BOUNDS ON THE GENERAL ECCENTRIC DISTANCE SUM OF GRAPHS

Yetneberk Kuma Feyissa

A Dissertation Submitted to the Department of Applied Mathematics,
School of Applied Natural Science

Presented in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy in Applied Mathematics

Office of Graduate Studies
Adama Science and Technology University

March, 2023
Adama, Ethiopia

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Declaration

I, hereby, declare that this dissertation entitled "**Bounds on the General Eccentric Distance Sum of Graphs**" is my original work. That is, it has not been submitted for the award of any academic degree, diploma or certificate in any other university. All sources of materials used for this thesis have been duly acknowledged through appropriate citations.

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Recommendation

We, the supervisors of this dissertation, hereby certify that we have read and revised the dissertation entitled "**Bounds on the General Eccentric Distance Sum of Graphs**" prepared under our guidance by **Yetneberk Kuma Feyissa** submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Applied Mathematics. Therefore, we recommend the submission of the dissertation to the department for further review and defense.

Prof. Dr. Tomáš Vetrík	____________________	____________________
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Approval page

We, hereby, certify that the recommendations and suggestions made by the board of examiners are appropriately incorporated into the final version of the dissertation entitled "**Bounds on the General Eccentric Distance Sum of Graphs**" by Yetneberk Kuma Feyissa.

Prof. Dr. Tomáš Vetrík	____________	____________
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Co-Advisor	Signature	Date

We, the undersigned, members of the Board of Examiners of the dissertation open defense by **Yetneberk Kuma Feyissa** have read and evaluated the dissertation entitled "**Bounds on the General Eccentric Distance Sum of Graphs**" and examined the candidate during open defense. This is, therefore, to certify that the dissertation is accepted for partial fulfillment of the requirement of the degree of Doctor of Philosophy in Applied Mathematics.

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Dedicated

To

My wife Tenaye Zerfu,

and

My sons Abem and Samuel Yetneberk.

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Acronyms and Abbreviations

$\mathbb{R}$	set of real numbers
G	graph
T	tree
$V(G)$	vertex set of G
$E(G)$	edge set of G
$deg_G(v)$	degree of a vertex v in G
$\Delta(G)$	maximum degree of G
$\delta(G)$	minimum degree of G
$r(G)$	radius of G
$d(G)$	diameter of G
$d_G(u,v)$	distance between vertices u and v in G
$ecc_G(v)$	eccentricity of a vertex v in G
$D_G(v)$	total distance of v in G
$\lfloor x \rfloor$	the biggest integer less than or equal to x
$\lceil x \rceil$	the smallest integer greater than or equal to x
χ	chromatic number
ν	matching number
K_n	complete graph of order n
$K_{p_1,p_2,\ldots,p_k}$	complete k-partite graph
K_{p_1,p_2}	complete bipartite graph
S_n	star graph of order n
P_n	path graph of order n
$EDS_{a,b}(G)$	general eccentric distance sum of G
$EDS(G)$	eccentric distance sum of G
$W(G)$	Wiener index of G
$DD(G)$	degree distance of G
$ECI(G)$	eccentric connectivity index of G
$M_1(G)$	first Zagreb index of G
$EM_1(G)$	first Zagreb eccentricity index of G
$EM_2(G)$	second Zagreb eccentricity index of G
QSAR	Quantitative structure-activity relationship
QSPR	Quantitative structure-property relationship

Abstract

A topological graph index is a mathematical formula that can be applied to any graph that models some molecular structure. Topological indices are used to study the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR)to predict the physicochemical properties of molecules. The eccentric distance sum of a graph G is one of these topological indices and it is defined by $EDS(G) = \sum_{v \in V(G)} ecc_G(v)D_G(v)$, where $ecc_G(v)$ is the distance between v and a vertex furthest from v in G and $D_G(v)$ is the sum of all distances from v to all other vertices in G. What we refer to as a general eccentric distance sum in this dissertation is obtained by raising $ecc_G(v)$ and $D_G(v)$ to powers of a and b $(a, b \in R)$, respectively, in the eccentric distance sum of a graph G. The focus of this study is finding bounds on the general eccentric distance sum of graphs. One of the motivations of this study is the great discriminating power of eccentric distance sum of graphs and its application in the study of structure activity/property relationships. For example, the anti-HIV activity of dihydroseselins was explored by using the structure-activity relationship of eccentric distance sum of its associated graph.

Motivated by [Vertik, T. (2021), General eccentric distance sum of graphs, Discrete Mathematics, Algorithms, and Applications, Vol. 13, No. 4: 2150046], we present bounds on the general eccentric distance sum for trees with a given bipartition. Moreover, we obtain bounds on the general eccentric distance sum for trees with a given order and specific diameter and domination number. Furthermore, we establish bounds on the general eccentric distance sum for bipartite graphs with a given order and matching number; and a given order and specific diameter. We also establish lower and upper bounds on the general eccentric distance sum for any graph with a given order and diameter; and for a join of two graphs with a given order and number of vertices of maximal degree. Graph transformation operations, proof by contradiction and direct proof techniques are used to obtain the main results in this dissertation.

Keywords: Graph, tree, bipartite graph, topological index, diameter, join, eccentric distance sum, bounds, extremal graph.

Publications

This PhD dissertation reports original results that contribute to the expansion of the frontiers of knowledge and scientific development of Mathematics. The original contributions of this PhD dissertation are contained in the following original papers which were published in international peer-review journals:

P1) Y. K. Feyissa and T. Vetrík, (2022). Bounds on the general eccentric distance sum of graphs. Discrete Math. Lett. 10: 99–109.

DOI: 10.47443/dml.2022.070.

P2) Y. K. Feyissa, M. Imran, T. Vetrík and N. Hunde, (2022). On the general eccentric distance sum of graphs and trees. Iranian J. Math. Chem. 13 (4): 239-252.

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CHAPTER 1

INTRODUCTION

This chapter includes definitions of basic graph theoretical terms that are used in the dissertation, and includes the motivations that provide relevant background to the study. Terms not defined in this chapter are defined in subsequent chapters, as the need arises.

1.1 Background of the Study

Graph Theory is an important area of contemporary mathematics with many applications in computer science, genetics, chemistry, engineering, industry, business and in social sciences. It is a relatively new field of study that was invented to address societal issues that traditional branches of mathematics like algebra or calculus are unable to address.

In this study, we are concerned with the part of graph theory that can be applied in chemistry which is called chemical graph theory. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory. It is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Its vertices are labeled with the kinds of the corresponding atoms and edges are labeled with the types of bonds. In theoretical chemistry, molecular descriptors are often used to develop quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR). These descriptors are also used to establish the mathematical basis for connections between molecular structures and physicochemical properties.

1.1.1 Preliminary Concepts

In this section, basic terms of graph theory introduced and used throughout the dissertation. Note that terms and definitions which are stated in this section are referred from (Bondy and Murty, 1976) and (West, 2001).

A lot of real-world situations can conveniently be described by means of a diagram consisting of a set of points (commonly called vertices) along with line segments (also commonly called edges) or arcs joining certain pairs of those vertices. For instance, the vertices could represent people, with edges joining pairs of friends; or the vertices may be communication centers, with edges representing communication links. Graphs are used to represent the competition of various species in a niche; they are used to represent who influences whom in a company, too. Notice that in such diagrams, one is especially curious about whether two given vertices are connected by an edge.

Definition 1.1. *A graph G consists of a finite non-empty set, $V(G)$, of vertices together with a (possibly empty) set, $E(G)$, of unordered pairs of vertices, called edges.*

The number of elements in the vertex set $V(G)$ is called the order of G, and the number of edges that G contains is called its size. If the order of G is 1, then G is said to be a trivial graph; otherwise G is called a nontrivial graph. For $e \in E(G)$, if edge $e = \{u, v\}$ (or, simply $e = uv$), we say that u and v are adjacent vertices, whereas e is said to be incident with u (or v). We also say that e joins vertices u and v.

Definition 1.2. *The degree of a vertex $v \in V(G)$, $deg_G(v)$, is the number of vertices (edges) adjacent (incident) to v. When it is obvious that we mean graph G, then we omit G and use $deg(v)$. A vertex of degree 1 is called a pendant vertex or a leaf.*

The minimum degree of G, denoted by $\delta(G) = \delta$, is the smallest of the degrees of the vertices in G, and the maximum degree of G, denoted by $\Delta(G) = \Delta$, is the largest of the degrees of the vertices in G. A simple graph of order n in which all distinct pairs of vertices are adjacent is called complete graph, denoted by K_n.

Definition 1.3. *A subgraph H of a graph G is a graph in which all its vertices belong to a set $U \subseteq V(G)$ and all its edges belong to $E(G)$ and connect vertices in U. If a subgraph of G contains precisely all the vertices of G, it is called a spanning subgraph of G.*

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

The graph denoted by $P_n : v_1 v_2 \dots v_n$ is a path of order n with vertex $V(P_n) = \{v_1, v_2, \dots, v_n\}$ and $E(P_n) = \{v_1v_2, v_2v_3, \dots, v_{n-1}v_n\}$. For $n \geq 3$, adding an edge between v_1 and v_n in the path P_n yields a cycle graph of order n, denoted by C_n.

Definition 1.4. *A graph G is connected if there is at least one path between every pair of vertices; otherwise it is disconnected.*

Definition 1.5. *For $k \geq 2$, a k-partite graph is a graph G whose vertex set $V(G)$ can be partitioned into k pairwise disjoint sets, so that no two vertices within the same set are adjacent.*

That is, $V(G) = V_1 \cup V_2 \cup \cdots \cup V_k$ and $V_i \cap V_j = \emptyset$ for $i \neq j$; $i, j = 1, 2, \ldots, k$ any edge in G connects two vertices from different partite sets. A complete k-partite graph is k-partite graph in which every two vertices from different partite sets are adjacent. It is denoted by $K_{p_1, p_2, \ldots, p_k}$ if the number of vertices in the i^{th} partite set is p_i, i.e. $|V_i| = p_i$ for $i = 1, 2, \ldots, k$. For a vertex $v \in V_i$ where $i = 1, 2, \ldots, k$, we have $deg(v) = n - p_i$ and the size (number of edges) of $K_{p_1, p_2, \ldots, p_k}$ is equal to $\sum_{i \neq j} p_i p_j$. When the number of partite sets is 2, we call such a graph 2-partite (commonly known as bipartite graph). When the two partite sets of vertices of a bipartite graph G contain s and t vertices, where $s + t = n$, then we say that G has an (s,t)-bipartition. If it is complete, it said to be complete bipartite graph which is denoted by $K_{s,t}$.

Definition 1.6.

1. *A planar graph is a graph which can be drawn on plane without edge crossing.*
2. *An outerplanar graph is a graph that can be embedded in the plane such that all vertices lie on the outer face.*

Outerplanar graphs are planar and, by their definition, connected graphs.

Definition 1.7. *For a graph G:*

1. *The distance $d_G(u, v)$ between two vertices u and v is the length of a shortest path between u and v in G.*
2. *The eccentricity of a vertex v in G, denoted by $ecc_G(v)$, is the distance between v and a vertex furthest from v in G.*
3. *The total distance of a vertex v in G, denoted by $D_G(v)$, is the the sum of all distance from v to all the other vertices in G, i.e. $D_G(v) = \sum_{u \in V(G)} d_G(v, u)$.*

The radius of G, denoted by $r(G)$, is the minimum eccentricity among the vertices of G, while the diameter of G, denoted by $d(G)$, is the maximum eccentricity. Therefore, we have the relation $r(G) \leq ecc_G(v) \leq d(G)$ for any vertex v of G. Let $d(G) = d$, a diametral path in G is a shortest path connecting two distinct vertices u and v of G such that the distance between u and v in G is the diameter of G, that is, $d_G(u, v) = d$.

Definition 1.8. *A tree is an acyclic graph (that is a graph that does not contain a cycle).*

A graph G with at least two vertices is a tree if and only if there is a unique path joining any pair of distinct vertices in G (West, 2001). The existence of the path corresponds to the connectedness property and the uniqueness of the path corresponds to the acyclic property of a tree. Every tree is a bipartite graph (West, 2001). There are different kinds of trees such as the path P_n, star S_n and caterpillars. A caterpillar is a tree T in which any vertex $v \in V(T)$ belongs to a diametral path or v is adjacent to a vertex in that diametral path. Let $C_{n,d}$ be a caterpillar obtained from $P_d : v_0 v_1 \cdots v_d$ by attaching $n-d-1$ pendent vertices to vertex $v_{\lfloor \frac{d}{2} \rfloor}$. For integers $l \geq 2$ and $n_1 \geq n_2 \geq 1$, $P_l(n_1,n_2)$ is a tree obtained from the path P_l by joining one end vertex of P_l to n_1 new pendant vertices and the other end vertex of P_l to n_2 pendant vertices; see Figure 5.1. The tree $P_l(n_1,n_2)$ has n_1+n_2 pendant vertices and has order n_1+n_2+l.

Definition 1.9. *A unicyclic graph G is a graph which contains a unique cycle in it.*

In a unicyclic graph, $|E(G)| = |V(G)|$. It can be obtained by adding an edge between two nonadjacent vertices of a tree. The girth of a graph is the length of a shortest cycle contained in a graph (which is not a tree).

Definition 1.10. *A coloring of a graph is the assignment of a color to each vertex of the graph so that any two adjacent vertices are colored differently. The minimum number of colors needed to color graph G is called the chromatic number of G and it is denoted by $\chi(G)$.*

If a graph G has chromatic number $\chi \geq 2$, the vertex set can be partitioned into χ sets such that no two vertices in the same set are adjacent. Thus, the graph is said to be an χ-partite graph.

Definition 1.11.

1. *An independent set of a graph G is a set $I \subseteq V(G)$ such that no two vertices in I are adjacent and independence number of G, denoted by $\alpha(G)$, is defined as* $\alpha(G) = \max\{|I| : I \text{ is independent set of } G\}$.

2. *A matching (sometimes called edge independent set) of a graph G is a set of edges such that any two distinct edges of the set do not have a common vertex. A matching number of a graph G, denoted by $\nu(G)$, is the maximum of the cardinalities of all matchings of a graph G.*

Tree is bipartite and so each partite set is an independent set. Thus, one of the two partite sets has at least $\frac{n}{2}$ vertices. Therefore, for any tree T with order n, we have $\frac{n}{2} \leq \alpha(T) \leq n-1$ (Balachandran and Vetrík, 2021) and the upper bound is achieved if and only if T is S_n.

A vertex cut of a graph G is a set $S \subseteq V(G)$ such that $G-S$ has more than one component, where $G-S$ is a subgraph obtained by deleting all vertices in S. The connectivity of G, written $\kappa(G)$, is the minimum cardinality of a vertex set S such that $G-S$ is disconnected or has only one vertex. A graph is κ-connected if its connectivity is at least κ and note that $\kappa(G) \leq \delta(G)$ where $\delta(G)$ is the minimum degree of G.

Definition 1.12.

1. *A dominating set V_D of G is a set $V_D \subseteq V(G)$ such that every vertex not in V_D is adjacent to at least one vertex in V_D and the domination number of G, denoted by $\gamma(G)$, is the minimum cardinality of all dominating sets.*

2. *A vertex cover of G is a set of vertices such that each edge of G is incident with at least one vertex of the set. A vertex cover number (simply covering) of G, denoted by $\beta(G)$, is the minimum of the cardinalities of all vertex covers.*

3. *An edge cover of G is a set of edges such that each vertex of G is incident with at least one edge of the set. An edge cover number of G, denoted by $\beta'(G)$ is the minimum of the cardinalities of all edge covers.*

From the fact that any tree is bipartite and each partite set is a dominating set. One of these partite set has at most $\frac{n}{2}$ vertices. Thus, for any tree T with order n, $1 \leq \gamma(T) \leq \frac{n}{2}$ (Ore, 1962). West (2001) related $\alpha(G)$, $\beta(G)$, $\nu(G)$ and $\beta'(G)$ for G of order n as stated in Lemma 1.1.

Lemma 1.1. *(West, 2001) For a graph G of order n, we have*

$$\alpha(G) + \beta(G) = n \ \text{ and } \ \nu(G) + \beta'(G) = n.$$

West (2001) also showed that for any bipartite graph with no isolated vertex,

$$\alpha(G) = \beta'(G) \ \text{ and } \ \nu(G) = \beta(G).$$

Xu and Feng (2011) also related the domination γ and matching number ν of graph G, as $\gamma(G) \leq \nu(G)$.

1.1.2 Graph Operations

Now, we define graph operations such as union and join. Later in section 3.4, we will include the definitions of other graph operations such as Cartesian product, composition, disjunction, symmetric difference and corona product.

Definition 1.13. *Let G_1 and G_2 be graphs with disjoint vertex sets. The union $G \cong G_1 \cup G_2$ has $V(G) = V(G_1) \cup V(G_2)$ and $E(G) = E(G_1) \cup E(G_2)$.*

If G consists of $k \geq 2$ disjoint copies of a graph H, then we write $G \cong kH$. For instance, the graph $G \cong 2K_1 \cup 3K_2 \cup K_{1,3}$ is shown in the Figure 1.1.

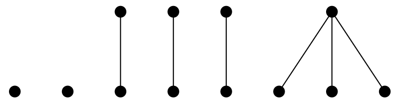

Figure 1.1: Graph $2K_1 \cup 3K_2 \cup K_{1,3}$.

Definition 1.14. *The join* $G \cong G_1 + G_2$ *has* $V(G) = V(G_1) \cup V(G_2)$ *and* $E(G) = E(G_1) \cup E(G_2) \cup \{uv \mid u \in V(G_1)$ *and* $v \in V(G_2)\}$.

The graph G obtained from G_1 and G_2 is shown in Figure 1.2.

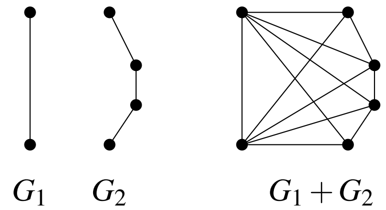

Figure 1.2: Graph $G_1 + G_2$.

In a simple manner, Definition 1.14 can be generalized to $t \geq 3$ graphs as stated in Definition 1.15.

Definition 1.15. *Let* $G_1, G_2, \dots, G_t$ *be pairwise vertex disjoint graphs. The sequential join* $G_1 + G_2 + \cdots + G_t$ *is* $(G_1 + G_2) \cup (G_2 + G_3) \cup \cdots \cup (G_{t-1} + G_t)$.

The sequential join of t disjoint copies of G will be denoted by $[t]G$, and so $[s]G_1 + G_2 + [k]G_3$ will denote the sequential join $(G_1 + G_1 + \cdots + G_1) + G_2 + (G_3 + G_3 + \cdots + G_3)$, where the sequential join contains s copies of G_1 and k copies of G_3.

For terms not defined in the dissertation, we referred from books like (Bondy and Murty, 1976) and (West, 2001). More specialized terminology not presented here are defined in the corresponding chapter where needed. Throughout this dissertation, we consider a graph which is nontrivial, simple, undirected and connected graphs.

1.1.3 Topological Indices

In graph theoretical notation, topological indices are the numerical parameters of a graph which are invariant under graph isomorphisms. Topological indices are expected to correlate with physical observable measures by experiments in a way that theoretical predictions can be used to gain chemical insights even for not yet existing molecules (Estrada and Bonchev, 2013). A topological index is a mathematical formula that is applied to any graph that describes a structure of molecule. It is a numerical value computed mathematically from a molecule's structural graph in a straightforward and unambiguous manner. Thus, it is possible to analyze mathematical values and explore some physiochemical aspects of a molecule using a topological index. As a result, it is a good approach to avoid more investment and time consuming analysis. In mathematical chemistry, topological indices play a really important role, especially in an exceedingly quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies.

Hosoya (1971) was the first person to introduce the concept of a topological index. He investigated the relationship between the physiochemical properties of a molecule and the matching number.

A lot of recent research in pharmaceutical drug design has focused on identifying properties of chemicals directly from their molecular structure. Biological, physicochemical, environmental and toxicological properties of molecules are being quantified by topological indices. Since both trial and error synthesis of compounds and their random screening for activity are time consuming and uneconomical, preliminary investigations using this quantitative structure-activity relationship (QSAR) permit a decrease in the number of compounds synthesized, by making it possible to select the most promising compounds (Grover et al., 2000).

One of the most serious problems affecting the use of topological descriptors in mathematical chemistry is their degeneracy-the fact that there are two or more graphs with same value of given descriptor (Došlić et al., 2010). The recently considered eccentric connectivity index and its derivatives were found to exhibit quite low degeneracy. This fact, along with simplicity of required computations, makes them potentially very useful for predicting various properties of many classes of chemical compounds.

Recently, some other topological indices based on distance have been introduced and investigated by mathematicians, chemists and biologists. Under this subsection, we give the definition of some of these commonly used distance-based topological indices.

A graph used to model a chemical compound and studying eccentric distance sum of this chemical compound provides important information on its structure-activity and/or structure-property relationship. Studying eccentric distance sum is helpful to explore some physiochemical aspects of molecules. It is very useful for predicting various properties of many classes of chemical compounds.

Topological indices are one of the oldest and most widely used descriptors in QSAR (Dutt and Madan, 2010). They have many advantages over other descriptors utilized in QSAR, like geometrical, electrostatic, electronic and quantum descriptors (Grover et al., 2000).

In chemistry and biology, researchers study molecules with desired physiochemical properties, for instance, boiling points, molecular volumes, flavor threshold concentration antiviral activity, energy levels, etc. These properties are often quantitatively represented by some values of a particular index.

A vast number of topological indices exists in the literature (Todeschini and Consonni, 2008, 2010) and (Gutman and Furtula, 2010). But, in this dissertation, we pay our attention to only the topological index named general eccentric distance sum. It is the topological index which depend on only the distance between two vertices of the graph. Now we give the definition for some of the topological indices which could be mentioned later in the dissertation.

