given by equations (6.9) and (6.10) give a good approximation of $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_k[n]$ nanocones. However, it is not certain that (6.9) and (6.10) can give a good approximation of $\mathcal{E}$ and $\mathcal{EE}$ for larger values of k. The reader is invited to choose a better approximation technique to find more exact values of $\mathcal{E}$ and $\mathcal{EE}$ of these as well as other nanostructures.

6.5 Computational results for the molecular graphs of nanotubes

Now we explain the procedure of calculating $\mathcal{E}$ and $\mathcal{EE}$ of $TUC_4C_8[m,n]$.

$[k,n]$		Energy	Estrada index
$[5,12]$	Exact	1307.4939259	2699.2638986
	Estimated	1301.693015	2691.051099
$[5,13]$	Exact	1518.1460546	3135.8826852
	Estimated	1506.840599	3117.446990
$[7,4]$	Exact	264.4223902	537.4529550
	Estimated	261.2510052	532.8954912
$[7,5]$	Exact	383.1230028	782.325393
	Estimated	381.2505556	780.5646281
$[8,4]$	Exact	302.0061802	614.2283756
	Estimated	298.5758631	609.8857596
$[8,5]$	Exact	437.7879216	894.08259023
	Estimated	435.7182063	892.9459060
$[9,5]$	Exact	492.5828863	1005.8424178
	Estimated	490.1858572	1005.643401
$[9,6]$	Exact	673.4318294	1379.5631373
	Estimated	673.3275706	1384.185845
$[10,5]$	Exact	547.34180729	1117.6026258
	Estimated	544.6535079	1118.621264

Table 6.4: Comparison of exact values of $\mathcal{E}$ and $\mathcal{EE}$ of $CNC_k[n]$ nanocones calculated by using equations (2.11) and (2.12) with the corresponding estimated values calculated by using (6.9) and (6.10).

For each m and n, $1 \leq m,n \leq 15$, the graphs $TUC_4C_8[m,n]$ are constructed in a software package HyperChem [86]. For every graph $TUC_4C_8[m,n]$, the adjacency matrix $A(TUC_4C_8[m,n])$ is obtained with the software TopoCluj [30]. Then the $\mathcal{E}$ and $\mathcal{EE}$ are calculated using MATLAB. For a constant value of m and $1 \leq n \leq 15$, a quadratic function is approximated with the exact values of $\mathcal{E}$ and $\mathcal{EE}$ of $TUC_4C_8[m,n]$ by using "cftoolbox" of MATLAB. These values are presented in Table 6.5.

Using the data given by Table 6.5, a quadratic polynomial is fitted to the coefficients of n^k, where $1 \leq m \leq 15$ and $k \in \{0,1,2\}$. The results are displayed in Table 6.6. Finally, the general curves in two dimensions, representing the $\mathcal{E}$ and $\mathcal{EE}$ of the graph $TUC_4C_8[m,n]$ are given by equation (6.11) and equation (6.12), respectively. A comparison between the plots of the two surfaces given by equation (6.11) and equation (6.12), has been made in Figure 6.3.

$$\begin{aligned}\mathcal{E}(G) &= 0.000001534n^2m^2 + 0.0003427n^2m + 0.0004565n^2 + 0.0003725nm^2 + 5.875nm \\ &\quad +5.195n + 0.0001713m^2 - 0.6824m - 0.6915 \end{aligned} \tag{6.11}$$

$$\begin{aligned}\mathcal{EE}(G) &= -2.973 \times 10^{-16}n^2m^2 + 2.189 \times 10^{-11}n^2m + 2.116 \times 10^{-11}n^2 + 0.0001721nm^2 \\ &\quad +13.53nm + 11.51n + 0.00001026m^2 - 2.029m - 1.982 \end{aligned} \tag{6.12}$$

$TUC_4C_8[m,n]$	Energy	Estrada index
$[1,n]$	$0.0008665n^2 + 11.1n - 1.284$	$0.00000000004306n^2 + 25.04n - 4.011$
$[2,n]$	$0.0009902n^2 + 16.93n - 2.226$	$0.00000000006495n^2 + 38.57n - 6.04$
$[3,n]$	$0.00159n^2 + 22.8n - 2.617$	$0.00000000008684n^2 + 52.1n - 8.068$
$[4,n]$	$0.001897n^2 + 28.71n - 3.55$	$0.0000000001087n^2 + 65.64n - 10.1$
$[5,n]$	$0.002164n^2 + 34.56n - 3.958$	$0.0000000001306n^2 + 79.17n - 12.13$
$[6,n]$	$0.002585n^2 + 40.47n - 4.886$	$0.0000000001525n^2 + 92.7n - 14.15$
$[7,n]$	$0.002815n^2 + 46.34n - 5.372$	$0.0000000001744n^2 + 106.2n - 16.18$
$[8,n]$	$0.00347n^2 + 52.22n - 6.185$	$0.0000000001963n^2 + 119.8n - 18.21$
$[9,n]$	$0.003525n^2 + 58.12n - 6.791$	$0.0000000002182n^2 + 133.3n - 20.24$
$[10,n]$	$0.004045n^2 + 63.98n - 7.525$	$0.0000000002401n^2 + 146.8n - 22.27$
$[11,n]$	$0.004669n^2 + 69.87n - 8.136$	$0.0000000002619n^2 + 160.4n - 24.3$
$[12,n]$	$0.004536n^2 + 75.75n - 8.891$	$0.0000000002838n^2 + 173.9n - 26.33$
$[13,n]$	$0.00524n^2 + 81.64n - 9.512$	$0.0000000003057n^2 + 187.4n - 28.36$
$[14,n]$	$0.005502n^2 + 87.52n - 10.25$	$0.0000000003276n^2 + 201n - 30.38$
$[15,n]$	$0.005983n^2 + 93.4n - 10.87$	$0.0000000003495n^2 + 214.5n - 32.41$