Many topological indices have been defined, but only a limited number have been found to successfully predict activity (Morgan et al., 2014). The first of these, introduced in 1947, is the well-studied Wiener index. The Wiener index is the oldest distance based topological index which was introduced by Harold Wiener (1947) as the path number when he studied on boiling points of paraffin, bi-product of petroleum. In the original work by Wiener, the Wiener number was not, strictly speaking, formulated in graph-theoretical terms. It was defined within the framework of chemical graph theory later in 1971 by Hosoya, who pointed out that the Wiener index can be defined as stated in Definition 1.16. Wiener index deserves high rank in theoretical chemistry and chemical graph theory due to its theoretical as well as applicable nature.

Definition 1.16. *For a graph G the Wiener index of G is defined as*

$$W(G) = \sum_{\{u,v\}\in V(G)} d_G(u,v) = \frac{1}{2}\left(\sum_{v\in V(G)} D_G(v)\right).$$

The Wiener index appears to be a convenient measure of the compactness of the molecule (Trinajstić, 1936). That is the smaller the Wiener number, the larger the compactness of the molecule. With Wiener's discovery of a close correlation between the boiling points of certain alkanes and the sum of the distances between vertices in the graphs representing their molecular structures (Wiener, 1947) it became apparent that graph parameters, or topological indices, can potentially be used to predict properties of chemical compounds. The Wiener index has been investigated in the mathematical, chemical and computer science literature under many different names and with slight differences in the definition, it is sometimes also called the distance or the total distance of a graph.

Gupta et al. (2002b) introduced the eccentric distance sum as a novel eccentricity based graph invariant in 2002. They investigated the structure-activity relationship of the eccentric distance sum with regard to the anti-HIV activity of dihydroseselins. The authors in (Gupta et al., 2002b) have shown that some structure activity and quantitative structure property studies using eccentric distance sum were better than the corresponding values obtained using the Wiener index.

Definition 1.17. *The eccentric distance sum of a graph G is defined as*

$$EDS(G) = \sum_{v \in V(G)} ecc_G(v) D_G(v).$$

Comparatively, the eccentric distance sum exhibited a much better correlation and lesser average errors than the Wiener index. Though both EDS and Wiener index showed almost the same predictability of anti-HIV activity of dihydroseselins, but eccentric distance sum exhibited far superior discriminating power and correlating ability with regard to physical properties.

Vetrík (2021) introduced the general form of the eccentric distance sum as defined in Definition 1.18.

Definition 1.18. *For $a, b \in \mathbb{R}$, the general eccentric distance sum of a graph G is defined as*

$$EDS_{a,b}(G) = \sum_{v \in V(G)} [ecc_G(v)]^a [D_G(v)]^b.$$

The eccentric distance sum is a special case of the general eccentric distance sum $EDS_{a,b}$ for $a = b = 1$. Thus, some results for $EDS_{a,b}$ are also valid for the eccentric distance sum. The eccentric distance sum showed high discriminating power in terms of both physical properties and biological activity. The structure activity relationship of eccentric distance sum was studied with respect to anti-HIV activity of dihydroseselins (Gupta et al., 2002b). It would be interesting to investigate the quantitative structure activity/property relationships when using one or both parameters (a and b) for $EDS_{a,b}$ different from 1.

Definition 1.19. *The total eccentricity, $ecc(G)$, of a graph G is defined as*

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

Definition 1.20. *The eccentric connectivity index of a graph G is defined as*

$$ECI(G) = \sum_{v \in V(G)} ecc_G(v) deg_G(v).$$

The eccentric connectivity index (Sharma et al., 1997), has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature.

Dobrynin and Kochetova (1994) introduced the degree distance index which is a weighted version of Wiener index.

Definition 1.21. *The degree distance of a graph G is defined as*

$$DD(G) = \sum_{v \in V(G)} deg_G(v) D_G(v).$$

Gutman and Trinajstić (1972) introduced the first Zagreb index 50 years ago. It is one of degree based topological indices.

Definition 1.22. *The first Zagreb index of a graph G is defined as* $M_1(G) = \sum_{v \in V(G)} [deg_G(v)]^2$.

Ghorbani and Hosseinzadeh (2012) and Vukičević and Graovac (2010), independently, introduces the first and second Zagreb eccentricity indices.

Definition 1.23. *The first and second Zagreb eccentricity indices of a graph G are defined as*

$$EM_1(G) = \sum_{v \in V(G)} [ecc_G(v)]^2 \text{ and } EM_2(G) = \sum_{uv \in E(G)} ecc_G(u) ecc_G(v).$$

1.2 Statement of the Problem

A graph used to model a chemical compound and studying eccentric distance sum of this chemical compound provides important information on its structure-activity and/or structure-property relationship. Studying eccentric distance sum is helpful to explore some physiochemical aspects of molecules. It is very useful for predicting various properties of many classes of chemical compounds.

The eccentric distance sum is one of the most well-known distance-based topological indices. The eccentric distance sum showed high discriminating power in terms of both physical properties and biological activity. The structure activity relationship of the eccentric distance sum was studied with respect to the anti-HIV activity of dihydroseselins (Gupta et al., 2002b). The general eccentric distance sum generalizes the eccentric distance sum and a few other distance-based topological indices.

Most of the bounds obtained so far are only on the eccentric distance sum and a few bounds on the general eccentric distance sum for some types of graphs with certain graphs parameters was presented in (Vetrík, 2021). Motivated by [Vetrík, T. (2021). General eccentric distance sum of graphs. Discrete Mathematics, Algorithms and Applications, 13(04):2150046], we present bounds on the general eccentric distance sum for graphs of given order, chromatic number, and diameter 3, and trees of given bipartition, order, diameter 3, domination number 2 and bipartite graphs with the given order, matching number and diameter 3. We also address the general eccentric distance sum for the join of two graphs with a given order and number of vertices having the maximum possible degree. We provide extremal graphs for each bound presented in the study. Finally, the dissertation recommends some open problems for future work depending on the choice of the real numbers a and b.

1.3 Objective of the Study

1.3.1 General Objective

The general objective of this dissertation was to study bounds for general eccentric distance sum of graphs such as trees, bipartite graphs and graphs in general for $a, b \in \mathbb{R}$.

1.3.2 Specific Objectives

The specific objectives of the study were intended to:

1. Determine bounds on the general eccentric distance sum of trees with respect to some graph parameters such as diameter, domination number and bipartition for $a, b \in \mathbb{R}$.
2. Find bounds on the general eccentric distance sum of bipartite graphs with respect to some graph parameters such as order, diameter and matching number for $a, b \in \mathbb{R}$.
3. Obtain bounds on the general eccentric distance sum of graphs with respect to some graph parameters such as order, chromatic number and diameter 3 for $a, b \in \mathbb{R}$.
4. Provide the extremal graphs for all bounds addressed in objectives 1, 2 and 3 above.

1.4 Significance of the Study

Topological indices play an important role in chemistry, materials science, pharmaceutical sciences and engineering because we can correlate them with many physical and chemical properties of molecules. Graph theory is used to characterize these chemical structures. Topological indices are very important numerical invariants used in drug formulation to get a better drug from the old one by studying their molecular structures.

The eccentric distance sum is a well-known distance based topological index. The eccentric distance sum has been used with respect to both biological activity and physical properties. The structure activity relationship of the eccentric distance sum was studied with respect to the anti-HIV activity of dihydroselins (Gupta et al., 2002b).

The general eccentric distance sum is one of these numerical invariants. It is the general form of the eccentric distance sum. Studying this index provides information about the interval where those numerical values fall. This index generalizes several distance-based indices, such as the eccentric distance sum, the total eccentricity index, the first Zagreb eccentricity index, and the Wiener index, depending on the choice of the parameters a and b.

1.5 Scope of the Study

This study focused on finding the extremal values and extremal graphs for general eccentric distance sum of graphs such as trees, bipartite graphs and graphs for $a, b \in \mathbb{R}$ with different intervals for a and b.

Bounds on the general eccentric distance sum for graphs, bipartite graphs and trees with given order and diameter 3, graphs with given order and domination number 2, and for the join of two graphs with given order and number of vertices having the maximum possible degree are presented. The dissertation also gives some bounds on the general eccentric distance sum for graphs with specified order and chromatic number, trees with specified bipartition and bipartite graphs with the given order and matching number. Bounds for bipartite graphs also hold if the matching number is replaced by the independence number, the vertex cover number, or the edge cover number. Finally, extremal graphs are presented for all the bounds and some open problems are presented for the reader.

1.6 Limitation of the Study

The scope of the study is limited to determining the bounds on the general eccentric distance sum for certain graphs. The study did not focus on the applications and interpretation of the bounds.

1.7 Organization of the Dissertation

This dissertation includes seven chapters. As previously stated, the first chapter introduces the mathematical context against which this dissertation is set.It begins with giving definitions for the terminologies of graph theory and the concept behind topological indices. It also included the definitions of some of the topological indices, such as the eccentric distance sum, degree distance, eccentric connectivity index and Wiener index, with their historical backgrounds. This chapter contains the following sections: background of the study, statement of the problem, objectives of the study, significance of the study, scope of the study, and limitations of the study.

The second chapter introduces the literature review on topological indices, including the eccentric distance sum and general eccentric distance sum. Moreover, it introduces how the concept of topological indices is applied in the study of mathematical chemistry. The works of different researchers on the eccentric distance sum and general eccentric distance sum are briefly presented.

The third chapter is all about the discussion of preliminary results on the eccentric distance sum and the general eccentric distance sum obtained by different researchers, that are related to the results presented in chapters 5 and 6. We divided those results into five sections. The first section discusses graphs in general, while the second section discusses trees and unicyclic graphs. The third section compares the eccentric distance sum with other topological indices. The fourth section discusses the eccentric distance sum related to graph operations and results obtained on the general eccentric distance sum discussed in the final section of the chapter. The final section also includes two important preliminary results that help in finding the results of the dissertation.

The fourth chapter discusses the research methods that the dissertation includes. It discusses the method of analysis, the assumptions, the formulation and the mathematical procedures applied in the research work. The fifth chapter presents all results which are obtained on he general eccentric distance sum of trees with respect to different graph parameters. The six chapter provide all results which are obtained on he general eccentric distance sum of graphs such as bipartite graph and graph in general related to different graph parameters.

The last chapter includes conclusions and suggested problems on the general eccentric distance sum that could be addressed in the future.

CHAPTER 2

LITERATURE REVIEW

Topological indices have a crucial use in medical, industrial and environmental research. Here we present some background material that is emphasized on the eccentric distance sum and general eccentric distance sum of a graph. In chemistry, a molecular graph represents the topology of a molecule, by considering how the atoms are connected. This could be modeled by a graph, where the vertices represent the atoms and the edges symbolize the covalent bonds between the atoms. Multiple bonds, if any, are represented by a single edge forming the molecular graph.

Chemical graph theory uses topological indices as a strong tool for establishing relationships between the structure of a molecular graph and its properties or activities. For instance, structural features like size, shape, branching, symmetry, bonding patterns and therefore the neighborhood patterns of atoms within the molecules is measured by a topological index (Basak et al., 1995, 2000; Dureja et al., 2008).

Recent studies in pharmaceutical drug design are focused on identifying the properties of chemicals directly from their molecular structure. In pharmaceutical research, both trial and error syntheses of compounds and their random screening for activity are time consuming and uneconomical (Grover et al., 2000). So, preliminary investigations using QSAR and QSPR are done to pick out the foremost promising compounds for the required property and hence decrease the quantity of compounds that require to be synthesized during the method of designing new drugs (Bajaj et al., 2005; Grover et al., 2000; Lather and Madan, 2005).

Topological indices are computed easily and rapidly for any known compound, or may be one not yet synthesized. Many software programs, like CODES SA, SciQSAR and POLLY are readily available for both the calculation of the descriptor values and subsequent multivariate statistical analysis (Grover et al., 2000; Randić and Zupan, 2001). Furthermore, not only they are powerful tools for drug design, but they are also getting used for virtual screening, lead optimization, isomer discrimination, chemical documentation, combinatorial library design (Dureja et al., 2008) and environmental toxicology assessment.

Therefore, one of the most interesting problems on topological indices is to check the extremal properties of topological indices and characterize the extremal structures. Another direction is to review the relation between topological indices and a few other graph invariants, which helps researchers to grasp the indices better and find more internal information. The quantification of chemical structures could be a basic problem in structure-activity relationships which is a vital tool for developing safer and more potent drugs. The procedure for quantification of chemical structures is by translation of chemical structures into characteristic topological indices (Balaban et al., 1983; Basak et al., 1994). This procedure provides a correlation between quantitative biological activity and qualitative chemical structures.

Another active area of chemical research deals with nanotubes, nanotori, nanostars and other dendrimers. These polymeric materials are of major chemical importance as they are finding applications in a kind of engineering use, both biomedical such as MRI diagnostics, coating agents to safeguard or deliver drugs to specific parts of the body, as anti-bacterial and anti-viral agents, as vectors in gene therapy and industrial (Klajnert and Bryszewska, 2001). Explicit values for various topological indices and specifically, the eccentric connectivity index and eccentric distance sum, are being calculated for these classes of compounds (see, for example (Ashrafi et al., 2011a,b; Saheli and Ashrafi, 2010)).

The Wiener index has successfully characterized properties such as the boiling point, density, critical pressure, refractive indices and vaporization of various hydrocarbons (Dobrynin and Kochetova, 1994). This quantitative relationship between the structure of a molecule and its properties (or activities) is the basis of the quantitative structure versus property (activity) relationship studies.

The eccentric distance sum has a lot of potential in terms of activity/property linkages in structures. Some structure-activity and quantitative structure-property studies utilizing eccentric distance sum were better than the corresponding values obtained using the Wiener index (Dobrynin et al., 2001). On the other hand, it can provide valuable leads for the development of safe and potent therapeutic agents of diverse nature. Comparatively, the eccentric distance sum exhibited a much better correlation and lesser average errors than the Wiener index. The excellent prediction of the physical properties by the eccentric distance sum can be attributed to the probable contribution of distance sum in addition to eccentricity. The physical properties are significantly responsible for the biological activity of a chemical compound (Gupta et al., 2002a).

The eccentric distance sum of each analog within the information set was computed, as well as the active range was obtained. Then, biological activity was given to each analog within the information set, which was then compared to dihydroseselin analogs' reported anti-HIV activity. In all six data sets used in (Gupta et al., 2002b), excellent correlations were obtained using the eccentric distance sum. In data sets using eccentric distance sum, relationship between the variables ranging from 93% to more than 99% were obtained. The eccentric distance sum has inspired a lot of attention in the mathematical and chemical worlds in recent years and several results and structural properties of the eccentric distance sum have been developed. The investigation of the mathematical properties of eccentric distance sum started recently after the works of Hua et al. (2011); Ilić et al. (2011) and Yu et al. (2011). The problem of finding an upper bound on the eccentric distance sum of a graph can now be restricted to finding an edge on the eccentric distance sum of trees. Ilić et al. (2011) proved that a path graph has the maximum eccentric distance sum among graphs of a given order. Further, in the same research, they established bounds on the eccentric distance sum in terms of other graph invariants, like the Wiener index, degree distance, eccentric connectivity index, independence number, connectivity, matching number, chromatic number and clique number. When we come to lower bounds, clearly, the complete graph minimizes the eccentric distance sum among all graphs of a given order. This simple bound on the index was improved for trees and for unicyclic graphs. Among trees of a given order, the star was identified to be the unique graph that minimizes the index (Yu et al., 2011). In the same research, Yu et al. (2011) established the lower bound for eccentric distance sum for trees of a given order and diameter.

Ilić et al. (2011) presented a lower bound on eccentric distance sum for graphs of a given order and connectivity. An upper bound on eccentric distance sum for graphs of order n and minimum degree was provided in (Mukungunugwa and Mukwembi, 2014). A lower bound for trees with prescribed order was given in (Yu et al., 2011) and (Hua et al., 2011). A lower bound on eccentric distance sum for trees with given order and domination number was given in (Geng et al., 2013). Eccentric distance sum for trees was studied in (Pei and Pan, 2020) as well. Eccentric distance sum for several basic graphs was presented in (Padmapriya and Mathad, 2017), graphs related to groups were investigated in (Abdussakir et al., 2019), cubic transitive graphs in (Xie and Xu, 2019), graph operations in (Azari and Iranmanesh, 2013), bipartite graphs in (Chen and Wu, 2020) and (Li et al., 2015), fullerances in (Hemmasi et al., 2014), Sierpiński networks in (Chen et al., 2019) and relations between eccentric distance sum and a few other indices were studied in (Hua and Bao, 2016). Alizadeh and Klavžar (2021), Chen et al. (2018) and Ilić et al. (2011) studied its relationship with the eccentric connectivity index as well as Hua et al. (2018) also studied its relationship with the degree distance.

Vetrík (2021) proved that the $EDS_{a,b}$ decreases (increases) for $a \geq 0$ and $b > 0$ (for $a \leq 0$ and $b < 0$ respectively) with addition of edge. In the same way, the $EDS_{a,b}$ increases (decreases) for $a \geq 0$ and $b > 0$ (for $a \leq 0$ and $b < 0$ respectively) by removing of an edge provided that the resulting graph is connected. This result becomes a corner stone in finding more results on the general eccentric distance sum graphs. He presented bounds on the general eccentric distance sum for graphs, bipartite graphs and trees of given order, graphs of given order and connectivity and graphs of given order and number of pendant vertices. He also presented the extremal graphs for all bounds he obtained.

In dissertation, we find extremal values and extremal graphs for general eccentric distance sum of graphs such as trees, bipartite graphs and graphs for $a,b \in \mathbb{R}$ with different intervals for a and b. We also provide open problems for future work on the general eccentric distance sum to find extremal values and extremal graphs for different classes of graphs.

CHAPTER 3

PRELIMINARY RESULTS ON THE ECCENTRIC DISTANCE SUM

Gupta et al. (2002b) conceptualized the eccentric distance sum in structure activity/property relationships and with respect to both biological activity and physical features. This topological index has a great discriminating power. The anti-HIV activity of dihydroseselins was explored by using structure-activity relationship of eccentric distance sum. This graph invariant was proposed as an eccentricity weighted version of the Wiener index. According to Gupta et al. (2002b), some structure activity and quantitative structure-property studies utilizing eccentric distance sum were better than the corresponding values obtained using the Wiener index. The mathematical features of eccentric distance sum have recently been thoroughly researched. The examination of the scientific properties of eccentric distance sum begun in 2002. The issue of finding an upper bound on the eccentric distance sum of a graph can presently be confined to finding an upper bound on the eccentric distance sum of trees.

In the next sections, we present some preliminary results on the eccentric distance sum and the general eccentric distance sum for varies graphs with certain graph parameters in detail. Many researchers have an interest in finding bounds for graph invariants, and therefore the related problem of determining the graphs achieving the extremal values of the eccentric distance sum and the general eccentric distance sum is elaborated.

3.1 Eccentric Distance Sum for Graphs

Ilić et al. (2011) studied the eccentric distance sum with respect to independence number, connectivity, matching number, chromatic number and clique number. They showed that eccentric distance sum decreases (increases) with addition of edge (removing of edges) provided that the resulting graph is connected. Ilić et al. (2011) showed that for any graph G of order n

$$EDS(K_n) \leq EDS(G) \leq EDS(P_n).$$

Li and Wu (2016) proved the relation

$$EDS(K_{1,n-1}) > EDS(K_{2,n-2}) > \cdots > EDS\left(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}\right)$$

among all bipartite graphs of order $n \geq 4$ and diameter 2. Chen et al. (2018) provided the extremal value of eccentric distance sum for bipartite graph of a given diameter and extremal values of eccentric distance sum for graph of a given connectivity and minimum degree and a given connectivity and independence number. They provided the lower bound

$$EDS(G) \geq 2n^2 + (4\delta + 2 - 5\kappa)n + (4\kappa - 8 - 4\delta)\delta + 5\kappa - 4$$

for any graph G of order n with connectivity κ and minimum degree $\delta \geq 2$. They also proved the bound

$$EDS(G) \geq 2n^2 + (2 - \kappa)n + 2\alpha^2 - 6\alpha - 3\kappa$$

for any graph G of order n with connectivity κ and independence number α. Mukungunugwa and Mukwembi (2014) provided an asymptotically upper bound on eccentric distance sum of graphs with respect to order and minimum degree. They and also Chen et al. (2018), provided lower and upper bounds for a graph of order n and minimum degree $\delta \geq 2$. They identified that the lower bound holds if and only if G is $K_\delta + (K_1 \cup K_{n-\delta-1})$, whereas the upper bound is asymptotically for a fixed δ.

A wheel graph W_n for $n \geq 4$ is a graph obtained by connecting a new vertex to all the vertices of a cycle C_{n-1}. A Halin graph is a planar graph constructed from a tree T of at least 4 vertices. Let C be a cycle connecting the leaves of T in a way such that C forms the boundary of the unbounded face. Note that a wheel W_n is a special Halin graph. Let $\mathscr{H}_{p,q}$ be a Halin graph obtained from a tree $P_2(p-1, q-1)$ where $p+q=n$ and $p \geq q \geq 3$. Huang et al. (2019) determined the minimum eccentric distance sum of Halin graphs. They showed that

$$EDS(G) \geq 4n^2 - 12n + 4k + 4$$

for any Halin graph G of order n having $k \geq 2$ interior vertices. They also obtained lower bounds for Halin graph G with respect to order n as

$$EDS(G) \geq 4n^2 - 13n + 9,$$

where equality holds if and only if G is W_n.

Huang et al. (2019) gave lower bound for eccentric distance sum of graphs of a given girth $g \geq 3$. They also determined the minimum eccentric distance sum of triangle-free and quadrangle-free graphs as

$$EDS(G) \geq 2n(n^2 - 2 - \sqrt{n-1}),$$

where equality holds if and only if G is $K_{1,4}$ or a Petersen graph (which is a graph with 10 vertices and diameter 2, where every vertex has degree 3). But Li and Wu (2016) provided the lower bound $4n(n-1)-4\lfloor\frac{n^2}{4}\rfloor$ for triangle-free graph G of order $n \geq 4$ and the bound is attained when the graph G is $K_{\lceil\frac{n}{2}\rceil,\lfloor\frac{n}{2}\rfloor}$. A Nordhaus-Gaddum type result is a lower or upper bound on the sum or product of a parameter of a graph and its complement. Huang et al. (2019) established a Nordhaus-Gaddum bound for eccentric distance sum of a graph G of order $n \geq 5$ and whose complement $\overline{G}$ is connected as

$$6n(n-1) \leq EDS(G) + EDS(\overline{G}) \leq EDS(P_n) + EDS(\overline{P_n}).$$

The minimum eccentric distance sum of a bipartite graph was obtained for a given even diameter (Huang et al., 2019), odd diameter and connectivity (Li et al., 2015). Here, we assume that for the complete bipartite graph K_{p_1,p_2}, we have $p_1 \geq p_2$. Li et al. (2015) defined a graph $O_\kappa \vee_1 (K_{p_1,p_2} \cup K_{p_1',p_2'})$ where O_κ $(\kappa \geq 1)$ is an empty graph of order κ and $\vee_1$ is a graph operation that joins all the vertices in O_κ to the vertices belonging to the partitions of cardinality p_1 in K_{p_1,p_2} and p_1' in $K_{p_1',p_2'}$, respectively.

Theorem 3.1. *(Li et al., 2015) Let G be a bipartite graph of order n with connectivity* κ, $1 \leq \kappa \leq \lfloor\frac{n}{2}\rfloor$, *and having the minimum eccentric distance sum. Let* $G_1 \cong O_\kappa \vee_1 K_{\lceil\frac{7n-\kappa-6}{10}\rceil,\lfloor\frac{3n-9\kappa-4}{10}\rfloor}$ *and* $G_2 \cong O_\kappa \vee_1 K_{\lfloor\frac{7n-\kappa+4}{10}\rfloor,\lceil\frac{3n-9\kappa-14}{10}\rceil}$. *Then*

1. *For* $2 \leq \kappa < \frac{n-12}{8}$ *and* $p < \frac{7n-\kappa-6}{10}$, *one has* $G \cong G_1$*;*
2. *For* $2 \leq \kappa < \frac{n-12}{8}$ *and* $\frac{7n-\kappa-6}{10} \leq p\frac{7n-\kappa+4}{10}$, *one has* $G \cong G_1$ *or* $G \cong G_2$ *if* $7n-\kappa-6 \equiv 0$ $(mod\ 10)$ *and* $G \cong G_1$ *if* $7n-\kappa-6 \equiv 1,2,\ldots,9$ $(mod\ 10)$*;*
3. *For* $2 \leq \kappa < \frac{n-12}{8}$ *and* $p > \frac{7n-\kappa-6}{10}$, *one has* $G \cong G_2$*;*
4. *For* $\kappa = 1$ *and* $\frac{n-12}{8} \leq \lfloor\frac{n}{2}\rfloor$, *one has* $G \cong K_{\kappa,n-\kappa}$
   if $\frac{n-12}{8} \notin \mathbb{Z}$ *and* $G \in \{K_{\kappa,n-\kappa}, O_\kappa \vee_1 (K_1 \cup K_{n-\kappa-2,1})\}$, *otherwise.*

A graph obtained from two disjoint cycles, C_n by connecting their corresponding vertices is called the ladder, L_n. Actually, $L_n \cong C_n \times K_2$. The Möbius ladder, M_n is the graph obtained from the cycle $C_{2n} = v_1v_2\ldots v_{2n}v_1$ by adding edges v_iv_{n+i}, $(1 \leq i \leq n)$.

Xie and Xu (2019) declared that ladder, L_n and Möbius ladder, M_n are cubic graphs. Li and Wu (2016) provided the upper bound on eccentric distance sum of κ-connected graph G with an even κ. Later, Xie and Xu (2019) obtained the bound for odd κ but only for some cubic graphs (3-connected graphs). It still remains open problem for any κ-connected graph. For integer k, let $K_{n-k} \star S_{k+1}$ be a graph obtained by identifying the center of the star S_{k+1} with a vertex of complete graph K_{n-k}, where $1 \leq k \leq n-1$.

Theorem 3.2. *(Hua et al., 2012) Let G be a graph on n vertices with k bridges with $1 \leq k \leq n-1$ and $k \neq n-2$. Then*

$$EDS(G) \geq 2n^2 + (4k-3)n - 2k^2 - 6k + 1,$$

with equality if and only if G is $K_{n-k} \star S_{k+1}$.

Theorem 3.3. *(Ilić et al., 2011) Let G be a graph of order n with connectivity κ. Then*

$$EDS(G) \geq 2n^2 + 2n - n\kappa - 3\kappa - 4,$$

with equality if and only if G is $K_\kappa + (K_1 \cup K_{n-\kappa-1})$.

Hua et al. (2012) established a lower bound for any graph G of order n with the connectivity κ as

$$EDS(G) \geq 2n^2 + 2n - n\kappa - 3\kappa - 4$$

in which the equality holds when G is $K_\kappa + (K_1 \cup K_{n-\kappa-1})$. This bound also works when κ is replaced by minimum degree δ and edge connectivity λ due to the relation, $\kappa \leq \lambda \leq \delta$. Li et al. (2015) provided the extremal graph $K_{\nu,n-\nu}$, which attains the lower bound of eccentric distance sum among all bipartite graphs having a matching number ν. According to the relationship stated in Lemma 1.1 for a bipartite graph, the graph $K_{\sigma,n-\sigma}$ is the extremal graph which attains the lower bound of eccentric distance sum for any bipartite graph of order n having vertex cover number or vertex independence number or edge cover number σ. Li and Wu (2016) showed that

$$EDS(G) \geq 4n^2 - 18n + 26$$

for any planar graph of order $n \geq 6$ and they also proved that

$$EDS(G) \geq 4n^2 - 13n + 13$$

for any outerplanar graph of order $n \geq 6$. Chen and Wu (2020) presented lower bounds of eccentric distance sum for a bipartite graph in relation to the number of bridges $k \leq n-4$, as stated in Theorem 3.4 and the extremal graph is $B_k(x, n-k-x)$ for different values of k, where $B_k(x, n-k-x)$ is a bipartite graph obtained by attaching k pendant vertices to a vertex with degree $n-k-x$ in $K_{x,n-k-x}$, where x, k, n are positive integers such that $2 \leq x \leq \frac{n-k}{2}$. The only bipartite graph with $k = n-1$ bridges is S_n.

Theorem 3.4. *(Chen and Wu, 2020) Let G be a bipartite graph of order $n \geq 5$ with k bridges.*

1. *If $\frac{3n-23}{11} \leq k \leq n-4$, then $EDS(G) \geq 4n^2 + 2kn - 11n + 8k + 16$, with equality if and only if G is $B_k(2, n-k-2)$.*

2. *If $1 \leq k < \frac{3n-23}{11}$ and $3n - 11k + 3 \equiv i$ (mod 10) for $0 \leq i \leq 5$, then*

$$EDS(G) \geq \frac{71n^2 - 121k^2 + 31 + i(i)}{20} + \frac{53kn - 59n - 107k}{10},$$

with equality if and only if G is $B_k(\frac{3n-11k+3-i}{10}, \frac{7n+k-3+i}{10})$.

3. *If $1 \leq k < \frac{3n-23}{11}$ and $3n - 11k + 3 \equiv 6$ (mod 10), then $EDS(G) \geq \frac{71n^2-121k^2+47}{20} + \frac{53kn-59n-107k}{10}$, with equality if and only if G is $B_k(\frac{3n-11k+7}{10}, \frac{7n+k-7}{10})$.*

4. *If $1 \leq k < \frac{3n-23}{11}$ and $3n - 11k + 3 \equiv 7$ (mod 10), then $EDS(G) \geq \frac{71n^2-121k^2+40}{20} + \frac{53kn-59n-107k}{10}$, with equality if and only if G is $B_k(\frac{3n-11k+6}{10}, \frac{7n+k-6}{10})$.*

5. *If $1 \leq k < \frac{3n-23}{11}$ and $3n - 11k + 3 \equiv 8$ (mod 10), then $EDS(G) \geq \frac{71n^2-121k^2+35}{20} + \frac{53kn-59n-107k}{10}$, with equality if and only if G is $B_k(\frac{3n-11k+5}{10}, \frac{7n+k-5}{10})$.*

6. *If $1 \leq k < \frac{3n-23}{11}$ and $3n - 11k + 3 \equiv 9$ (mod 10), then $EDS(G) \geq \frac{71n^2-121k^2+32}{20} + \frac{53kn-59n-107k}{10}$, with equality if and only if G is $B_k(\frac{3n-11k+4}{10}, \frac{7n+k-4}{10})$.*

3.2 Eccentric Distance Sum of Trees and Unicyclic Graphs

A spanning tree T of an graph G is a subgraph that is a tree which includes all of the vertices of G. We can apply addition/removal of an edge to/from a graph and for any spanning tree T of G, we have $EDS(G) \leq EDS(T)$. For a tree of the form $P_l(n_1, n_2)$, where $n_1 + n_2 = n - l$ and $n_1, n_2 \geq 1$ Geng et al. (2013) provided the relation

$$EDS(P_l(1, n-l-1)) < EDS(P_l(2, n-l-2)) < \cdots < EDS\left(P_l\left(\left\lfloor\frac{n-l}{2}\right\rfloor, \left\lceil\frac{n-l}{2}\right\rceil\right)\right). \quad (3.1)$$

From the relation in equation 3.1, one can easily understand that $P_l(1, n-l-1)$ and $P_l\left(\left\lceil\frac{n-l}{2}\right\rceil, \left\lfloor\frac{n-l}{2}\right\rfloor\right)$ are the extremal trees which give lower and upper bounds among tress of the form $P_l(n_1, n_2)$. Ilić et al. (2011) proved that the star S_n and caterpillar $C_{n,d}$ attain the minimum eccentric distance sum among all trees of order n and trees with order n and diameter d, respectively. The tree $P_{n-p}\left(\left\lfloor\frac{p}{2}\right\rfloor, \left\lceil\frac{p}{2}\right\rceil\right)$ was classified as an extremal tree among all trees of order n and having p pendent vertices which attains the minimum eccentric distance sum (Geng et al., 2013).

It is known that any tree is a bipartite graph, so it has an (s,t)-bipartition where $s+t=n$ and it is clear that S_n has $(1,n-1)$-bipartition and $P_3(n_1,n-n_1-3)$ has $(2,n-2)$-bipartition. From the relation in equation 3.1 we have

$$EDS(P_3(0,n-3)) < EDS(P_3(1,n-4)) < \cdots < EDS\left(P_3\left(\left\lfloor\frac{n-3}{2}\right\rfloor,\left\lceil\frac{n-3}{2}\right\rceil\right)\right).$$

Geng et al. (2013) showed that $EDS(T) \geq 6(s+t-2)^2+6st+3(s+t)-8$, with equality if and only if $T \cong P_2(s-1,t-1)$ for any tree T having an (s,t)-bipartition and $s \geq 3$,.

Let ν be a matching number and $T_{n,\nu}$ be a tree obtained from the star graph $S_{n-\nu+1}$ by attaching a pendant edge to each of certain $\nu-1$ non-central vertices of $S_{n-\nu+1}$. Thus, $T_{n,\nu}$ contains an ν-matching. We denote it as $T_{2\nu,\nu}$ if $n=2\nu$ that is, it has a perfect matching. In other way, $T_{2\nu,\nu}$ is obtained from the star $S_{\nu+1}$ by attaching a pendant edge to each of certain $\nu-1$ non-central vertices of $S_{\nu+1}$. If $\nu=1$ and $\nu=2$, the corresponding trees with $n=2\nu$ are P_2 and P_4 only respectively. Li et al. (2012) considered for $\nu \geq 3$ and presented the lower bound

$$EDS(T) \geq 43\nu^2-72\nu+34$$

for all trees of order $n=2\nu$. The only tree of order n with matching number $\nu=1$ and $\nu=2$ are S_n and $P_2(p,n-p-2)$ where $1 \leq p \leq n-3$, respectively. So Li et al. (2012) considered $\nu \geq 3$ and provided the lower bound

$$EDS(T) \geq 6n^2+\nu^2-9n\nu-22n-28\nu+34$$

in which the lower bound is achieved when the tree T is $T_{n,\nu}$. Ilić et al. (2011) showed that K_n is the graph with the minimum eccentric distance sum among all graphs of order n and thus we conclude that it is also the graph with the minimum eccentric distance sum among all graphs of order n and matching number $\nu = \left\lfloor\frac{n}{2}\right\rfloor$.

Corollary 3.1. *(Miao et al., 2015) Let T be a tree of order n with matching number ν. Then*

$$EDS(T) \leq EDS\left(P_{2\nu-1}\left(\left\lfloor\frac{n+1}{2}\right\rfloor-\nu,\left\lceil\frac{n+1}{2}\right\rceil-\nu\right)\right).$$

By Lemma 1.1, $\alpha+\beta=n$ and $\nu=\beta$, that is $\alpha=n-\nu$. From Corollary 3.1 $l=2\nu-1=2(n-\alpha)-1$ and Miao et al. (2015) obtained the bounds for all trees of order n and independence number α as

$$EDS(T_{n,n-\alpha}) \leq EDS(T) \leq EDS\left(P_{2(n-\alpha)-1}\left(\left\lfloor \frac{n+1}{2} \right\rfloor - (n-\alpha), \left\lceil \frac{n+1}{2} \right\rceil - (n-\alpha)\right)\right).$$

For $n \leq 3$, the domination number γ is 1 and the corresponding tree is a star graph S_n. For $n = 4$, the domination number γ can be 1 or 2 and the corresponding tree is S_4 and P_4 respectively. For $n = 5$, the domination number γ can be 1 or 2. For $\gamma = 2$ the corresponding trees are $P_2(2,1)$ and $P_3(1,1) \cong P_5$. Thus, P_4, P_5 and $P_2(2,1)$ are the only trees with order $n \leq 5$ and domination number, $\gamma = 2$. Geng et al. (2013) showed that $EDS(T) \geq 6n^2 + \gamma^2 - 9n\gamma - 22n - 28\gamma + 34$ for any tree of order n and with domination number γ and the bound is achieved when T is $T_{n,\gamma}$. They also provided the result stated in Theorem 3.5 for trees of order $n = 2\gamma$.

Theorem 3.5. *(Geng et al., 2013) Let T be a tree of order n with $\gamma = \frac{n}{2}$ where n is even, then $EDS(T) \leq EDS(T^\star)$, where $T^\star$ is a tree obtained by attaching a pendent edge to each vertex of $P_{\frac{n}{2}}$.*

According to Ilić et al. (2011), P_n is the extremal tree having the maximum eccentric distance sum among all order n trees and different researchers including Masre and Vetrík (2021) showed that $\gamma(P_n) = \left\lceil \frac{n}{3} \right\rceil$. Thus, we can conclude that P_n is the extremal tree having the maximum eccentric distance sum among order n trees and having domination number $\left\lceil \frac{n}{3} \right\rceil$. For tree T of order $n \geq 4$ and domination number γ, with $2 \leq \gamma \leq \left\lceil \frac{n}{3} \right\rceil$, Geng et al. (2013) and Miao et al. (2017, 2015) presented the upper bound

$$EDS(T) \leq EDS\left(P_{3\gamma-2}\left(\left\lceil \frac{n-3\gamma}{2} \right\rceil + 1, \left\lfloor \frac{n-3\gamma}{2} \right\rfloor + 1\right)\right).$$

Miao et al. (2020) obtained the lower bound on eccentric distance sum among all trees of order n and maximum degree. A set $V_K \subseteq V(G)$ is a distance k-dominating set of G if for every vertex $v \in V(G) \setminus V_K$, $d_G(u,v) \leq k$ for some vertex $u \in V_K$. The minimum cardinality among all distance k-dominating sets of G is called the distance k-domination number γ_k of G. Note that the domination number of a graph is the special case of distance k-domination number when $k = 1$. Pei and Pan (2020) characterized trees with distance k-domination number γ_k for $k \geq 2$. Let T_{n,k,γ_k} be a tree obtained from star $S_{n-k\gamma_k+1}$ by attaching exactly one path P_k to each of $\gamma_k - 1$ non-central vertices of $S_{n-k\gamma_k+1}$ and by attaching exactly one path P_{k-1} to another non-central vertex of $S_{n-k\gamma_k+1}$. They showed that the star S_n is the extremal tree among all trees of order n with distance k-domination number, $\gamma_k = 1$.

Theorem 3.6. *(Pei and Pan, 2020) Let T be a tree of order n with distance k-domination number, $\gamma_k \geq 2$. Then $EDS(T) \geq EDS(T_{n,k,\gamma_k})$, with equality if and only if $T \cong T_{n,k,\gamma_k}$.*

Let $\mathcal{U}_n(k)$ be the set of unicyclic graphs of order n with girth k and $\mathcal{U}_n$ be the set of all unicyclic graphs of order n. The set $\mathcal{U}_n(n-1)$, contains a unique graph. So we consider for $3 \leq k \leq n-2$. Yu et al. (2011) gave a lower bound for trees of given order and diameter. They showed that $H_{n,k}$ is the extremal graph with the minimum eccentric distance sum among all unicyclic graphs of order n and girth k. They also provided that $EDS(G) \geq 4n^2 - 9n + 1$ for any unicyclic graphs of order $n > 5$ and Hua et al. (2011) provided a short proof for this bound. A cactus is a graph in which any two cycles have at most one vertex in common. Cacti is the plural form of cactus. Equivalently, it is a graph in which every edge belongs to at most one cycle. Hua et al. (2011) also provided a lower bound of eccentric distance sum for a cactus of order n and k cycles as stated in Theorem 3.7.

Theorem 3.7. *(Hua et al., 2011) Let G be a cactus of order $n \geq 4$ and $k \geq 0$ cycles. Then*

$$EDS(G) \geq 4n^2 - 9n - 4k + 5,$$

with equality if and only if G is cactus obtained by introducing k independent edges among pendent vertices of S_n.

Later Bielak and Broniszewska (2017) presented a lower bound for the eccentric distance sum for some generalization of cacti. This result extends the result of Theorem 3.7. Li et al. (2013) presented a lower bound on eccentric distance sum for unicyclic graphs of order n and matching number $\nu \geq 2$.

A hexagonal cactus is a 6-uniform cactus, that is, a cactus in which every block is a hexagon. A vertex shared by two or more hexagons is called a cut-vertex. If each hexagon of a hexagonal cactus G has at most two cut-vertices and each cut-vertex is shared by exactly two hexagons, we say that G is a chain hexagonal cactus. Qu and Yu (2014) characterized the chain hexagonal cactus with the extremal eccentric distance sum among all chain hexagonal cacti of length n, respectively. Moreover, They presented exact formulas for eccentric distance sum of two types of hexagonal cacti.

3.3 Eccentric Distance Sum and Other Topological Indices

In this section, we review some results on the relationship between the eccentric distance sum and some other topological indices such as the first Zagreb index, Wiener index, eccentric connectivity index, total eccentricity and degree distance as they are defined in section 1.1.3.

Now, we are going to review some of the results on the relation between the eccentric distance sum and the above indices.

Suppose $K_n - ke$ is a graph obtained by deleting k independent edges from the complete graph K_n, where $k = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$. Alizadeh and Klavžar (2021) obtained bounds on the difference between the eccentric distance sum and eccentric connectivity index of graphs and trees.

Theorem 3.8. *(Alizadeh and Klavžar, 2021) Let G be a graph of order n and size m. Then*

1. *$EDS(G) - ECI(G) \geq 2(n - 1 - \Delta(G))ecc(G)$, with equality if and only if G is a regular graph with $d(G) \leq 2$.*
2. *$EDS(G) - ECI(G) \leq 2n(W(G) - m) + M_1(G) - DD(G)$, with equality if and only if G is P_4 or $G \cong K_n - ke$, for $k = 0, 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$. .*

Theorem 3.9. *(Alizadeh and Klavžar, 2021) Let T be a tree of order n and diameter d. Then*

$$EDS(T) - ECI(T) \geq EDS(C_{n,d}) - ECI(C_{n,d}).$$

Theorem 3.10. *(Alizadeh and Klavžar, 2021) Let T be a tree of order n. Then*

$$EDS(S_n) - ECI(S_n) \leq EDS(T) - ECI(T) \leq EDS(P_n) - ECI(P_n).$$

Recall that a graph G is said to be self-centered if all vertices have the same eccentricity. If this eccentricity is ε, we further say that G is ε-self-centered.

Theorem 3.11. *(Alizadeh and Klavžar, 2021) Let G be a graph on n vertices with maximum degree $\Delta \leq \frac{2}{3}(n-1)$. Then*

$$EDS(G) \geq 2ECI(G),$$

where equality holds if and only if G is 2-self-centered and $\frac{2}{3}(n-1)$-regular graph.

Alizadeh and Klavžar (2021) provided a lower bound on the eccentric distance sum of a graph with respect to order n, radius r and total eccentricity, $ecc(G)$

$$EDS(G) \geq \left(n - 1 + \binom{r}{2}\right) ecc(G),$$

with equality if and only if G is K_n. Zhang et al. (2019) obtained bounds on the eccentric distance sum of graphs with respect to the minimum degree and diameter 2. They gave the difference between eccentric distance sum and eccentric connectivity index among all graphs of diameter 2 with a given minimum degree, connectivity and independence number. Zhang et al. (2019) considered graphs with diameter 2 and independence number α, where $n \geq \alpha + 1$

to find $EDS(G) - ECI(G)$. They showed that

$$EDS(G) - ECI(G) \geq 4\alpha^2 - 4\alpha,$$

where equality holds if and only if G is $\overline{K}_\alpha + K_{n-\alpha}$. Bounds on the difference between the eccentric distance sum and degree distance among all graphs, trees and self-centered graphs, respectively presented in (Hua et al., 2018). Also, they introduced those extremal graphs attaining the bounds. Hua et al. (2018) provided extremal trees which give lower and upper bounds on the difference between the eccentric distance sum and degree distance for all trees T of order n as

$$EDS(S_n) - DD(S_n) \leq EDS(T) - DD(T) \leq EDS(P_n) - DD(P_n).$$

They also found extremal graphs which give lower and upper bounds on the difference between the eccentric distance sum and degree distance for all graphs G of order n as

$$EDS(K_n) - DD(K_n) \leq EDS(G) - DD(G) \leq EDS(P_n) - DD(P_n).$$

They also considered self-centered graphs G of order $n \geq 3$ and provided the bounds

$$EDS(K_n) - DD(K_n) \leq EDS(G) - DD(G) \leq EDS(C_n) - DD(C_n).$$

Li and Wu (2016) showed that among all graphs of diameter 2, $K_n - e$ with $e \in E(K_n)$ is the graph with the minimum eccentric distance sum. Zhang et al. (2019) showed that $EDS(G) - ECI(G) \geq 8$, where the equality holds if and only if G is $K_n - e$ with $e \in E(K_n)$. Hua et al. (2018) compared the eccentric distance sum with degree distance for a graph with respect to minimum degree, maximum degree, radius and diameter and they also obtained the difference for self-centered graphs with respect to order. They showed that $DD(G) \leq EDS(G)$ for any graph G of order n and radius $r \geq \frac{n}{2}$.