Table 6.5: The quadratic curves, each for $1 \leq n \leq 15$, fitted to the $\mathcal{E}$ and $\mathcal{EE}$ of $TUC_4C_8(R)[m,n]$.

	Energy	Estrada index
n^2	$0.000001534m^2 + 0.0003427m$ $+0.0004565$	$-2.973 \times 10^{-16}m^2 + 2.189 \times 10^{-11}m$ $+2.116 \times 10^{-11}$
n	$0.0003725m^2 + 5.875m + 5.195$	$0.0001721m^2 + 13.53m + 11.51$
1	$-0.0001713m^2 + 0.6824m + 0.6915$	$-0.00001026m^2 + 2.029m + 1.982$

Table 6.6: The quadratic curves fitted to the coefficients of the curves presented in Table 6.5.

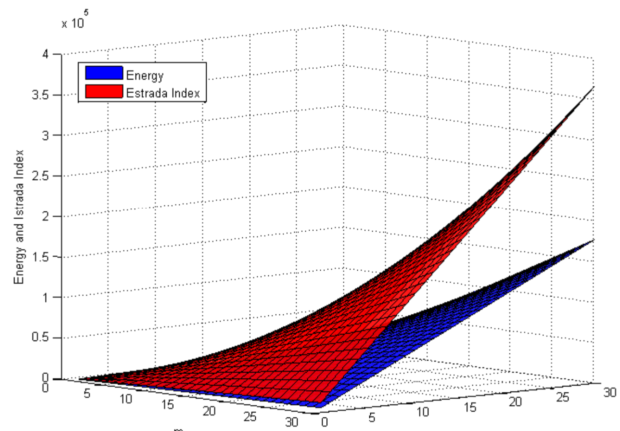

Figure 6.3: The invariants $\mathcal{E}$ and $\mathcal{EE}$ for $TUC_4C_8[m,n]$ nanotubes.

6.6 Analysis of the results on nanotubes

The study of computational results using software tools is important since obtaining algebraic results on large graphs is hard. Software tools makes it possible to estimate and predict results for large graphs by using few given exact values. The estimated and exact values of $\mathcal{E}$ and $\mathcal{EE}$ of the graph $TUC_4C_8[m,n]$ are presented in Table 6.7 and Table 6.8, respectively.

[m,n]	Energy	Estrada index
[15,1]	175.9424361000000	396.5827535013978
[15,2]	269.3759593500000	611.0814760031450
[15,3]	362.8213669000000	825.5801985055912
[15,4]	456.2786587500000	1040.078921008736
[15,5]	549.7478348999999	1254.577643512580
[15,6]	643.2288953499999	1469.076366017123
[15,7]	736.7218401000000	1683.575088522364
[15,8]	830.2266691499999	1898.073811028305
[15,9]	923.7433824999999	2112.572533534944

Table 6.7: The estimated values of $\mathcal{E}$ and $\mathcal{EE}$ of the graph $TUC_4C_8[m,n]$.

$[m,n]$	Energy	Estrada index
$[15,1]$	176.4719283781837	396.5932571216588
$[15,2]$	268.9602139104927	611.0965536459598
$[15,3]$	362.6373316374283	825.5998502177959
$[15,4]$	456.3125271135441	1040.103146789630
$[15,5]$	549.4664397693208	1254.606443361467
$[15,6]$	643.2525811733453	1469.109739933303
$[15,7]$	736.7771997058154	1683.613036505137
$[15,8]$	830.2341258472407	1898.116333076973
$[15,9]$	923.8919048450422	2112.619629648809

Table 6.8: The exact values of $\mathcal{E}$ and $\mathcal{EE}$ of the graph $TUC_4C_8[m,n]$.

It can be seen that the values of desired parameters ($\mathcal{E}(TUC_4C_8[m,n])$ and $\mathcal{EE}(TUC_4C_8[m,n])$) can be obtained with small errors. These errors can be reduced by applying a better estimation technique to the data and some other important molecular graphs can also be studied in this perspective, which is open to the readers.

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