Theorem 3.12. *(Hua et al., 2018) Let G be a graph on n vertices with maximum degree Δ, minimum degree δ, radius r and diameter d. Then*

1. *If $\delta \geq d$, then $DD(G) \geq EDS(G)$,*
2. *If $r \geq \Delta$, then $DD(G) \leq EDS(G)$.*

Hua (2020) presented bounds on the quotient of the eccentric distance sum and eccentric connectivity index for graphs of diameter 2 as

$$\frac{3}{4n-5} \leq \frac{ECI(G)}{EDS(G)} \leq \frac{n^2+n-6}{n^2+n+2},$$

where the left and right equalities hold if and only if G is S_n and $K_n - e$, respectively. Ilić et al. (2011) related the eccentric distance sum with other invariants such as the Wiener index and degree distance as $EDS(G) \leq 2n(W(G)) - DD(G)$, where equality holds if and only if G is $K_n - ke$, for $k = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$. They also added a relation between the eccentric distance sum and eccentric connectivity index as $ECI(G) \leq EDS(G)$ for any graph G of order $n \geq 3$ where the equality holds if and only if G is K_n. Hua et al. (2020) proved that $EDS(G) \geq EM_1(G)$ for any graph G, whereas $EDS(T) > EM_2(T)$ for any tree T. They also compared eccentric distance sum with the second Zagreb eccentricity index for graphs under some restricted conditions.

3.4 Eccentric Distance Sum and Graph Operations

In this section, we discuss the eccentric distance sum for some graph operations. The operations are the Cartesian product, join, composition, disjunction and corona product. Note that a vertex $v \in V(G)$ is called well-connected, if it is adjacent to all other vertices of G. Let $N(G)$ be the set of all well-connected vertices of G.

Azari and Iranmanesh (2013) and Altassan et al. (2022), independently, gave precise formulas for determining the eccentric distance sum of the most common graph operations, including the Cartesian product, join, composition, disjunction, symmetric difference and corona product. By specializing components of these graph operations, they were able to determine this distance-related invariant for various essential classes of molecular graphs and nanostructures.

3.4.1 Cartesian Product

The Cartesian product $G \cong \prod_{i=1}^{k} G_i$ of graphs $G_1, G_2, \ldots, G_k$ has vertex set $V(G) = V(G_1) \times V(G_2) \times \cdots \times V(G_k)$ and two vertices $u = (u_1, u_2, \ldots, u_k)$ and $v = (v_1, v_2, \ldots, v_k)$ are adjacent if they differ in exactly one position, say in i^{th} and $u_i v_i$ is an edge of G_i. Imrich et al. (2000) showed for $G \cong \prod_{i=1}^{k} G_i$ and vertices $u = (u_1, u_2, \ldots, u_k), v = (v_1, v_2, \ldots, v_k) \in V(G)$, $d_G(u,v) = \sum_{i=1}^{k} d_{G_i}(u_i, v_i)$ and this implies that $ecc_G(u) = \sum_{i=1}^{k} ecc_{G_i}(u_i)$. In particular, the Cartesian product, $G \cong G_1 \times G_2$, of two graphs G_1 and G_2 has vertex set $V(G) = V(G_1) \times V(G_2)$ and two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ are adjacent if and only if

$$u_1 = v_1 \textit{ and } u_2 v_2 \in E(G_2) \;\; \textit{or} \;\; u_2 = v_2 \textit{ and } u_1 v_1 \in E(G_1).$$

Also, we have

$$d_{G_1\times G_2}((u_1,u_2),(v_1,v_2)) = d_{G_1}(u_1,v_1)+d_{G_2}(u_2,v_2)$$

and

$$ecc_{G_1\times G_2}((u_1,u_2),(v_1,v_2)) = ecc_{G_1}(u_1,v_1)+ecc_{G_2}(u_2,v_2).$$

Theorem 3.13. *(Azari and Iranmanesh, 2013) Let $G_1, G_2, \dots, G_k$ be graphs with $|V(G_i)| = n_i$ and $n = \prod_{i=1}^{k} n_i$. Then*

$$EDS\left(\prod_{i=1}^{k} G_i\right) = n^2\left[\sum_{i=1}^{k}\frac{EDS(G_i)}{n_i^2}\right] + 2n^2\left[\sum_{i=1}^{k}\frac{ecc(G_i)}{n_i}\sum_{j=1,j\neq i}^{k}\frac{W(G_j)}{n_j^2}\right].$$

Let U be a non-empty sebset of $V(G_1)$. Consider the induced subgraph $G_1(U)$ of G_1, the generalized hierarchical product $G_1(U)\sqcap G_2$ is the same as $G_1(U)\times G_2$ and the eccentric distance sum of $G_1(U)\sqcap G_2$ was obtained as stated in Corollary 3.2.

Corollary 3.2. *(Eskender and Vumar, 2013)*

$$\begin{aligned}EDS(G_1(U)\sqcap G_2) = {} & n_2^2 EDS(G_1(U)) + n_1^2 EDS(G_2)\\ & + 2n_1 ecc(G_1(U))W(G_2) + 2n_2 ecc(G_2)W(G_1(U)).\end{aligned}$$

3.4.2 Join

We consider the sequential join which was introduced in Section 1.1.2. For vertices $u, v \in V(G_1+G_2+\cdots+G_t)$, we have

$$d_{G_1+G_2+\cdots+G_t}(u,v) = \begin{cases} 1 & \text{if } [uv\in E(G_i), 1\le i\le t] \text{ or } [u\in V(G_i), v\in V(G_j), 1\le i\neq j\le t],\\ 2, & \text{otherwise.}\end{cases}$$

For the eccentricities, we have

$$ecc_{G_1+G_2+\cdots+G_t}(u) = \begin{cases} 1, & \text{if } u\in N(G_i),\ 1\le i\le t,\\ 2, & \text{otherwise.}\end{cases}$$

Theorem 3.14. *(Azari and Iranmanesh, 2013) Let $G_1, G_2, \dots, G_t$ be graphs with $|V(G_i)| = n_i$, $|E(G_i)| = e_i$ and $|N(G_i)| = m_i$ for $1\le i\le t$. Then*

$$EDS(G_1+G_2+\cdots+G_t) = \left(1-\sum_{i=1}^{t} n_i\right)\left[\sum_{i=1}^{t} m_i\right] + 2\sum_{i=1}^{t}\left[n_i^2 - 2n_i - 2e_i + n_i\sum_{j=1}^{t} n_j\right].$$

3.4.3 Composition

Let G_1 and G_2 be graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$ and let $G_1 \ncong K_1$. The composition $G_1[G_2]$ of graphs G_1 and G_2 is a graph with the vertex set $V(G_1) \times V(G_2)$ and $u = (u_1, u_2)$ is adjacent to $v = (v_1, v_2)$ whenever (u_1 is adjacent to v_1 in G_1) or ($u_1 = v_1$ and u_2 is adjacent to v_2 in G_2). By the above definition, for vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G_1[G_2]$, we have

$$d_{G_1[G_2]}(u,v) = \begin{cases} d_{G_1}(u_1,v_1), & \text{if } u_1 \neq v_1, \\ 1 & \text{if } u_1 = v_1,\ u_2v_2 \in E(G_2), \\ 2, & \text{if } u_1 = v_1,\ u_2v_2 \notin E(G_2). \end{cases}$$

For the eccentricities, we have

$$ecc_{G_1[G_2]}((u_1,u_2)) = \begin{cases} ecc_{G_1}(u_1), & \text{if } u_1 \notin N(G_1), \\ 1, & \text{if } u_1 \in N(G_1),\ u_2 \in N(G_2), \\ 2, & \text{if } u_1 \in N(G_1),\ u_2 \notin N(G_2). \end{cases}$$

Theorem 3.15. *(Azari and Iranmanesh, 2013) Let G_1 and G_2 be graphs with $G_1 \neq K_1$. $|V(G_i)| = n_i$, $|E(G_i)| = e_i$ and $|N(G_i)| = m_i$ for $1 \leq i \leq 2$. Then*

$$EDS(G_1[G_2]) = (1 - n_1n_2)(m_1m_2) + [n_2^2(n_1+1) - 2(n_2+e_2)]m_1 + 2[n_2(n_2-1) - e_2]ECI(G_1) + n_2^2 EDS(G_1).$$

3.4.4 Disjunction

Let G_1 and G_2 be graphs with $G_i \neq K_1$ for $i = 1, 2$. The disjunction $G_1 \vee G_2$ of graphs G_1 and G_2 is a graph with the vertex set $V(G_1) \times V(G_2)$ and vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ are adjacent whenever $u_1v_1 \in E(G_1)$ or $u_2v_2 \in E(G_2)$. By the above definition, for vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G_1 \vee G_2$, we have

$$d_{G_1 \vee G_2}(u,v) = \begin{cases} 1 & \text{if } u_1v_1 \in E(G_1) \text{ or } u_2v_2 \in E(G_2), \\ 2, & \text{otherwise.} \end{cases}$$

For the eccentricities, we have

$$ecc_{G_1 \vee G_2}((u_1,u_2)) = \begin{cases} 1, & \text{if } u_1 \in N(G_1),\ u_2 \in N(G_2), \\ 2, & \text{otherwise.} \end{cases}$$

Theorem 3.16. *(Azari and Iranmanesh, 2013) Let G_1 and G_2 be graphs with $|V(G_i)| = n_i > 1$, $|E(G_i)| = e_i$ and $|N(G_i)| = m_i$ for $1 \leq i \leq 2$. Then*

$$EDS(G_1 \vee G_2) = (4n_1n_2 - m_1m_2)(n_1n_2 - 1) - 4e_1n_2^2 - 4e_2n_1^2 + 8e_1e_2.$$

3.4.5 Symmetric Difference

Let G_1 and G_2 be graphs with $G_i \neq K_1$ for $i = 1,2$. The symmetric difference $G_1 \oplus G_2$ of graphs G_1 and G_2 is a graph with the vertex set $V(G_1) \times V(G_2)$ and edge set $E(G_1 \oplus G_2) = \{(u_1,u_2)(v_1,v_2) : \text{either } u_1v_1 \in E(G_1) \text{ or } u_2v_2 \in E(G_2)\}$. By this definition, for vertices $u = (u_1,u_2)$ and $v = (v_1,v_2)$ of $G_1 \oplus G_2$, we have

$$d_{G_1 \oplus G_2}(u,v) = \begin{cases} 1 & \text{if } u_1v_1 \in E(G_1) \text{ or } \ u_2v_2 \in E(G_2) \text{ but not both,} \\ 2, & \text{otherwise.} \end{cases}$$

For the eccentricities, we have $ecc_{G_1 \oplus G_2}(u) = 2$, for any $u \in V(G_1 \oplus G_2)$.

Theorem 3.17. *(Azari and Iranmanesh, 2013) Let G_1 and G_2 be graphs with $|V(G_i)| = n_i > 1$, $|E(G_i)| = e_i$ and $|N(G_i)| = m_i$ for $1 \leq i \leq 2$. Then*

$$EDS(G_1 \oplus G_2) = 4\left(4n_1^2n_2^2 - n_1n_2 - e_1n_2^2 - e_2n_1^2 + 4e_1e_2\right).$$

3.4.6 Corona Product

Let G_1 and G_2 be graphs. The corona product $G_1 \circ G_2$ of graphs G_1 and G_2 is a graph obtained by taking one copy of G_1 and $|V(G_1)| = n_1$ copies of G_2 and joining the i^{th} vertex of G_1 to every vertex in i^{th} copy of G_2. For $1 \leq i \leq n_1$, the i^{th} copy of G_2 and i^{th} element of G_1 will be denoted by G_2^i and w_i respectively. Let $V(G_1) = \{w_1, w_2, \ldots, w_{n_1}\}$. By this definition, for vertices u and v of $G_1 \circ G_2$, we have

$$d_{G_1 \circ G_2}(u,v) = \begin{cases} d_{G_1}(u,v), & \text{if } u,v \in V(G_1), \\ d_{G_1}(u,w_i) + 1, & \text{if } u \in V(G_1),\ v \in V(G_2^i),\ 1 \leq i \leq n_1, \\ 1 & \text{if } uv \in E(G_2^i),\ 1 \leq i \leq n_1, \\ 2 & \text{if } u,v \in V(G_2^i);\ uv \notin E(G_2^i),\ u \neq v,\ 1 \leq i \leq n_1, \\ d_{G_1}(w_i,w_j) + 2, & \text{if } u \in V(G_2^i),\ v \in V(G_2^j),\ 1 \leq i \neq j \leq n_1. \end{cases}$$

For the eccentricities, we have

$$ecc_{G_1 \circ G_2}(u) = \begin{cases} ecc_{G_1}(u)+1, & \text{if } u \in V(G_1), \\ ecc_{G_1}(w_i)+2, & u \in V(G_2^i),\ 1 \le i \le n_1. \end{cases}$$

Theorem 3.18. *(Azari and Iranmanesh, 2013) Let G_1 and G_2 be graphs with $|V(G_i)| = n_i$, $|E(G_i)| = e_i$. Then*

$$\begin{aligned} EDS(G_1 \circ G_2) =& (n_2+1)^2 EDS(G_1) + 2(n_2+1)(2n_2+1)W(G_1) \\ & + 2(n_1 n_2^2 + n_1 n_2 - n_2 - e_2)ECI(G_1) + n_1^2 n_2(4n_2+3) - 4n_1(n_2+2_2). \end{aligned}$$

3.5 General Eccentric Distance Sum

Masre and Vetrík (2021) proved Lemma 3.1, which is used to compare the $EDS_{a,b}$ of various graphs and Lemma 3.2 was used to obtain bounds for the $EDS_{a,b}$ of graphs. Lemma 3.1 and 3.2 are used in the proof of the results of the dissertation.

Lemma 3.1. *(Masre and Vetrík, 2021) Let $1 \le x < y$ and $c > 0$. Then for $b > 1$ or $b < 0$,*

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

If $0 < b < 1$, then

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

Lemma 3.2. *(Vetrík, 2021) Let G be a graph with two non-adjacent vertices u and v.*

Then for $a \ge 0$ and $b > 0$, we have

$$EDS_{a,b}(G+uv) < EDS_{a,b}(G).$$

For $a \le 0$ and $b < 0$, we have

$$EDS_{a,b}(G+uv) > EDS_{a,b}(G).$$

That is, $EDS_{a,b}$ decreases (increases) for $a \ge 0$ and $b > 0$ (for $a \le 0$ and $b < 0$) with the addition of an edge. In the same way, $EDS_{a,b}$ increases (decreases) for $a \ge 0$ and $b > 0$ (for $a \le 0$ and $b < 0$) by removing of an edge provided that the resulting graph is connected.

Among all graphs of order $n \ge 2$, the complete graph K_n has the minimum (maximum) $EDS_{a,b}$ for $a \ge 0$ and $b > 0$ (for $a \le 0$ and $b < 0$) as stated in Theorem 3.19 (Vetrík, 2021).

Thus, we can conclude that, it is also a graph with the minimum (maximum) $EDS_{a,b}$ for $a \geq 0$ and $b > 0$, (for $a \leq 0$ and $b < 0$) among all graphs of order n and matching number $\nu = \left\lfloor \frac{n}{2} \right\rfloor$.

Theorem 3.19. *(Vetrík, 2021) Let G be any graph of order $n \geq 2$. Then for $a \geq 0$ and $b > 0$*

$$EDS_{a,b}(G) \geq n(n-1)^b.$$

For $a \leq 0$ and $b < 0$

$$EDS_{a,b}(G) \leq n(n-1)^b.$$

The equalities hold if and only if $G \cong K_n$.

Vetrík (2021) also presented that the star S_n has the minimum (maximum) $EDS_{a,b}$ for $a \geq 0$ and $b > 0$ (for $a \leq 0$ and $b < 0$) among all trees of order n. These extremal graphs were obtained by Ilić et al. (2011) for the particular case, $a = b = 1$.

Theorem 3.20. *(Vetrík, 2021) Let T be a tree with order n. Then for $a \geq 0$ and $b > 0$*

$$EDS_{a,b}(G) \geq (n-1)^b + (n-1)2^a(2n-3)^b.$$

For $a \leq 0$ and $b < 0$

$$EDS_{a,b}(G) \leq (n-1)^b + (n-1)2^a(2n-3)^b.$$

The equalities hold if and only if $G \cong S_n$.

Vetrík (2021) also presented the $EDS_{a,b}$ for graphs with respect to order, connectivity and number of pendent vertices and bipartite graphs of order n as stated in Theorems 3.21-3.23.

Theorem 3.21. *(Vetrík, 2021) Let G be any bipartite graph of order n other than the star S_n, where $n \geq 4$. Then for $a \geq 0$ and $b \geq 1$,*

$$EDS_{a,b}(G) \geq 2^a \left\lceil \frac{n}{2} \right\rceil \left(n + \left\lceil \frac{n}{2}2 \right\rceil - 2\right)^b + 2^a \left\lfloor \frac{n}{2} \right\rfloor \left(n + \left\lfloor \frac{n}{2} \right\rfloor - 2\right)^b.$$

The equalities hold if and only if $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

Theorem 3.22. *(Vetrík, 2021) Let G be any graph of order n and connectivity κ, where $1 \leq \kappa \leq n-2$.*

Then for $a \geq 0$ and $0 < b \leq 1$

$$EDS_{a,b}(G) \geq (n-\kappa-1)2^a n^b + 2^a(2n-\kappa-2)^b + \kappa(n-1)^b.$$

For $a \leq 0$ and $b < 0$

$$EDS_{a,b}(G) \leq (n-\kappa-1)2^a n^b + 2^a(2n-\kappa-2)^b + \kappa(n-1)^b.$$

The equalities hold if and only if $G \cong K_\kappa + (K_{n-\kappa-1} \cup K_1)$.

Theorem 3.23. *(Vetrík, 2021) Let G be any graph of order n and p pendent vertices, where $1 \leq p \leq n-3$.*

Then for $a \geq 0$ and $b > 1$

$$EDS_{a,b}(G) \geq (n-p-1)2^a(n+p-1)^b + p2^a(2n-3)^b + (n-1)^b.$$

For $a \leq 0$ and $b < 0$

$$EDS_{a,b}(G) \leq (n-p-1)2^a(n+p-1)^b + p2^a(2n-3)^b + (n-1)^b.$$

The equalities hold if and only if $G \cong K_{n-p} \star S_{p+1}$.

This study focused on finding the extremal values and extremal graphs for general eccentric distance sum of graphs such as trees, bipartite graphs and graphs for $a, b\mathbb{R}$ with different intervals for a and b. This study mainly focuses on general eccentric distance sum of graphs with graph parameters not considered under this chapter.

CHAPTER 4

RESEARCH METHODOLOGY

This dissertation is devoted to present extremal values and extremal graphs on the general eccentric distance sum for graphs, bipartite graphs and trees with a given order and some other graph parameters. We outline the techniques and procedures in this chapter to accomplish the general and specific objectives of this dissertation. In order to do this, we quickly go over the methods of problem-solving and mathematical procedures.

4.1 Mathematical Procedures

Mathematical procedures that the dissertation follows are described below.

1. **Document Analysis**

   At this stage, we review different published papers on both the eccentric distance sum and the general eccentric distance sum for different types of graphs with respect to different graph parameters.

2. **Abstraction**

   At this point, we attempt to reconsider those extremal small-order graphs for given graph parameters on the eccentric distance sum in order to investigate their general eccentric distance sum value using small-order graphs and a fixed value of a and b.

3. **Generalization/Extension**

   At this stage, we try to construct a conjuncture or hypothesis for the general eccentric distance sum from those graphs discussed in the above stage.

4. **Proof**

   We give a proof for the hypothesis or conjunction that was established above. Some changes are sometimes made to the previously hypothesized results. Finally, we have theorems and corollaries.

4.2 Assumptions and Formulation

To achieve the objectives of this dissertation, we employ different types of problem solving methods, such as proof by contradiction and direct proof techniques, as well as graph transformation techniques to find the extremal values and graphs. We also study the nature of the parameters, such as chromatic number, matching number, diameter, and pendent vertices, in finding the extremal values and graphs for the general eccentric distance sum. Then we introduce some preliminary lemmas (especially a lemma that defines the nature of the general eccentric distance sum on graphs) from other researchers' work that could help us in finding extremal values. At the same time, for the total distance and eccentricity of a vertex, the mathematical properties and changes they have during graph transformation operations on graphs were investigated in order to find the extremal values. We consider only connected graph types due to the distance property in a graph.

4.3 Research Design

Parameters such as order, chromatic number, matching number, and diameter with at most 4 are considered in finding the extremal values. We draw some graphs with a small number of vertices satisfying our parameters to find extremal graphs. Next, we compute the general eccentric distance sum for those graphs and identify the graph with the minimum and maximum general eccentric distance sum for some $a, b \in \mathbb{R}$ (for instance, we may choose $a = 2$ and $b = 0.5$ or $b = 2$). Then we compare whether those extremal values and the extremal value of the eccentric distance sum while we put $a = b = 1$. Finally, we give proof for the general arbitrary graph achieving the extremal value. In the proof, we commonly apply graph transformation operation in addition to proof by contradiction and direct proof techniques to get the extremal values and extremal graphs.

CHAPTER 5

RESULTS ON THE GENERAL ECCENTRIC DISTANCE SUM OF TREES

In this chapter, we give bounds on $EDS_{a,b}$ for trees with given order and bipartition, lower bounds are obtained for $a \geq 0$ and $0 < b \leq 1$ and upper bounds are obtained for $a \leq 0$ and $b < 0$. We present bounds on the general eccentric distance sum for trees with given order and diameter 3, trees with a given order and domination number 2. All the bounds are and extremal graphs are presented.

Recall that a bipartite graph with two partite sets U_1 and U_2 has an (s,t)-bipartition if $|U_1| = s$ and $|U_2| = t$. Clearly, for the order n of G, we have $n = s+t$. Note that any tree is a bipartite graph and thus, it has an (s,t)-bipartition. In Theorems 5.1 and 5.2, we consider trees having an (s,t)-bipartition with $s \geq t \geq 2$, because the unique tree having an $(s,1)$-bipartition is a star with $s+1$. For $a = b = 1$, Theorem 5.1 was presented in (Geng et al., 2013). For $a = 2$ and $b = 0$, Theorem 5.1 was given in (Qi and Du, 2017).

Theorem 5.1. *Let $a \geq 0$, $0 < b \leq 1$ and $s \geq t \geq 2$. For any tree T with an (s,t)-bipartition,*

$$\begin{aligned} EDS_{a,b}(T) \; &\geq (s-1)3^a(3t+2s-4)^b + (t-1)3^a(3s+2t-4)^b \\ &+2^a(2t+s-2)^b + 2^a(2s+t-2)^b, \end{aligned}$$

with equality if and only if T is $P_2(s-1,t-1)$.

Proof. Among trees with an (s,t)-bipartition, we denote a tree with the smallest $EDS_{a,b}$ by T'. For simplification, let $T^* = P_2(s-1,t-1)$. Let us prove by contradiction that T' is $T^* = P_2(s-1,t-1)$.

Assume that $T' \neq T^*$. A tree with diameter $d \leq 2$ does not exist for $s \geq t \geq 2$ and the only tree having diameter 3 is T^*. Thus $d \geq 4$. We denote a diametral path in T' by $u_0u_1 \ldots u_d$ (so $d_{T'}(u_0,u_d) = d$) and the leaves adjacent to u_{d-1} by $w_1, w_2, \ldots, w_p$, where u_d is one of them and $p \geq 1$. Without loos of generality, we assume that $D_{T'}(u_1) \leq D_{T'}(u_{d-1})$. Let $T'' = T' - \{u_{d-1}w_1, u_{d-1}w_2, \ldots, u_{d-1}w_p\} + \{u_{d-3}w_1, u_{d-3}w_2, \ldots, u_{d-3}w_p\}$. Clearly, T'' has an (s,t)-bipartition.

Let us use u_1 and u_{d-1} to obtain a contradiction. We have $ecc_{T'}(u_1) = ecc_{T'}(u_{d-1}) =$

$ecc_{T''}(u_{d-1}) = d-1$ and $d-2 \leq ecc_{T''}(u_1) \leq d-1$. We obtain

$$D_{T''}(u_1) = D_{T'}(u_1) - 2p \text{ and } D_{T''}(u_{d-1}) = D_{T'}(u_{d-1}) + 2p.$$

For any vertex $z \in V(T') \setminus \{u_1, u_{d-1}\}$, we have $ecc_{T'}(z) \geq ecc_{T''}(z)$ and $D_{T'}(z) \geq D_{T''}(z)$, therefore

$$[ecc_{T'}(z)]^a [D_{T'}(z)]^b \geq [ecc_{T''}(z)]^a [D_{T''}(z)]^b$$

for $a \geq 0$ and $0 < b < 1$. Moreover, there are some vertices $z \in V(T') \setminus \{u_1, u_{d-1}\}$ (for example u_0), for which $D_{T'}(z) > D_{T''}(z)$, therefore

$$[ecc_{T'}(z)]^a [D_{T'}(z)]^b > [ecc_{T''}(z)]^a [D_{T''}(z)]^b$$

for those vertices. Thus

$$\begin{aligned}
& EDS_{a,b}(T') - EDS_{a,b}(T'') \\
= & \sum_{z \in V(T') \setminus \{u_1, u_{d-1}\}} ([ecc_{T'}(z)]^a [D_{T'}(z)]^b - [ecc_{T''}(z)]^a [D_{T''}(z)]^b) \\
& + [ecc_{T'}(u_1)]^a [D_{T'}(u_1)]^b - [ecc_{T''}(u_1)]^a [D_{T''}(u_1)]^b \\
& + [ecc_{T'}(u_{d-1})]^a [D_{T'}(u_{d-1})]^b - [ecc_{T''}(v_{u-1})]^a [D_{T''}(u_{d-1})]^b \\
> & [ecc_{T'}(u_1)]^a [D_{T'}(u_1)]^b - [ecc_{T''}(u_1)]^a [D_{T''}(u_1)]^b \\
& + [ecc_{T'}(u_{d-1})]^a [D_{T'}(u_{d-1})]^b - [ecc_{T''}(v_{u-1})]^a [D_{T''}(u_{d-1})]^b \\
= & (d-1)^a [D_{T'}(u_1)]^b - [ecc_{T''}(u_1)]^a [D_{T'}(u_1) - 2p]^b \\
& + (d-1)^a ([D_{T'}(u_{d-1})]^b - [D_{T'}(u_{d-1}) + 2p]^b) \\
\geq & (d-1)^a \left([D_{T'}(u_1)]^b - [D_{T'}(u_1) - 2p]^b + [D_{T'}(u_{d-1})]^b - [D_{T'}(u_{d-1}) + 2p]^b \right) \\
\geq & 0,
\end{aligned}$$

because for $b = 1$,

$$[D_{T'}(u_1)]^b - [D_{T'}(u_1) - 2p]^b + [D_{T'}(u_{d-1})]^b - [D_{T'}(u_{d-1}) + 2p]^b = 0,$$

and for $0 < b < 1$, from Lemma 3.1, we obtain

$$[D_{T'}(u_1)]^b - [D_{T'}(u_1) - 2p]^b > [D_{T'}(u_{d-1}) + 2p]^b - [D_{T'}(u_{d-1})]^b.$$

Therefore $EDS_{a,b}(T') > EDS_{a,b}(T'')$. Hence T' does not have the minimum $EDS_{a,b}$. We have a contradiction.

So T' is T^* which contains two vertices which are not leaves, say v and v', where v is adjacent to $s-1$ leaves v_i, $i = 1,2,\ldots,s-1$ and v' is adjacent to $t-1$ leaves v'_j, $j = 1,2,\ldots,t-1$. We have

$$\begin{aligned}
ecc_{T^*}(v) &= 2, \quad D_{T^*}(v) = s+2(t-1),\\
ecc_{T^*}(v') &= 2, \quad D_{T^*}(v') = t+2(s-1),\\
ecc_{T^*}(v_i) &= 3, \quad D_{T^*}(v_i) = 1+2(s-1)+3(t-1),\\
ecc_{T^*}(v'_j) &= 3, \quad D_{T^*}(v'_j) = 1+2(t-1)+3(s-1).
\end{aligned}$$

Hence

$$\begin{aligned}
EDS_{a,b}(P_2(s-1,t-1)) &= EDS_{a,b}(T^*)\\
&= (s-1)3^a(3t+2s-4)^b + (t-1)3^a(3s+2t-4)^b\\
&\quad + 2^a(2t+s-2)^b + 2^a(2s+t-2)^b.
\end{aligned}$$

□

Theorem 5.2. *Let $a \le 0$, $b < 0$ and $s \ge t \ge 2$. For any tree T with an (s,t)-bipartition,*

$$\begin{aligned}
EDS_{a,b}(T) &\le (s-1)3^a(3t+2s-4)^b + (t-1)3^a(3s+2t-4)^b\\
&\quad +2^a(2t+s-2)^b + 2^a(2s+t-2)^b,
\end{aligned}$$

with equality if and only if T is $P_2(s-1,t-1)$.

Proof. Only those parts of the proof are presented which differ from the proof of Theorem 5.1.

Among trees with an (s,t)-bipartition, we denote a tree with the largest $EDS_{a,b}$ by T'.

Since $ecc_{T''}(u_1) \le d-1$, we have

$$[ecc_{T''}(u_1)]^a \ge (d-1)^a$$

for $a \le 0$.

For any vertex $z \in V(T') \setminus \{u_1, u_{d-1}\}$, we have $ecc_{T'}(z) \ge ecc_{T''}(z)$ and $D_{T'}(z) \ge D_{T''}(z)$, therefore $[ecc_{T'}(z)]^a \le [ecc_{T''}(z)]^a$ for $a \le 0$ and $[D_{T'}(z)]^b \le [D_{T''}(z)]^b$ for $b < 0$, so

$$[ecc_{T'}(z)]^a[D_{T'}(z)]^b \le [ecc_{T''}(z)]^a[D_{T''}(z)]^b.$$

Thus

$$
\begin{aligned}
& EDS_{a,b}(T') - EDS_{a,b}(T'') \\
\le\ & [ecc_{T'}(u_1)]^a[D_{T'}(u_1)]^b - [ecc_{T''}(u_1)]^a[D_{T''}(u_1)]^b \\
& +[ecc_{T'}(u_{d-1})]^a[D_{T'}(u_{d-1})]^b - [ecc_{T''}(v_{u-1})]^a[D_{T''}(u_{d-1})]^b \\
=\ & (d-1)^a[D_{T'}(u_1)]^b - [ecc_{T''}(u_1)]^a[D_{T'}(u_1)-2p]^b \\
& +(d-1)^a([D_{T'}(u_{d-1})]^b - [D_{T'}(u_{d-1})+2p]^b) \\
\le\ & (d-1)^a\left([D_{T'}(u_1)]^b - [D_{T'}(u_1)-2p]^b + [D_{T'}(u_{d-1})]^b - [D_{T'}(u_{d-1})+2p]^b\right) \\
<\ & 0,
\end{aligned}
$$

because for $b<0$, from Lemma 3.1, we obtain

$$[D_{T'}(u_1)]^b - [D_{T'}(u_1)-2p]^b < [D_{T'}(u_{d-1})+2p]^b - [D_{T'}(u_{d-1})]^b.$$

Therefore $EDS_{a,b}(T') < EDS_{a,b}(T'')$. Hence T' does not have the maxmum $EDS_{a,b}$. We have a contradiction. $\square$

For integers $l \ge 2$ and $n_1 \ge n_2 \ge 1$, $P_l(n_1,n_2)$ is a tree presented in Figure 5.1.

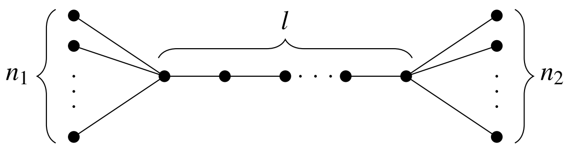

Figure 5.1: Tree $P_l(n_1,n_2)$.

In Theorems 5.3 and 5.4, we compare the $EDS_{a,b}$ indices of these graphs if l and the order are fixed. Theorem 5.3 is used in the proofs of Theorems 5.5 and 5.8.

Theorem 5.3. *Let* $2 \le l \le n-2$. *For* $a,b \in \mathbb{R}$ *where* $0 < b \le 1$,

$$EDS_{a,b}(P_l(1,n-l-1)) < EDS_{a,b}(P_l(2,n-l-2)) < \cdots < EDS_{a,b}\left(P_l\left(\left\lfloor\frac{n-l}{2}\right\rfloor,\left\lceil\frac{n-l}{2}\right\rceil\right)\right).$$

Proof. In the tree $T_1 = P_l(n_1,n_2)$, where $n_1 \ge n_2 \ge 2$, let $u_1u_2\ldots u_l$ be the path which does not contain pendant vertices of $P_l(n_1,n_2)$. We denote the pendant vertices adjacent to u_1 by $v_1,v_2,\ldots,v_{n_1}$ and the pendant vertices adjacent to u_l by $v'_1,v'_2,\ldots,v'_{n_2}$.

Let $V(T_2)=V(T_1)$ and $E(T_2)=\{u_1v'_{n_2}\}\cup E(T_1)\setminus\{u_lv'_{n_2}\}$. Note that T_2 is the tree $P_l(n_1+1,n_2-1)$. To prove Theorem 5.3, it suffices to show that $EDS_{a,b}(T_2) < EDS_{a,b}(T_1)$.

For any $v \in V(T_1)$, we obtain $ecc_{T_1}(v) = ecc_{T_2}(v)$. Note that for $i = 1, 2, \ldots, \lfloor \frac{l+1}{2} \rfloor$,

$$ecc_{T_1}(u_i) = ecc_{T_1}(u_{l+1-i}) = l+1-i, \text{ and } ecc_{T_1}(v) = l+1$$

for all the pendant vertices $v \in V(T_1)$.

For $j = 1, 2, \ldots, n_1$ and $k = 1, 2, \ldots, n_2 - 1$,

- in T_1, there are $n_1 - 1$ pendant vertices of distance 2 from v_j and n_2 pendant vertices of distance $l+1$ from v_j,
- in T_2, there are n_1 pendant vertices of distance 2 from v_j and $n_2 - 1$ pendant vertices of distance $l+1$ from v_j,
- in T_1, there are $n_2 - 1$ pendant vertices of distance 2 from v'_k and n_1 pendant vertices of distance $l+1$ from v'_k,
- in T_2, there are $n_2 - 2$ pendant vertices of distance 2 from v'_k and $n_1 + 1$ pendant vertices of distance $l+1$ from v'_k,

thus

$$D_{T_2}(v_j) < D_{T_1}(v_j) \leq D_{T_1}(v'_k) < D_{T_2}(v'_k), \tag{5.1}$$

where

$$D_{T_1}(v_j) - D_{T_2}(v_j) = D_{T_2}(v'_k) - D_{T_1}(v'_k) = l-1. \tag{5.2}$$

Similarly,

$$D_{T_2}(v'_{n_2}) < D_{T_1}(v'_{n_2}), \ \ thus \ \ [D_{T_2}(v'_{n_2})]^b < [D_{T_1}(v'_{n_2})]^b \tag{5.3}$$

for $0 < b \leq 1$.

For $i = 1, 2, \ldots, \lfloor \frac{l}{2} \rfloor$,

- in T_1, there are n_1 pendant vertices of distance i from u_i and n_2 pendant vertices of distance $l+1-i$ from u_i,
- in T_2, there are $n_1 + 1$ pendant vertices of distance i from u_i and $n_2 - 1$ pendant vertices of distance $l+1-i$ from u_i,
- in T_1, there are n_2 pendant vertices of distance i from u_{l+1-i} and n_1 pendant vertices of distance $l+1-i$ from u_{l+1-i},
- in T_2, there are $n_2 - 1$ pendant vertices of distance i from u_{l+1-i} and $n_1 + 1$ pendant vertices of distance $l+1-i$ from u_{l+1-i},

thus

$$D_{T_2}(u_i) < D_{T_1}(u_i) \le D_{T_1}(u_{l+1-i}) < D_{T_2}(u_{l+1-i}), \tag{5.4}$$

where

$$D_{T_1}(u_i) - D_{T_2}(u_i) = D_{T_2}(u_{l+1-i}) - D_{T_1}(u_{l+1-i}) = l+1-2i. \tag{5.5}$$

Note that if l is odd, then $D_{T_2}(u_{\frac{l+1}{2}}) = D_{T_1}(u_{\frac{l+1}{2}})$. We have

$$\begin{aligned}
&EDS_{a,b}(T_1) - EDS_{a,b}(T_2) \\
&= \sum_{v \in V(T_1)} [ecc_{T_1}(v)]^a([D_{T_1}(v)]^b - [D_{T_2}(v)]^b) \\
&= \sum_{j=1}^{n_1} [ecc_{T_1}(v_j)]^a([D_{T_1}(v_j)]^b - [D_{T_2}(v_j)]^b) \\
&\quad + \sum_{k=1}^{n_2} [ecc_{T_1}(v'_k)]^a([D_{T_1}(v'_k)]^b - [D_{T_2}(v'_k)]^b + \sum_{i=1}^{l} [ecc_{T_1}(u_i)]^a([D_{T_1}(u_i)]^b - [D_{T_2}(u_i)]^b).
\end{aligned}$$

From (5.2) and (5.3),

$$\begin{aligned}
&\sum_{j=1}^{n_1} [ecc_{T_1}(v_j)]^a([D_{T_1}(v_j)]^b - [D_{T_2}(v_j)]^b) + \sum_{k=1}^{n_2} [ecc_{T_1}(v'_k)]^a([D_{T_1}(v'_k)]^b - [D_{T_2}(v'_k)]^b) \\
&= (l+1)^a[[D_{T_1}(v'_{n_2})]^b - [D_{T_2}(v'_{n_2})]^b] \\
&\quad + (l+1)^a[n_1([D_{T_1}(v_1)]^b - [D_{T_2}(v_1)]^b) + (n_2-1)([D_{T_1}(v'_1)]^b - [D_{T_2}(v'_1)]^b) +] \\
&> (l+1)^a[n_1([D_{T_2}(v_1)+l-1]^b - [D_{T_2}(v_1)]^b) + (n_2-1)([D_{T_1}(v'_1)]^b - [D_{T_1}(v'_1)+l-1]^b)] \\
&> (l+1)^a(n_2-1)([D_{T_2}(v_1)+l-1]^b - [D_{T_2}(v_1)]^b + [D_{T_1}(v'_1)]^b - [D_{T_1}(v'_1)+l-1]^b) \\
&\ge 0,
\end{aligned}$$

since $(l+1)^a > 0$, for $b=1$,

$$[D_{T_2}(v_1)+l-1]^b - [D_{T_2}(v_1)]^b + [D_{T_1}(v'_1)]^b - [D_{T_1}(v'_1)+l-1]^b = 0,$$

and for $0 < b < 1$, by (5.1) and Lemma 3.1,

$$[D_{T_2}(v_1)+l-1]^b - [D_{T_2}(v_1)]^b > [D_{T_1}(v'_1)+l-1]^b - [D_{T_1}(v'_1)]^b.$$

From (5.5),

$$
\begin{aligned}
&\sum_{i=1}^{l}[ecc_{T_1}(u_i)]^a([D_{T_1}(u_i)]^b-[D_{T_2}(u_i)]^b)\\
&=\sum_{i=1}^{\lfloor\frac{l}{2}\rfloor}[ecc_{T_1}(u_i)]^a([D_{T_1}(u_i)]^b-[D_{T_2}(u_i)]^b)+[ecc_{T_1}(u_{l+1-i})]^a([D_{T_1}(u_{l+1-i})]^b-[D_{T_2}(u_{l+1-i})]^b)\\
&=\sum_{i=1}^{\lfloor\frac{l}{2}\rfloor}(l+1-i)^a([D_{T_2}(u_i)+l+1-2i]^b-[D_{T_2}(u_i)]^b\\
&\quad+[D_{T_1}(u_{l+1-i})]^b-[D_{T_1}(u_{l+1-i})+l+1-2i]^b)\\
&\geq 0,
\end{aligned}
$$

since $(l+1-i)^a>0$, for $b=1$,

$$[D_{T_2}(u_i)+l+1-2i]^b-[D_{T_2}(u_i)]^b+[D_{T_1}(u_{l+1-i})]^b-[D_{T_1}(u_{l+1-i})+l+1-2i]^b=0,$$

and for $0<b<1$, by (5.4) and Lemma 3.1,

$$[D_{T_2}(u_i)+l+1-2i]^b-[D_{T_2}(u_i)]^b>[D_{T_1}(u_{l+1-i})+l+1-2i]^b-[D_{T_1}(u_{l+1-i})]^b.$$

Hence $EDS_{a,b}(T_1)-EDS_{a,b}(T_2)>0$. □

Theorem 5.4. *Let $2\leq l\leq n-2$. For $a,b\in\mathbb{R}$ where $b<0$,*

$$EDS_{a,b}(P_l(1,n-l-1))>EDS_{a,b}(P_l(2,n-l-2))>\cdots>EDS_{a,b}\left(P_l\left(\left\lfloor\frac{n-l}{2}\right\rfloor,\left\lceil\frac{n-l}{2}\right\rceil\right)\right).$$

Proof. We present those parts of the proof of Theorem 5.4, which differ from the proof of Theorem 5.3. We show that $EDS_{a,b}(T_1)<EDS_{a,b}(T_2)$, where $T_1=P_l(n_1,n_2)$, $T_2=P_l(n_1+1,n_2-1)$ and $n_1\geq n_2\geq 2$,

For $j=1,2,\ldots,n_1$ and $k=1,2,\ldots,n_2-1$, we have

$$D_{T_2}(v_j)<D_{T_1}(v_j)\leq D_{T_1}(v'_k)<D_{T_2}(v'_k), \tag{5.6}$$

where

$$D_{T_1}(v_j)-D_{T_2}(v_j)=D_{T_2}(v'_k)-D_{T_1}(v'_k)=l-1. \tag{5.7}$$

Similarly,

$$D_{T_2}(v'_{n_2})<D_{T_1}(v'_{n_2}),\ \text{ so }\ [D_{T_2}(v'_{n_2})]^b>[D_{T_1}(v'_{n_2})]^b \tag{5.8}$$

for $b<0$.

For $i=1,2,\dots,\lfloor \frac{l}{2}\rfloor$, we have

$$D_{T_2}(u_i) < D_{T_1}(u_i) \le D_{T_1}(u_{l+1-i}) < D_{T_2}(u_{l+1-i}), \tag{5.9}$$

where

$$D_{T_1}(u_i) - D_{T_2}(u_i) = D_{T_2}(u_{l+1-i}) - D_{T_1}(u_{l+1-i}) = l+1-2i. \tag{5.10}$$

By (5.7) and (5.8),

$$\begin{aligned}
&\sum_{j=1}^{n_1}[ecc_{T_1}(v_j)]^a([D_{T_1}(v_j)]^b-[D_{T_2}(v_j)]^b)+\sum_{k=1}^{n_2}[ecc_{T_1}(v'_k)]^a([D_{T_1}(v'_k)]^b-[D_{T_2}(v'_k)]^b)\\
&=(l+1)^a[[D_{T_1}(v'_{n_2})]^b-[D_{T_2}(v'_{n_2})]^b]\\
&\quad+(l+1)^a[n_1([D_{T_1}(v_1)]^b-[D_{T_2}(v_1)]^b)+(n_2-1)([D_{T_1}(v'_1)]^b-[D_{T_2}(v'_1)]^b)+]\\
&<(l+1)^a[n_1([D_{T_2}(v_1)+l-1]^b-[D_{T_2}(v_1)]^b)+(n_2-1)([D_{T_1}(v'_1)]^b-[D_{T_1}(v'_1)+l-1]^b)]\\
&<(l+1)^a(n_2-1)([D_{T_2}(v_1)+l-1]^b-[D_{T_2}(v_1)]^b+[D_{T_1}(v'_1)]^b-[D_{T_1}(v'_1)+l-1]^b)\\
&<0,
\end{aligned}$$

since $(l+1)^a>0$ and by (5.6) and Lemma 3.1, for $b<0$,

$$[D_{T_2}(v_1)+l-1]^b-[D_{T_2}(v_1)]^b < [D_{T_1}(v'_1)+l-1]^b-[D_{T_1}(v'_1)]^b.$$

By (5.10),

$$\begin{aligned}
&\sum_{i=1}^{l}[ecc_{T_1}(u_i)]^a([D_{T_1}(u_i)]^b-[D_{T_2}(u_i)]^b)\\
&=\sum_{i=1}^{\lfloor \frac{l}{2}\rfloor}[ecc_{T_1}(u_i)]^a([D_{T_1}(u_i)]^b-[D_{T_2}(u_i)]^b)+[ecc_{T_1}(u_{l+1-i})]^a([D_{T_1}(u_{l+1-i})]^b-[D_{T_2}(u_{l+1-i})]^b)\\
&=\sum_{i=1}^{\lfloor \frac{l}{2}\rfloor}(l+1-i)^a([D_{T_2}(u_i)+l+1-2i]^b-[D_{T_2}(u_i)]^b\\
&\quad+[D_{T_1}(u_{l+1-i})]^b-[D_{T_1}(u_{l+1-i})+l+1-2i]^b)\\
&<0,
\end{aligned}$$

since $(l+1-i)^a>0$ and for $b<0$, by (5.9) and Lemma 3.1,

$$[D_{T_2}(u_i)+l+1-2i]^b-[D_{T_2}(u_i)]^b < [D_{T_1}(u_{l+1-i})+l+1-2i]^b-[D_{T_1}(u_{l+1-i})]^b.$$

Hence $EDS_{a,b}(T_1) - EDS_{a,b}(T_2) < 0$. $\square$

Let us present bounds on $EDS_{a,b}(T)$ for trees T of given order and diameter 3.

Theorem 5.5. *Let T be a tree of order $n \geq 4$ and diameter 3. Let $a, b \in \mathbb{R}$ where $0 < b \leq 1$. Then*

$$EDS_{a,b}(P_2(n-3,1)) \leq EDS_{a,b}(T) \leq EDS_{a,b}\left(P_2\left(\left\lceil \frac{n}{2} \right\rceil - 1, \left\lfloor \frac{n}{2} \right\rfloor - 1\right)\right)$$

with equalities if and only if T is $P_2(n-3,1)$ and $P_2(\lceil \frac{n}{2} \rceil - 1, \lfloor \frac{n}{2} \rfloor - 1)$, respectively.

Proof. Every tree of order n and diameter 3 has the form $P_2(n-k,k)$, where $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$. For $0 < b \leq 1$, by Theorem 5.3, $P_2(n-3,1)$ and $P_2(\lceil \frac{n}{2} \rceil - 1, \lfloor \frac{n}{2} \rfloor - 1)$ are the unique trees with the smallest and largest $EDS_{a,b}$ index, respectively. $\square$

Similarly, using Theorem 5.4, we obtain the following bounds for negative b.

Theorem 5.6. *Let T be a tree of order $n \geq 4$ and diameter 3. Let $a, b \in \mathbb{R}$ where $b < 0$. Then*

$$EDS_{a,b}\left(P_2\left(\left\lceil \frac{n}{2} \right\rceil - 1, \left\lfloor \frac{n}{2} \right\rfloor - 1\right)\right) \leq EDS_{a,b}(T) \leq EDS_{a,b}(P_2(n-3,1))$$

with equalities if and only if T is $P_2(\lceil \frac{n}{2} \rceil - 1, \lfloor \frac{n}{2} \rfloor - 1)$ and $P_2(n-3,1)$, respectively.

We present the values of $EDS_{a,b}(P_2(n-3,1))$ and $EDS_{a,b}(P_2(\lceil \frac{n}{2} \rceil - 1, \lfloor \frac{n}{2} \rfloor - 1))$. We have

$$EDS_{a,b}(P_2(n-3,1)) = 3^a[(n-3)(2n-2)^b + (3n-6)^b] + 2^a[(2n-4)^b + n^b]$$

and

$$\begin{aligned}
&EDS_{a,b}\left(P_2\left(\left\lceil \frac{n}{2} \right\rceil - 1, \left\lfloor \frac{n}{2} \right\rfloor - 1\right)\right) \\
&= 3^a\left[\left(\left\lceil \frac{n}{2} \right\rceil - 1\right)\left(2n + \left\lfloor \frac{n}{2} \right\rfloor - 4\right)^b + \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right)\left(2n + \left\lceil \frac{n}{2} \right\rceil - 4\right)^b\right] \\
&\quad + 2^a\left[\left(n + \left\lfloor \frac{n}{2} \right\rfloor - 2\right)^b + \left(n + \left\lceil \frac{n}{2} \right\rceil - 2\right)^b\right].
\end{aligned}$$

Let us compare the $EDS_{a,b}$ indices of $P_l(n_1,n_2)$ and $P_{l+1}(n_1-1,n_2)$, which are trees having the same order, but different number of pendant vertices (and different diameter). Theorem 5.7 is used in the proof of Theorem 5.8.

Theorem 5.7. *Let $l \geq 2$, $n_1 \geq 2$ and $n_2 \geq 1$, where $n_1 \geq n_2$. Then for $a \geq 0$ and $b \geq 1$,*

$$EDS_{a,b}(P_l(n_1,n_2)) < EDS_{a,b}(P_{l+1}(n_1-1,n_2)).$$

Proof. In the tree $T_1 = P_l(n_1,n_2)$, let $u_1u_2\dots u_l$ be the path which does not contain pendant vertices of $P_l(n_1,n_2)$. We denote the pendant vertices adjacent to u_1 by $v_1,v_2,\dots,v_{n_1}$ and the pendant vertices adjacent to u_l by $v'_1,v'_2,\dots,v'_{n_2}$.

Let $V(T_2)=V(T_1)$ and $E(T_2)=\{v_1v_2,v_1v_3\dots v_1v_{n_1}\}\cup E(T_1)\setminus\{u_1v_2,u_1v_3\dots u_1v_{n_1}\}$. Note that T_2 is the tree $P_{l+1}(n_1-1,n_2)$. For any $v\in V(T_1)$, we obtain $ecc_{T_2}(v)\geq ecc_{T_1}(v)$. For any $v\in V(T_1)\setminus\{v_1\}$, we have $D_{T_2}(v)>D_{T_1}(v)$, thus for $a\geq 0$ and $b\geq 1$,

$$[ecc_{T_2}(v)]^a[D_{T_2}(v)]^b > [ecc_{T_1}(v)]^a[D_{T_1}(v)]^b.$$

For v_1, we get $D_{T_2}(v_1)=D_{T_1}(v_1)-n_1+1$.

We use v_1 and v'_1 to compare $EDS_{a,b}(T_1)$ and $EDS_{a,b}(T_2)$. For v'_1, we have $D_{T_2}(v'_1) = D_{T_1}(v'_1)+n_1-1$. Since $n_1\geq n_2$, we obtain $D_{T_1}(v'_1)\geq D_{T_1}(v_1)$. Note that

$$ecc_{T_1}(v_1)=ecc_{T_2}(v_1)=ecc_{T_1}(v'_1)=l+1 \ \text{ and } \ ecc_{T_2}(v'_1)=l+2.$$

We obtain

$$\begin{aligned}
&EDS_{a,b}(T_2)-EDS_{a,b}(T_1)\\
&> [ecc_{T_2}(v_1)]^a[D_{T_2}(v_1)]^b-[ecc_{T_1}(v_1)]^a[D_{T_1}(v_1)]^b\\
&\quad +[ecc_{T_2}(v'_1)]^a[D_{T_2}(v'_1)]^b-[ecc_{T_1}(v'_1)]^a[D_{T_1}(v'_1)]^b\\
&=(l+2)^a[D_{T_1}(v_1)-n_1+1]^b-(l+1)^a[D_{T_1}(v_1)]^b\\
&\quad +(l+1)^a[D_{T_1}(v'_1)+n_1-1]^b-(l+1)^a[D_{T_1}(v'_1)]^b\\
&>(l+1)^a([D_{T_1}(v_1)-n_1+1]^b-[D_{T_1}(v_1)]^b+[D_{T_1}(v'_1)+n_1-1]^b-[D_{T_1}(v'_1)]^b)\\
&\geq 0,
\end{aligned}$$

because for $b=1$,

$$[D_{T_1}(v_1)-n_1+1]^b-[D_{T_1}(v_1)]^b+[D_{T_1}(v'_1)+n_1-1]^b-[D_{T_1}(v'_1)]^b=0,$$

and for $b>1$, by Lemma 3.1,

$$[D_{T_1}(v'_1)+n_1-1]^b-[D_{T_1}(v'_1)]^b>[D_{T_1}(v_1)]^b-[D_{T_1}(v_1)-n_1+1]^b,$$

since $D_{T_1}(v'_1)\geq D_{T_1}(v_1)>D_{T_1}(v_1)-n_1+1$. Hence, $EDS_{a,b}(T_2)>EDS_{a,b}(T_1)$. □

Let us give first an upper bound on $EDS_{a,1}(T)$ for trees T with given order and domination number 2.

Theorem 5.8. *Let T be a tree of order $n \geq 6$ and domination number 2. Then for $a \geq 0$,*

$$EDS_{a,1}(T) \leq \left(2n^2 + 6\left\lfloor \frac{n^2}{4} \right\rfloor - 20n + 24\right) 5^a + (5n-8)4^a + (5n-12)3^a$$

with equality if and only if T is $P_4(\lceil \frac{n-4}{2} \rceil, \lfloor \frac{n-4}{2} \rfloor)$.

Proof. Any tree of order n and domination number 2 has the form $P_l(n_1, n_2)$, where $2 \leq l \leq 4$ and $l + n_1 + n_2 = n$. By Theorem 5.3, a tree with the largest $EDS_{a,1}$ index is $P_2(\lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor)$ or $P_3(\lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor)$ or $P_4(\lceil \frac{n-4}{2} \rceil, \lfloor \frac{n-4}{2} \rfloor)$. By Theorem 5.7,

$$\begin{aligned} EDS_{a,1}\left(P_2\left(\left\lceil \frac{n-2}{2} \right\rceil, \left\lfloor \frac{n-2}{2} \right\rfloor\right)\right) &< EDS_{a,1}\left(P_3\left(\left\lceil \frac{n-3}{2} \right\rceil, \left\lfloor \frac{n-3}{2} \right\rfloor\right)\right) \\ &< EDS_{a,1}\left(P_4\left(\left\lceil \frac{n-4}{2} \right\rceil, \left\lfloor \frac{n-4}{2} \right\rfloor\right)\right), \end{aligned}$$

thus $P_4(\lceil \frac{n-4}{2} \rceil, \lfloor \frac{n-4}{2} \rfloor) = P_4(\lceil \frac{n}{2} \rceil - 2, \lfloor \frac{n}{2} \rfloor - 2)$ is the tree with the largest $EDS_{a,1}$ index. We have

$$EDS_{a,1}\left(P_4\left(\left\lceil \frac{n}{2} \right\rceil - 2, \left\lfloor \frac{n}{2} \right\rfloor - 2\right)\right) = \left(2n^2 + 6\left\lfloor \frac{n^2}{4} \right\rfloor - 20n + 24\right) 5^a + (5n-8)4^a + (5n-12)3^a.$$

□

CHAPTER 6

RESULTS ON THE GENERAL ECCENTRIC DISTANCE SUM OF GRAPHS

In this chapter, we give bounds on $EDS_{a,b}$ for bipartite graphs with given order and matching number, lower bounds are obtained for $a \geq 0$ and $0 < b \leq 1$ and upper bounds are obtained for $a \leq 0$ and $b < 0$. Bounds for bipartite graphs hold also if the matching number is replaced by the independence number, vertex cover number or edge cover number. We present some bounds on the general eccentric distance sum for bipartite graphs with given order and diameter 3.

A lower bound on $EDS_{a,b}$ for graphs with given order and chromatic number, where each color is used for at least two vertices, is presented for $a \geq 0$ and $b \geq 1$. We present some bounds on the general eccentric distance sum for graphs with a given order and diameter 3 and for join of two graphs with given order and number of vertices of maximum possible degree. Finally, for $a \geq 0$, we present a lower bound on $EDS_{a,1}(G)$ for graphs G of given order and size containing no vertex adjacent to all the other vertices and a lower bound on $EDS_{a,1}(G) + EDS_{a,1}(\overline{G})$ for graphs G of given order. All the bounds are and extremal graphs are presented.

Any graph has the matching number ν at most $\lfloor \frac{n}{2} \rfloor$. The stars are the unique bipartite graphs with matching number 1. Thus, let us consider bipartite graphs for $2 \leq \nu \leq \lfloor \frac{n}{2} \rfloor$. For $a = b = 1$, Theorem 6.1 was presented in (Li et al., 2015). The proofs of Theorems 6.1, 6.2 and 6.4 use Lemma 3.2 which was proved in (Vetrík, 2021).

Theorem 6.1. *Let $a \geq 0$ and $0 < b \leq 1$. For a bipartite graph G of order n and matching number ν, where $2 \leq \nu \leq \lfloor \frac{n}{2} \rfloor$, we have*

$$EDS_{a,b}(G) \geq \nu 2^a (n + \nu - 2)^b + (n - \nu) 2^a (2n - \nu - 2)^b.$$

The equality holds if and only if G is $K_{\nu,n-\nu}$.

Proof. Among bipartite graphs of order n and matching number ν, let us denote a graph with the minimum $EDS_{a,b}$ by G'. Without loss of generality, suppose that $|U_1| \leq |U_2|$, where U_1 and U_2 are the partite sets of G'. Let us show by contradiction that G' is $K_{\nu,n-\nu}$.

Suppose that G' is not $K_{\nu,n-\nu}$. Clearly, $|U_1| \geq \nu$ (otherwise if $|U_1| \leq \nu - 1$, the matching number of G' is at most $\nu - 1$). Note that G' cannot be a subgraph of $K_{\nu,n-\nu}$, (if G' would be a subgraph of $K_{\nu,n-\nu}$, by Lemma 3.2, we get $EDS_{a,b}(G') > EDS_{a,b}(K_{\nu,n-\nu})$). Therefore $\nu < |U_1| \leq |U_2|$.

Let us denote any matching in G' having ν edges by M'. For $j=1,2$, let U_j^ν be the subset of U_j containing ν vertices incident with the edges in M'. We have $|U_j| = \nu + l_j$ with $l_j > 0$ (and $2\nu + l_1 + l_2 = n$). Obviously, a vertex $u_1 \in U_1 \setminus U_1^\nu$ is not adjacent to a vertex $u_2 \in U_2 \setminus U_2^\nu$, otherwise there would be the matching $M' \cup \{u_1u_2\}$ in G' with $\nu+1$ edges.

Let us define the graph H' having the same vertices as G', and containing all the edges between U_1^ν and U_2^ν, between U_1^ν and $U_2 \setminus U_2^\nu$ and between $U_1 \setminus U_1^\nu$ and U_2^ν. The graph G' is a subgraph of H', thus from Lemma 3.2, we obtain $EDS_{a,b}(H') < EDS_{a,b}(G')$. The matching number of H' is at least $\nu+1$.

Now we construct a graph H'' from H' by deleting all the edges between $U_1 \setminus U_1^\nu$ and U_2^ν, and by adding all the edges between $U_1 \setminus U_1^\nu$ and U_1^ν. The graph H'' is bipartite, having the matching number ν and H'' is a subgraph of $K_{\nu,n-\nu}$. Thus, by Lemma 3.2, we have $EDS_{a,b}(K_{\nu,n-\nu}) < EDS_{a,b}(H'')$.

Let us compare the $EDS_{a,b}$ of the graphs H' and H''. For any $u_1 \in U_1^\nu$ and any $u_2 \in U_2^\nu$, we have $ecc_{H'}(u_1) = ecc_{H''}(u_1) = ecc_{H'}(u_2) = ecc_{H''}(u_2) = 2$ and

$$\begin{aligned}
D_{H'}(u_1) &= \nu + l_2 + 2l_1 + 2(\nu-1) = 3\nu + 2l_1 + l_2 - 2,\\
D_{H''}(u_1) &= \nu + l_2 + l_1 + 2(\nu-1) = 3\nu + l_1 + l_2 - 2,\\
D_{H'}(u_2) &= \nu + l_1 + 2l_2 + 2(\nu-1) = 3\nu + l_1 + 2l_2 - 2,\\
D_{H''}(u_2) &= \nu + 2l_1 + 2l_2 + 2(\nu-1) = 3\nu + 2l_1 + 2l_2 - 2,
\end{aligned}$$

so

$$D_{H'}(u_1) = D_{H''}(u_1) + l_1,\ \ D_{H'}(u_2) = D_{H''}(u_1) + l_2 \ \text{ and } \ D_{H''}(u_2) = D_{H''}(u_1) + l_1 + l_2.$$

For $u_1' \in U_1 \setminus U_1^\nu$, we have $ecc_{H'}(u_1') = 3$ and $ecc_{H''}(u_1') = 2$ and

$$\begin{aligned}
D_{H'}(u_1') &= \nu + 2\nu + 3l_2 + 2(l_1-1) = 3\nu + 3l_2 + 2l_1 - 2,\\
D_{H''}(u_1') &= \nu + 2\nu + 2l_2 + 2(l_1-1) = 3\nu + 2l_2 + 2l_1 - 2.
\end{aligned}$$

For $u_2' \in U_2 \setminus U_2^\nu$, we have $ecc_{H'}(u_2') = 3$ and $ecc_{H''}(u_2') = 2$ and

$$\begin{aligned}
D_{H'}(u_2') &= \nu + 2\nu + 3l_1 + 2(l_2-1) = 3\nu + 3l_1 + 2l_2 - 2,\\
D_{H''}(u_2') &= \nu + 2\nu + 2l_1 + 2(l_2-1) = 3\nu + 2l_1 + 2l_2 - 2.
\end{aligned}$$

So, for $j = 1, 2$, we have $D_{H'}(u'_j) > D_{H''}(u'_j)$ and $ecc_{H'}(u'_j) > ecc_{H''}(u'_j)$, thus

$$[ecc_{H'}(u'_j)]^a [D_{H'}(u'_j)]^b > [ecc_{H''}(u'_j)]^a [D_{H''}(u'_j)]^b$$

for $a \geq 0$ and $b > 0$. Consequently,

$$\begin{aligned}
& EDS_{a,b}(H') - EDS_{a,b}(H'') \\
= & \sum_{u_1 \in U_1^\nu} ([ecc_{H'}(u_1)]^a [D_{H'}(u_1)]^b - [ecc_{H''}(u_1)]^a [D_{H''}(u_1)]^b) \\
& + \sum_{u_2 \in U_2^\nu} ([ecc_{H'}(u_2)]^a [D_{H'}(u_2)]^b - [ecc_{H''}(u_2)]^a [D_{H''}(u_2)]^b) \\
& + \sum_{u'_1 \in U_1 \setminus U_1^\nu} ([ecc_{H'}(u'_1)]^a [D_{H'}(u'_1)]^b - [ecc_{H''}(u'_1)]^a [D_{H''}(u'_1)]^b) \\
& + \sum_{u'_2 \in U_2 \setminus U_2^\nu} ([ecc_{H'}(u'_2)]^a [D_{H'}(u'_2)]^b - [ecc_{H''}(u'_2)]^a [D_{H''}(u'_2)]^b) \\
> & \sum_{u_1 \in U_1^\nu} ([ecc_{H'}(u_1)]^a [D_{H'}(u_1)]^b - [ecc_{H''}(u_1)]^a [D_{H''}(u_1)]^b) \\
& + \sum_{u_2 \in U_2^\nu} ([ecc_{H'}(u_2)]^a [D_{H'}(u_2)]^b - [ecc_{H''}(u_2)]^a [D_{H''}(u_2)]^b) \\
= & \nu 2^a ([D_{H''}(u_1) + l_1]^b - [D_{H''}(u_1)]^b + [D_{H''}(u_1) + l_2]^b - [D_{H''}(u_1) + l_1 + l_2]^b) \\
\geq & 0,
\end{aligned}$$

since

$$[D_{H''}(u_1) + l_1]^b - [D_{H''}(u_1)]^b + [D_{H''}(u_1) + l_2]^b - [D_{H''}(u_1) + l_1 + l_2]^b = 0$$

if $b = 1$ and by Lemma 3.1,

$$[D_{H''}(u_1) + l_1]^b - [D_{H''}(u_1)]^b > [D_{H''}(u_1) + l_1 + l_2]^b - [D_{H''}(u_1) + l_2]^b.$$

for $0 < b < 1$.

We obtain $EDS_{a,b}(H'') < EDS_{a,b}(H')$, so

$$EDS_{a,b}(K_{\nu,n-\nu}) < EDS_{a,b}(H'') < EDS_{a,b}(H') < EDS_{a,b}(G').$$

We have a contradiction.

Thus G' is $K_{\nu,n-\nu}$. For ν vertices of $K_{\nu,n-\nu}$, say v_i, $i = 1, 2, \ldots, \nu$, we have

$$D_{K_{\nu,n-\nu}}(v_i) = n - \nu + 2(\nu - 1) = n + \nu - 2,$$

and for the other $n-\nu$ vertices, say v'_j, $j=1,2,\dots,n-\nu$, we get

$$D_{K_{\nu,n-\nu}}(v_i) = \nu + 2(n-\nu-1) = 2n-\nu-2.$$

Since the eccentricity of every vertex is 2, we obtain

$$EDS_{a,b}(K_{\nu,n-\nu}) = \nu 2^a (n+\nu-2)^b + (n-\nu)2^a(2n-\nu-2)^b.$$

$\square$

Theorem 6.2. *Let $a \le 0$ and $b < 0$. For a bipartite graph G of order n and matching number ν, where $2 \le \nu \le \lfloor \frac{n}{2} \rfloor$, we have*

$$EDS_{a,b}(G) \le \nu 2^a (n+\nu-2)^b + (n-\nu)2^a(2n-\nu-2)^b.$$

The equality holds if and only if G is $K_{\nu,n-\nu}$.

Proof. Only those parts of the proof are presented which differ from the proof of Theorem 6.1.

Among bipartite graphs of order n and matching number ν, let us denote a graph with the maximum $EDS_{a,b}$ by G'.

The graph G' is a subgraph of H', thus from Lemma 3.2, we obtain $EDS_{a,b}(H') > EDS_{a,b}(G')$. Similarly, by Lemma 3.2, we have $EDS_{a,b}(K_{\nu,n-\nu}) > EDS_{a,b}(H'')$.

For $j=1,2$, we have $D_{H'}(u'_j) > D_{H''}(u'_j)$ and $ecc_{H'}(u'_j) > ecc_{H''}(u'_j)$, thus for $a \le 0$ and $b<0$, we obtain $[ecc_{H'}(u'_j)]^a \le [ecc_{H''}(u'_j)]^a$ and $[D_{H'}(u'_j)]^b < [D_{H''}(u'_j)]^b$. Then

$$[ecc_{H'}(u'_j)]^a [D_{H'}(u'_j)]^b < [ecc_{H''}(u'_j)]^a [D_{H''}(u'_j)]^b$$

Consequently,

$$\begin{aligned}
& EDS_{a,b}(H') - EDS_{a,b}(H'') \\
< & \sum_{u_1 \in U_1^\nu} ([ecc_{H'}(u_1)]^a [D_{H'}(u_1)]^b - [ecc_{H''}(u_1)]^a [D_{H''}(u_1)]^b) \\
& + \sum_{u_2 \in U_2^\nu} ([ecc_{H'}(u_2)]^a [D_{H'}(u_2)]^b - [ecc_{H''}(u_2)]^a [D_{H''}(u_2)]^b) \\
= & \nu 2^a ([D_{H''}(u_1)+l_1]^b - [D_{H''}(u_1)]^b + [D_{H''}(u_1)+l_2]^b - [D_{H''}(u_1)+l_1+l_2]^b) \\
< & 0,
\end{aligned}$$

since by Lemma 3.1,

$$[D_{H''}(u_1)+l_1]^b - [D_{H''}(u_1)]^b < [D_{H''}(u_1)+l_1+l_2]^b - [D_{H''}(u_1)+l_2]^b.$$

for $b<0$.

We obtain $EDS_{a,b}(H'') > EDS_{a,b}(H')$, so

$$EDS_{a,b}(K_{\nu,n-\nu}) > EDS_{a,b}(H'') > EDS_{a,b}(H') > EDS_{a,b}(G').$$

□

Let us denote the independence number, vertex cover number and edge cover number by α, β and β', respectively. It is known that for a graph G of order n,

$$\alpha+\beta=n.$$

If G has no isolated vertices, then

$$\nu+\beta'=n.$$

If G is bipartite with no isolated vertices,

$$\alpha=\beta', \text{ thus } \nu=\beta;$$

see (West, 2001). So, from Theorems 6.1 and 6.2, we obtain the following corollary.

Corollary 6.1. *For a bipartite graph of order n and vertex cover number β, where $2\le\beta\le\lfloor\frac{n}{2}\rfloor$, we have*

$$EDS_{a,b}(G) \ge \beta 2^a(n+\beta-2)^b + (n-\beta)2^a(2n-\beta-2)^b$$

if $a\ge 0$ and $0<b\le 1$ and

$$EDS_{a,b}(G) \le \beta 2^a(n+\beta-2)^b + (n-\beta)2^a(2n-\beta-2)^b$$

if $a\le 0$ and $b<0$. The equalities hold if and only if G is $K_{\beta,n-\beta}$.

In Theorems 6.1 and 6.2, $2\le\nu\le\lfloor\frac{n}{2}\rfloor$, thus

$$\left\lceil\frac{n}{2}\right\rceil \le \beta' \le n-2.$$

Since $\nu+\beta'=n$, Theorem 6.1 says that if $a\ge 0$ and $0<b\le 1$, then for a bipartite graph G of

order n and matching number $n-\beta'$, we get

$$EDS_{a,b}(G) \geq (n-\beta')2^a(2n-\beta'-2)^b + \beta' 2^a(n+\beta'-2)^b.$$

Similarly, an upper bound can be obtained for $a \leq 0$ and $b < 0$. Thus, we obtain Corollary 6.2.

Corollary 6.2. *For a bipartite graph G of order n and edge cover number/independence number β', where $\lceil \frac{n}{2} \rceil \leq \beta' \leq n-2$, we have*

$$EDS_{a,b}(G) \geq \beta' 2^a(n+\beta'-2)^b + (n-\beta')2^a(2n-\beta'-2)^b$$

if $a \geq 0$ and $0 < b \leq 1$ and

$$EDS_{a,b}(G) \leq \beta' 2^a(n+\beta'-2)^b + (n-\beta')2^a(2n-\beta'-2)^b$$

if $a \leq 0$ and $b < 0$. The equalities hold if and only if G is $K_{\beta',n-\beta'}$.

Lemma 3.1 is used in the proofs of Theorem 6.3. A lower bound on $EDS_{a,b}(G)$ for bipartite graphs G is given in Theorem 6.3.

Theorem 6.3. *Let G be a bipartite graph G of order $n \geq 4$ and diameter 3. Then for $a \geq 0$ and $b \geq 1$, we have*

$$\begin{aligned} EDS_{a,b}(G) \geq\ & 3^a\left[\left(n+\left\lceil\frac{n}{2}\right\rceil\right)^b + \left(n+\left\lfloor\frac{n}{2}\right\rfloor\right)^b\right] \\ & + 2^a\left[\left(\left\lceil\frac{n}{2}\right\rceil - 1\right)\left(n+\left\lceil\frac{n}{2}\right\rceil-2\right)^b + \left(\left\lfloor\frac{n}{2}\right\rfloor - 1\right)\left(n+\left\lfloor\frac{n}{2}\right\rfloor-2\right)^b\right] \end{aligned}$$

with equality if and only if G is $K_1 + \overline{K_{\lceil \frac{n}{2} \rceil - 1}} + \overline{K_{\lfloor \frac{n}{2} \rfloor - 1}} + K_1$.

Proof. Suppose that G' is a graph of order n and diameter 3 with the minimum $EDS_{a,b}$ index. Let u_0 and u_3 be any two vertices of distance 3 in G'. For $i = 0,1,2,3$, let $U_i = \{v \in V(G') : d_{G'}(u_0,u) = i\}$. Then $V(G') = U_0 \cup U_1 \cup U_2 \cup U_3$, where $U_0 = \{u_0\}$. The graph $G'[U_i]$ must be empty, otherwise G' would have some cycle of odd length. According to Lemma 3.2, adding an edge will decrease $EDS_{a,b}$. Thus, $G'[U_{i-1} \cup U_i]$ is a complete bipartite graph for $i = 1,2,3$. Note that $|U_3| = 1$ (otherwise, if $|U_3| \geq 2$, we can add the edge u_0u_3 to G' to obtain G'' $EDS_{a,b}(G'') < EDS_{a,b}(G')$, by Lemma 3.2). So, G' has the form $K_1 + \overline{K_{n_1}} + \overline{K_{n_2}} + K_1$, where $n_1 + n_2 = n-2$.

Without loss of generality, assume that $|U_1| \geq |U_2|$. We prove that $|U_1| - |U_2| \leq 1$. Suppose to the contrary that $|U_1| - |U_2| \geq 2$. We choose $w \in U_1$. Let G''' has the same vertex set as

G' while $E(G''') = \{wu : u \in U_1 \cup \{u_3\}\} \cup E(G') \setminus \{wu : u \in \{u_0\} \cup U_2\}$. So, G''' is the graph $K_1 + \overline{K_{n_1-1}} + \overline{K_{n_2+1}} + K_1$.

For all $u \in V(G')$, we get $ecc_{G'''}(u) = ecc_{G'}(u)$. We have

$$D_{G'}(w) = 2|U_1| + |U_2| + 1 \text{ and } D_{G'''}(w) = |U_1| + 2|U_2| + 2.$$

Since $|U_1| - |U_2| \geq 2$, we obtain $D_{G'}(w) - D_{G'''}(w) > 0$. Thus

$$[ecc_{G'}(w)]^a [D_{G'}(w)]^b - [ecc_{G'''}(w)]^a [D_{G'''}(w)]^b > 0.$$

We obtain

$$\begin{aligned}
D_{G'}(u_0) &= |U_1| + 2|U_2| + 1, & D_{G'''}(u_0) &= |U_1| + 2|U_2| + 2, \\
D_{G'}(u_3) &= 2|U_1| + |U_2| + 1, & D_{G'''}(u_3) &= 2|U_1| + |U_2|, \\
D_{G'}(u) &= 2|U_1| + |U_2| + 1, & D_{G'''}(u) &= 2|U_1| + |U_2|, \\
D_{G'}(v) &= |U_1| + 2|U_2| + 1, & D_{G'''}(v) &= |U_1| + 2|U_2| + 2,
\end{aligned}$$

where $u \in U_1 \setminus \{w\}$ and $v \in U_2$.

Note that

$$ecc_{G'}(u) = ecc_{G'}(v) = 2 \text{ and } ecc_{G'}(u_0) = ecc_{G'}(u_3) = 3.$$

Then

$$\begin{aligned}
&EDS_{a,b}(G') - EDS_{a,b}(G''') \\
&= [ecc_{G'}(u_0)]^a([D_{G'}(u_0)]^b - [D_{G'''}(u_0)]^b) + [ecc_{G'}(u_3)]^a([D_{G'}(u_3)]^b - [D_{G'''}(u_3)]^b) \\
&\quad + \sum_{v \in U_2} [ecc_{G'}(v)]^a([D_{G'}(v)]^b - [D_{G'''}(v)]^b) + \sum_{u \in U_1 \setminus \{w\}} [ecc_{G'}(u)]^a([D_{G'}(u)]^b - [D_{G'''}(u)]^b) \\
&\quad + [ecc_{G'}(w)]^a([D_{G'}(w)]^b - [D_{G'''}(w)]^b) \\
&> 3^a([D_{G'}(u_0)]^b - [D_{G'}(u_0) + 1]^b + [D_{G'}(u_3)]^b - [D_{G'}(u_3) - 1]^b) \\
&\quad + 2^a \left[|U_2|([D_{G'}(v)]^b - [D_{G'}(v) + 1]^b) + (|U_1| - 1)([D_{G'}(u)]^b - [D_{G'}(u) - 1]^b) \right] \\
&> 3^a([D_{G'}(u_0)]^b - [D_{G'}(u_0) + 1]^b + [D_{G'}(u_3)]^b - [D_{G'}(u_3) - 1]^b) \\
&\quad + |U_2| 2^a([D_{G'}(v)]^b - [D_{G'}(v) + 1]^b + [D_{G'}(u)]^b - [D_{G'}(u) - 1]^b) \\
&\geq 0,
\end{aligned}$$

because for $b = 1$,

$$[D_{G'}(u_0)]^b - [D_{G'}(u_0)+1]^b + [D_{G'}(u_3)]^b - [D_{G'}(u_3)-1]^b = 0$$

and

$$[D_{G'}(v)]^b - [D_{G'}(v)+1]^b + [D_{G'}(u)]^b - [D_{G'}(u)-1]^b = 0,$$

and for $b > 1$, by Lemma 3.1,

$$[D_{G'}(u_3)]^b - [D_{G'}(u_3)-1]^b > [D_{G'}(u_0)+1]^b - [D_{G'}(u_0)]^b$$

and

$$[D_{G'}(u)]^b - [D_{G'}(u)-1]^b > [D_{G'}(v)+1]^b - [D_{G'}(v)]^b,$$

since $D_{G'}(u_3) > D_{G'}(u_0)+1$ and $D_{G'}(u) > D_{G'}(v)+1$.

Thus $EDS_{a,b}(G') > EDS_{a,b}(G''')$ for $a \geq 0$ and $b \geq 1$, a contradiction. So, $|U_1| - |U_2| \leq 1$. Hence G' is $K_1 + \overline{K_{\lceil \frac{n}{2} \rceil - 1}} + \overline{K_{\lfloor \frac{n}{2} \rfloor - 1}} + K_1$ and

$$\begin{aligned} EDS_{a,b}(G') = 3^a &\left[\left(n + \left\lceil \frac{n}{2} \right\rceil\right)^b + \left(n + \left\lfloor \frac{n}{2} \right\rfloor\right)^b \right] \\ &+ 2^a \left[\left(\left\lceil \frac{n}{2} \right\rceil - 1\right)\left(n + \left\lceil \frac{n}{2} \right\rceil - 2\right)^b + \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right)\left(n + \left\lfloor \frac{n}{2} \right\rfloor - 2\right)^b \right], \end{aligned}$$

□

The smallest number of colors needed to color the vertices of a graph G such that no two adjacent vertices have the same color is the chromatic number of G. Clearly, any nonempty graph has chromatic number at least 2. Graphs with a given order and chromatic number are investigated in Theorem 6.4. For $a = b = 1$, Theorem 6.4 was presented in (Ilić et al., 2011).

Theorem 6.4. *Let $a \geq 0$ and $b \geq 1$. For any graph G with n vertices and chromatic number χ, where each of the χ colors is used for at least two vertices, we have*

$$EDS_{a,b}(G) \geq EDS_{a,b}(K_{p_1,p_2,\ldots,p_\chi}).$$

The equality holds if only if G is $K_{p_1,p_2,\ldots,p_\chi}$, where $|p_j - p_l| \leq 1$ for any $1 \leq j < l \leq \chi$.

Proof. For the considered set of graphs, let us denote a graph with the minimum $EDS_{a,b}$ by G'. Since the graph G' does not contain edges between vertices colored by the same color, G' is a χ-partite graph. Each of the χ colors is used for at least two vertices, thus each partite set contains at least two vertices. By Lemma 3.2, any two vertices from different partite sets are adjacent, therefore G' is $K_{p_1,p_2,\ldots,p_\chi}$, where $p_j \geq 2$, $j = 1,2,\ldots,\chi$. Let us show that $|p_j - p_l| \leq 1$ for any $1 \leq j < l \leq \chi$.

Suppose to the contrary that there exist j and l, where $1 \leq j < l \leq \chi$, such that $|p_j - p_l| \geq 2$. We can suppose that $p_1 \geq p_2 + 2$. We compare $EDS_{a,b}(G')$ and $EDS_{a,b}(G'')$, where $G' = K_{p_1,p_2,\ldots,p_\chi}$ and $G'' = K_{p_1-1,p_2+1,\ldots,p_\chi}$. Every vertex in G' and G'' has eccentricity 2. For any u_1' from the first partite set and u_2' from the second partite set of G', we have

$$D_{G'}(u_1') = (n-p_1)+2(p_1-1) = n+p_1-2 \text{ and } D_{G'}(u_2') = (n-p_2)+2(p_2-1) = n+p_2-2.$$

For any u_1'' from the first partite set and u_2'' from the second partite set of G'', we get

$$D_{G''}(u_1'') = [n-(p_1-1)]+2(p_1-2) = n+p_1-3 \text{ and } D_{G''}(u_2'') = [n-(p_2+1)]+2p_2 = n+p_2-1.$$

For any other vertex x, we get $D_{G'}(x) = D_{G''}(x)$. Since $p_1 - 1 \geq p_2 + 1$, we obtain

$$\begin{aligned}
& EDS_{a,b}(G') - EDS_{a,b}(G'') \\
= \;& p_1 2^a (n+p_1-2)^b + p_2 2^a (n+p_2-2)^b - (p_1-1)2^a(n+p_1-3)^b \\
& -(p_2+1)2^a(n+p_2-1)^b \\
= \;& (p_1-1)2^a[(n+p_1-2)^b - (n+p_1-3)^b] - (p_2+1)2^a[(n+p_2-1)^b - (n+p_2-2)^b] \\
& +2^a(n+p_1-2)^b - 2^a(n+p_2-2)^b \\
> \;& (p_1-1)2^a[(n+p_1-2)^b - (n+p_1-3)^b] - (p_2+1)2^a[(n+p_2-1)^b - (n+p_2-2)^b] \\
\geq \;& (p_2+1)2^a[(n+p_1-2)^b - (n+p_1-3)^b + (n+p_2-2)^b - (n+p_2-1)^b]
\end{aligned}$$

which equals 0 if $b = 1$, and it is positive for $b > 1$, because from Lemma 3.1,

$$(n+p_1-2)^b - (n+p_1-3)^b > (n+p_2-1)^b - (n+p_2-2)^b.$$

Therefore $EDS_{a,b}(G') - EDS_{a,b}(G'') > 0$ and $EDS_{a,b}(G') > EDS_{a,b}(G'')$. We have a contradiction. Thus $|p_j - p_l| \leq 1$ for any $1 \leq j < l \leq \chi$, hence G' is $K_{p_1,p_2,\ldots,p_\chi}$. □

Recall that the join $G_1 + G_2$ of two graphs G_1 and G_2 has the vertex set $V(G_1+G_2) = V(G_1) \cup V(G_2)$ and the edge set $E(G_1+G_2) = E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1), v \in V(G_2)\}$. Let us present bounds on $EDS_{a,b}(G_1+G_2)$ for the join of two graphs.

Theorem 6.5. *For $i = 1,2$, let G_i be a graph of order n_i with k_i vertices of degree $n_i - 1$. Let*

$a,b \in \mathbb{R}$. Then for $b > 0$,

$$EDS_{a,b}(G_1+G_2) \geq (k_1+k_2)(n_1+n_2-1)^b + (n_1+n_2-k_1-k_2)2^a(n_1+n_2)^b,$$

and for $b < 0$,

$$EDS_{a,b}(G_1+G_2) \leq (k_1+k_2)(n_1+n_2-1)^b + (n_1+n_2-k_1-k_2)2^a(n_1+n_2)^b.$$

The equalities hold if and only if G_i contains $n_i - k_i$ vertices of degree $n_i - 2$, where $n_i - k_i$ is even; $i = 1,2$.

Proof. For $i = 1,2$, let us denote the set of vertices of degree $n_i - 1$ in $V(G_i)$ by S_i. We have $|V(G_i)| = n_i$ and $|S_i| = k_i$. Then $ecc_{G_1+G_2}(v) = 1$ and $D_{G_1+G_2}(v) = n_1+n_2-1$ for $v \in S_1 \cup S_2$. For $v \in (V(G_1)\setminus S_1) \cup (V(G_2)\setminus S_2)$, we get $ecc_{G_1+G_2}(v) = 2$. For $v_1 \in V(G_1)\setminus S_1$, we have

$$D_{G_1+G_2}(v_1) = n_2 + deg_{G_1}(v_1) + 2[n_1 - 1 - deg_{G_1}(v_1)] = n_2 + 2n_1 - 2 - deg_{G_1}(v_1) \geq n_1 + n_2,$$

since $deg_{G_1}(v_1) \leq n_1 - 2$. Similarly, $D_{G_1+G_2}(v_2) \geq n_1 + n_2$ for $v_2 \in V(G_2)\setminus S_2$. Thus, for $i = 1,2$, we obtain

$$[D_{G_1+G_2}(v_i)]^b \geq (n_1+n_2)^b$$

if $b > 0$ and

$$[D_{G_1+G_2}(v_i)]^b \leq (n_1+n_2)^b$$

if $b < 0$. Consequently, for $b > 0$,

$$\begin{aligned} EDS_{a,b}(G_1+G_2) \geq\ & k_1(n_1+n_2-1)^b + k_2(n_1+n_2-1)^b \\ & + (n_1-k_1)2^a(n_1+n_2)^b + (n_2-k_2)2^a(n_1+n_2)^b, \end{aligned}$$

and for $b < 0$,

$$\begin{aligned} EDS_{a,b}(G_1+G_2) \leq\ & k_1(n_1+n_2-1)^b + k_2(n_1+n_2-1)^b \\ & + (n_1-k_1)2^a(n_1+n_2)^b + (n_2-k_2)2^a(n_1+n_2)^b. \end{aligned}$$

The equalities are achieved when $deg_{G_i}(v_i) = n_i - 2$ for every $v_i \in V(G_i)\setminus S_i$, where $i = 1,2$. Note that $n_i - k_i$ must be even, since for a graph with k_i vertices of degree $n_i - 1$ and $n_i - k_i$

vertices of degree $n_i - 2$, from Handshaking lemma, we have

$$2|E(G_i)| = \sum_{v \in V(G_i)} deg_{G_i}(v) = k_i(n_i - 1) + (n_i - k_i)(n_i - 2) = n_i(n_i - 1) - (n_i - k_i).$$

$\square$

Lemma 3.2 is used in the proofs of Theorems 6.6, 6.7 and 6.8. Now, we focus on graphs of diameter 3 and 4. In Theorems 6.6 and 6.7, we give bounds on $EDS_{a,b}(G)$ for graphs G where as in Theorems 6.8 , we give bounds on $EDS_{a,1}(G)$ for graphs G of diameter 4. In Theorems 6.8, 6.9 and 6.10, we give bounds on $EDS_{a,b}(G)$ when $b = 1$.

Theorem 6.6. *Let G be a graph of order $n \geq 4$ and diameter 3. Then for $a \geq 0$ and $0 < b < 1$, we have*

$$EDS_{a,b}(G) \geq 3^a[(n+2)^b + (2n-2)^b] + 2^a(n-2)n^b$$

with equality if and only if G is $K_1 + K_{n-3} + K_1 + K_1$.

Proof. Suppose that G' is a graph of order n and diameter 3 with the minimum $EDS_{a,b}$ index. Let u_0 and u_3 be any two vertices of distance 3 in G'. For $i = 0, 1, 2, 3$, let $U_i = \{v \in V(G') : d_{G'}(u_0, u) = i\}$. Then $V(G') = U_0 \cup U_1 \cup U_2 \cup U_3$. According to Lemma 3.2, adding an edge will decrease $EDS_{a,b}$. Thus, $G'[U_{i-1} \cup U_i]$ is a complete graph for $i = 1, 2, 3$. Note that $|U_3| = 1$ (otherwise, if $|U_3| \geq 2$, we can add edges to G' to obtain G'' with $E(G'') = E(G') \cup \{uu_3 : u \in U_1\}$ and by Lemma 3.2, $EDS_{a,b}(G'') < EDS_{a,b}(G')$). So, G' has the form $G_p = K_1 + K_{n-p-2} + K_p + K_1$ where $1 \leq p \leq \lfloor \frac{n}{2} \rfloor - 1$. We have

$$ecc_{G_p}(u_0) = ecc_{G_p}(u_3) = 3, \;\; D_{G_p}(u_0) = n + p + 1 \;\text{ and }\; D_{G_p}(u_3) = 2n - p - 1.$$

For all $u \in V(G_p) \setminus \{u_0, u_3\}$, we have $ecc_{G_p}(u) = 2$ and $D_{G_p}(u) = n$. Thus

$$EDS_{a,b}(G_p) = 3^a[(n+p+1)^b + (2n-p-1)^b] + 2^a(n-2)n^b = f(p).$$

Then the derivative

$$f'(p) = 3^a b[(n+p+1)^{b-1} - (2n-p-1)^{b-1}].$$

Since $0 < b < 1$, we have $f'(p) > 0$ for $1 \leq p < \lfloor \frac{n}{2} \rfloor - 1$ and $f'(p) = 0$ for $p = \lfloor \frac{n}{2} \rfloor - 1$. Thus, $f(p)$ is increasing for $1 \leq p \leq \lfloor \frac{n}{2} \rfloor - 1$ and $0 < b < 1$. So, $EDS_{a,b}(G_1) < EDS_{a,b}(G_p)$, where

$2 \le p \le \lfloor \frac{n}{2} \rfloor - 1$. Hence G' is $K_1 + K_{n-3} + K_1 + K_1$ and

$$EDS_{a,b}(K_1 + K_{n-3} + K_1 + K_1) = 3^a[(n+2)^b + (2n-2)^b] + 2^a(n-2)n^b.$$

□

Theorem 6.7. *Let G be a graph of order $n \ge 4$ and diameter 3. Then for $a \le 0$ and $b < 0$, we have*

$$EDS_{a,b}(G) \le 3^a[(n+2)^b + (2n-2)^b] + 2^a(n-2)n^b$$

with equality if and only if G is $K_1 + K_{n-3} + K_1 + K_1$.

Proof. We present only those parts which are different from the proof of Theorem 6.6. Suppose that G' is a graph of order n and diameter 3 with the maximum $EDS_{a,b}$ index. According to Lemma 3.2, adding an edge will increase $EDS_{a,b}$. Thus $G'[U_{i-1} \cup U_i]$ is a complete graph for $i = 1,2,3$. Note that $|U_3| = 1$ (otherwise, if $|U_3| \ge 2$, we can add edges to G' to obtain G'' with $E(G'') = E(G') \cup \{uu_3 : u \in U_1\}$ and by Lemma 3.2, $EDS_{a,b}(G'') > EDS_{a,b}(G')$). So, G' has the form $G_p = K_1 + K_{n-p-2} + K_p + K_1$ where $1 \le p \le \lfloor \frac{n}{2} \rfloor - 1$. Since $b < 0$, we have $f'(p) < 0$ for $1 \le p < \lfloor \frac{n}{2} \rfloor - 1$ and $f'(p) = 0$ for $p = \lfloor \frac{n}{2} \rfloor - 1$. Thus, $f(p)$ is decreasing for $1 \le p \le \lfloor \frac{n}{2} \rfloor - 1$ and $b < 0$. So, $EDS_{a,b}(G_1) > EDS_{a,b}(G_p)$, where $2 \le p \le \lfloor \frac{n}{2} \rfloor - 1$. Hence G' is $K_1 + K_{n-3} + K_1 + K_1$. □

Theorem 6.8. *Let G be an order n graph with diameter 4. Then for $a \ge 0$,*

$$EDS_{a,1}(G) \ge n\left(4^{a+1} + 2 \cdot 3^a - 3 \cdot 2^a\right) + n^2 \cdot 2^a + 4 \cdot (3^a - 2^a)$$

with equality holds if and only if G is $K_1 + K_1 + K_{n-4} + K_1 + K_1$.

Proof. Suppose G' is a graph of order n and diameter 4 with the minimum $EDS_{a,1}$. Let u_0 and u_4 be any two vertices of distance 4 in G'. For $i = 0,1,2,3,4$, let $U_i = \{v \in V(G') : d_{G'}(u_0,u) = i\}$. Then $V(G') = U_0 \cup U_1 \cup U_2 \cup U_3 \cup U_4$, where $U_0 = \{u_0\}$. According to Lemma 3.2, adding an edge will decrease $EDS_{a,1}$. Thus, $G'[U_{i-1} \cup U_i]$ is a complete graph for $i = 1,2,3,4$. Note that $|U_4| = 1$ (otherwise, if $|U_4| \ge 2$, we can add edges to G' to obtain G'' with the graph transformation $G'' = G' + \{ux : x \in U_2\}$, and by Lemma 3.2, $EDS_{a,1}(G'') < EDS_{a,1}(G')$). So, G' has the vertex set $V(G') = \{u_0\} \cup U_1 \cup U_2 \cup U_3 \cup \{u_4\}$. Next, we show first $|U_1| = 1$ and then, $|U_3| = 1$.

Claim 6.8.1. $|U_1| = 1$.

Contrary assume that $|U_1| \geq 2$ and choose $u \in U_1 \setminus \{u_1\}$. By the graph transformation, $G'' = G' - uu_0 + \{ux : x \in U_3\}$. Then $\{u_0\} \cup (U_1 \setminus \{u\}) \cup (U_2 \cup \{u\}) \cup U_3 \cup \{u_4\}$ is a partition of $V(G'')$. From the transformation of G'' from G', we have $ecc_{G'}(v) = ecc_{G''}(v)$ for all $v \in V(G') \setminus \{u\}$. $ecc_{G'}(u) = 3 > ecc_{G''}(u) = 2$ and $D_{G'}(u) = D_{G''}(u) + |U_3|$. That is, $D_{G'}(u) > D_{G''}(u)$.

Thus

$$(ecc_{G'}(u))^a(D_{G'}(u)) > (ecc_{G''}(u))^a(D_{G''}(u)).$$

For all $v \in (U_1 \setminus \{u\}) \cup U_2$, we have $D_{G'}(v) = D_{G''}(v)$. Thus

$$(ecc_{G'}(v))^a(D_{G'}(v)) - (ecc_{G''}(v))^a(D_{G'}(v)) = 0.$$

For $v \in U_3 \cup U_4$, we have $D_{G'}(v) = D_{G''}(v) + 1$. That is, $D_{G'}(v) > D_{G''}(v)$. Thus

$$(ecc_{G'}(v))^a(D_{G'}(v)) > (ecc_{G''}(v))^a(D_{G'}(v)).$$

So, consider vertices u_0 and u_4 such that $ecc_{G'}(u_i) = ecc_{G''}(u_i) = 4$ for $i = 0, 4$, and

$$\begin{aligned} D_{G'}(u_0) &= |U_1| + 2|U_2| + 3|U_3| + 4, & D_{G''}(u_0) &= |U_1| + 2|U_2| + 3|U_3| + 5, \\ D_{G'}(u_4) &= 3|U_1| + 2|U_2| + |U_3| + 4, & D_{G''}(u_4) &= 3|U_1| + 2|U_2| + |U_3| + 3. \end{aligned}$$

Then $D_{G'}(u_4) - D_{G''}(u_4) = -1$ and $D_{G'}(u_0) - D_{G''}(u_0) = 1$. Henceforth

$$\begin{aligned} & EDS_{a,b}(G') - EDS_{a,b}(G'') \\ > \; & (ecc_{G'}(u_0))^a \left[D_{G'}(u_0) - D_{G''}(u_0)\right] + (ecc_{G'}(u_4))^a \left[D_{G'}(u_4) - D_{G''}(u_4)\right] \\ = \; & 4^a \left[D_{G'}(u_0) - D_{G''}(u_0) + D_{G'}(u_4) - D_{G''}(u_4)\right] = 0, \end{aligned}$$

because $D_{G'}(u_0) - D_{G''}(u_0) + D_{G'}(u_4) - D_{G''}(u_4) = 0$. Thus,

$EDS_{a,1}(G') > EDS_{a,1}(G'')$ for $a \geq 0$, a contradiction. Hence, $|U_1| = 1$.

Claim 6.8.2. $|U_3| = 1$ *and* $|U_2| = n - 4$.

Contrary assume that $|U_1| \geq 2$ and choose $w \in U_3 \setminus \{u_3\}$. Define a graph transformation as, $G''' = G' - wu_4 + wu_1$. Then $\{u_0\} \cup \{u_1\} \cup (U_2 \cup \{w\}) \cup (U_3 \setminus \{w\}) \cup \{u_4\}$ is a partition of $V(G''')$. From the transformation of G''' from G', we have $ecc_{G'}(v) = ecc_{G'''}(v)$ for all $v \in V(G') \setminus \{w\}$.

$D_{G'}(u_1) = D_{G''}(u_1) + 1$ i.e. $D_{G'}(u_1) > D_{G''}(u_1)$. Thus

$$(ecc_{G'}(u_1))^a(D_{G'}(u_1)) > (ecc_{G''}(u_1))^a(D_{G''}(u_1)).$$

But $ecc_{G'}(w) = 3 > ecc_{G''}(w) = 2$ and $D_{G'}(w) = D_{G''}(w)+1$, that is, we have $D_{G'}(w) > D_{G'''}(w)$. Thus

$$(ecc_{G'}(w))^a(D_{G'}(w)) > (ecc_{G'''}(w))^a(D_{G'''}(w)).$$

For all $v \in U_2 \cup (U_3 \setminus \{w\})$, we have $D_{G'}(v) = D_{G'''}(v)$. and

$$(ecc_{G'}(v))^a(D_{G'}(v)) - (ecc_{G'''}(v))^a(D_{G'''}(v)) = 0.$$

So, consider vertices u_0 and u_4 such that $ecc_{G'}(u_i) = ecc_{G'''}(u_i) = 4$ for $i = 0,4$, and

$$\begin{aligned} D_{G'}(u_0) &= |U_1|+2|U_2|+3|U_3|+4, & D_{G'''}(u_0) &= |U_1|+2|U_2|+3|U_3|+5,\\ D_{G'}(u_4) &= 3|U_1|+2|U_2|+|U_3|+4, & D_{G'''}(u_3) &= 3|U_1|+2|U_2|+|U_3|+3. \end{aligned}$$

Then $D_{G'}(u_4) - D_{G'''}(u_4) = -1$ and $D_{G'}(u_0) - D_{G'''}(u_0) = 1$. Henceforth

$$\begin{aligned} & EDS_{a,1}(G') - EDS_{a,1}(G''') \\ > \;& (ecc_{G'}(u_0))^a\left[(D_{G'}(u_0)) - (D_{G'''}(u_0))\right] + (ecc_{G'}(u_4))^a\left[(D_{G'}(u_4)) - (D_{G'''}(u_4))\right] \\ = \;& 4^a\left[D_{G'}(u_0) - D_{G'''}(u_0) + D_{G'}(u_4) - D_{G'''}(u_4)\right] = 0, \end{aligned}$$

because $D_{G'}(u_0) - D_{G'''}(u_0) + D_{G'}(u_4) - D_{G'''}(u_4) = 0$. Thus,

$EDS_{a,1}(G') > EDS_{a,1}(G''')$ for $a \geq 0$, a contradiction. Hence, $|U_3| = 1$ and since $|G'| = n$, we have $|U_2| = n-4$. So, G' has the form $K_1+K_1+K_{n-4}+K_1+K_1$ and

$$EDS_{a,1}(K_1+K_1+K_{n-4}+K_1+K_1) = n\left(4^{a+1}+2\cdot 3^a - 3\cdot 2^a\right) + n^2\cdot 2^a + 4\cdot(3^a-2^a).$$

□

Theorem 6.9. *Let $a \geq 0$. For any graph G of order n and size m not containing a vertex of degree $n-1$,*

$$EDS_{a,1}(G) \geq [n(n-1)-m]2^{a+1}$$

with equality if and only if the diameter of G is 2.

Proof. Since no vertex of G is adjacent to all the other vertices, we have $ecc_G(u) \geq 2$ for every $u \in V(G)$. Thus

$$[ecc_G(u)]^a \geq 2^a.$$

For every $u \in V(G)$,

$$D_G(u) \geq deg_G(u) + 2[n-1-deg_G(u)] = 2(n-1) - deg_G(u)$$

since the distance between u and any of the $n-1-deg_G(u)$ vertices not adjacent to u is at least 2. Since $\sum_{u\in V(G)} deg_G(u) = 2m$, we obtain

$$EDS_{a,1}(G) \geq \sum_{u\in V(G)} 2^a[2(n-1) - deg_G(u)] = 2^{a+1}[n(n-1) - m]$$

with equality if and only if the diameter of G is 2. □

For any graph G, we have

$$n-1 \leq m \leq \binom{n}{2} = \frac{n(n-1)}{2}.$$

We show that there exist graphs with a small size (size close to $n-1$) as well as for some graphs with a large size (size close to $\frac{n(n-1)}{2}$) which attain the bound presented in Theorem 6.9.

Note that C_n is the cycle of order n and $\frac{n}{2}K_2$ is the set of $\frac{n}{2}$ independent edges. The graphs $K_{c,n-c}$ for $2 \leq c \leq \lfloor \frac{n}{2} \rfloor$, $\overline{\frac{n}{2}K_2}$ for even n and $\overline{C_n}$ have diameter 2 and they do not contain a vertex of degree $n-1$, therefore they belong to the extremal graphs for Theorem 6.9. The graphs $K_{c,n-c}$ have a small size if c is small. We have $|E(K_{c,n-c})| = c(n-c)$. Thus, for $c=2$,

$$|E(K_{2,n-2})| = 2n-4.$$

The graphs $\overline{\frac{n}{2}K_2}$ for even n and $\overline{C_n}$ have a large size. We have

$$\left|E\left(\overline{\frac{n}{2}K_2}\right)\right| = \frac{n(n-2)}{2} \quad \text{and} \quad |E(\overline{C_n})| = \frac{n(n-3)}{2}.$$

For $a=1$, the bound given in Theorem 6.10 was presented in (Hua et al., 2012) and (Huang et al., 2019). The extremal graph declared in (Hua et al., 2018) is not sharp enough while the extremal graph presented in (Huang et al., 2019) is a little bit better with a condition satisfying $ecc_G(v) = ecc_{\overline{G}}(v) = 2$ for any vertex v in a graph G.

Theorem 6.10. *Let $a \geq 0$. If G and $\overline{G}$ are graphs of order $n \geq 5$, then*

$$EDS_{a,1}(G) + EDS_{a,1}(\overline{G}) \geq 3n(n-1)2^a$$

with equality if and only if $d(G) = d(\overline{G}) = 2$.

Proof. Since G is connected, $\overline{G}$ does not contain vertices of degree $n-1$. Analogously, since $\overline{G}$ is connected, G does not contain vertices of degree $n-1$. So, from Theorem 6.9, we have

$$EDS_{a,1}(G) \geq [n(n-1)-m]2^{a+1}$$

and

$$EDS_{a,1}(\overline{G}) \geq [n(n-1)-\overline{m}]2^{a+1},$$

where m and $\overline{m}$ are the sizes of G and $\overline{G}$, respectively. By Theorem 6.9, the equalities hold if and only if G and $\overline{G}$ have diameter 2, respectively.

Since $m+\overline{m} = \binom{n}{2} = \frac{n(n-1)}{2}$, we obtain

$$\begin{aligned} EDS_{a,1}(G)+EDS_{a,1}(\overline{G}) &\geq 2n(n-1)2^{a+1}-(m+\overline{m})2^{a+1} \\ &= 4n(n-1)2^{a}-n(n-1)2^{a} \\ &= 3n(n-1)2^{a} \end{aligned}$$

with equality if and only if $d(G) = d(\overline{G}) = 2$. □

We show that there exist graphs G such that $d(G) = d(\overline{G}) = 2$ for every $n \geq 5$ which implies that the bound presented in Theorem 6.10 is sharp for every $n \geq 5$. Let G_1, G_2, G_3, G_4, G_5 be any (possibly disconnected) graphs of orders $n_1, n_2, n_3, n_4, n_5 \geq 1$. Let G be the graph obtained from G_1, G_2, G_3, G_4, G_5 by joining any vertex of G_1 and any vertex of G_5, and by joining any vertex of G_i and any vertex of G_{i+1} for $i = 1,2,3,4$.

Note that $\overline{G}$ is the graph obtained from $\overline{G_1}$, $\overline{G_2}$, $\overline{G_3}$, $\overline{G_4}$, $\overline{G_5}$ by joining any vertex of G_i and any vertex of G_{i+2} for $i = 1,2,3$, and by joining any vertex of G_i and any vertex of G_{i+3} for $i = 1,2$. Clearly, $|V(G)| = |V(\overline{G})| = n_1+n_2+n_3+n_4+n_5$.

CONCLUSION AND FUTURE WORKS

Conclusion

Topological indices have a crucial use in medical, industrial and environmental research. In chemistry, a molecular graph represents the topology of a molecule, by considering how the atoms are connected. This could be modeled by a graph, where the vertices represent the atoms and also the edges symbolize the covalent bonds between the atoms. Multiple bonds, if any, are represented by a single edge in forming the molecular graph. Chemical graph theory uses topological indices as a strong tool for establishing relationships between the structure of the molecular graph and its properties or activities. For instance, structural features like size, shape, branching, symmetry, bonding patterns and therefore the neighborhood patterns of atoms within the molecules are measured by a topological index.

The eccentric distance sum belongs to the most well-known distance-based indices. For $a,b \in \mathbb{R}$, the general eccentric distance sum is defined as

$$EDS_{a,b}(G) = \sum_{u \in V(G)} [ecc_G(u)]^a [D_G(u)]^b,$$

where $D_G(u) = \sum\limits_{v \in V(G)} d_G(u,v)$ and $ecc_G(u)$ is the eccentricity of vertex u in G and $d_G(u,v)$ is the distance between vertices u and v in G. The general eccentric distance sum generalizes the eccentric distance sum when $a = b = 1$ and a few other distance-based topological indices.

In this dissertation, we mainly focused on the mathematical aspect of the topological indices. Here we presented some background results on the classical and general eccentric distance sum of a graph which motivated us for further study. The dissertation mainly focuses on finding lower and upper bounds when $a,b \in \mathbb{R}$. It also includes bounds when $b = 1$.

In this dissertation, we presented some results on the eccentric distance sum which are obtained by different researchers and some results on the general eccentric distance sum. We provided both lower and upper bounds for a tree of order n with an (s,t)-bipartition where $s \geq t \geq 2$ for $a \geq 0$, $0 < b \leq 1$ and $a \leq 0$, $b < 0$ respectively. We also presented lower and upper bounds for a bipartite graph of order n and matching number ν, where $2 \leq \nu \leq \lfloor \frac{n}{2} \rfloor$ for $a \geq 0$, $0 < b \leq 1$ and $a \leq 0$, $b < 0$ respectively. The bounds for bipartite graphs hold also if the matching number is replaced by the independence number, vertex cover number, or edge cover number. For any graph G with n vertices and chromatic number χ, where each of the χ colors is used for at least two vertices, we presented a lower bound for $a \geq 0$ and $b \geq 1$.

We presented bounds on the general eccentric distance sum for graphs, bipartite graphs and trees with given order and diameter 3. We obtained the general eccentric distance sum for join of two graphs with given order and number of vertices of maximum possible degree. We presented four more results for $b = 1$. Extremal graphs are presented for all the bounds.

Future Works

Work on the general eccentric distance sum for trees, unicyclic graphs and graphs with specified graph parameters can be done in the future. For the general eccentric distance sum for trees, unicyclic graphs and graphs, we present a few open problems. In Theorem 6.5, we presented bounds on $EDS_{a,b}(G_1 + G_2)$ for the join of two graphs G_1 and G_2. We suggest studying other graph products.

Problem 6.1. *Study the $EDS_{a,b}$ for the Cartesian product, Corona product and symmetric difference of two graphs.*

In Theorems 5.5, 5.6, 6.3, 6.6 and 6.7, we obtained bounds on the $EDS_{a,b}$ for graphs, bipartite graphs and trees of diameter 3. We recommend studying graphs of larger diameters.

Problem 6.2. *Find upper or lower bounds on $EDS_{a,b}(G)$ for trees, bipartite graphs or graphs G with given order and diameter greater than* 3.

In Theorem 5.8, we presented an upper bound on $EDS_{a,b}(T)$ of trees T only for domination number 2 and $b = 1$. We suggest studying related problems if both a and b are general.

Problem 6.3. *Find upper or lower bounds on $EDS_{a,b}(G)$ for trees or graphs G with given order and domination number, where both a and b are general.*

Vetrík (2021) presented an upper bounds on $EDS_{a,b}$ of graphs and trees for $a \leq 0$ and $b < 0$ as stated in Theorem 3.19 and 3.20.

Problem 6.4. *Find a graph with the largest $EDS_{a,b}$ among graphs/trees of given order for positive a and b.*

Problem 6.5. *Find bounds on $EDS_{a,b}$ for planar graphs and outerplanar graphs of given order.*

Problem 6.6. *Find bounds on $EDS_{a,b}$ for graphs with given order and number of bridges.*

Problem 6.7. *Find bounds on $EDS_{a,b}$ for trees of given order and number of segments.*

Problem 6.8. *Give a relation between $EDS_{a,b}$ and other topological indices of a graph.*

We suggest also to study Problems 6.1–6.8 for one general parameter and the other parameter being 1.

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